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Soliton excitations in one-dimensional diatomic lattices

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We present a systematic analytical study of the soliton excitations in a one-dimensional diatomic lattice with nonlinear on-site potential and a quartic interaction between nearest neighbors. We show that (1) the *decoupling ansatz* widely used in literature for the motion of two different masses is unncessary and can be naturally derived in our approach; (2) the system may support some new types of gap solitons and resonant kinks, two of which have been observed recently in a nonlinear diatomic pendulum lattice experiment; (3) for nonlinear on-site potential when the wave number of carrier waves is near the edge of the Brillouin zone and the difference of mass between two kinds of atoms becomes small, the results coincide with that of Kivshar and Flytzanis about the gap solitons in diatomic lattices; and (4) the theoretical results, being without any divergence, are valid in the whole Brillouin zone and can be applied to other nonlinear lattices.

I. INTRODUCTION

The pioneering works of Fermi, Pasta, and Ulam[1] and of Zabusky and Kruskal[2] have stimulated a great variety of research on dynamics of nonlinear lattices especially lattice solitons. Most of the work in this area has focused on models of one-dimensional (1D) monatomic chains, the prototype of which is the Toda lattice.[3] The nonlinear excitations in diatomic lattices have also received much attention[4-9] due to their applications to some physical systems. Models of diatomic lattices have been used as prototypes to approach the transport of energy,[10] the proton conductivity in hydrogen-bonded chains,[11] and the structural phase transition and associated soft-mode and central-peak phenomena which occur in materials like ferroelectric perovskites which present a quasi-1D diatomic structure along certain crystallographic directions.[12]

On the other hand, the so-called intrinsic localized modes in anharmonic lattices proposed by Sievers and Takeno[13] have been greatly studied.[14-17] Since these modes are localized in only a few particles, they can be viewed as strong localized nonpropagating envelope solitons.[18] Recently the interest has turned to the gap solitons in nonlinear diatomic lattices.[19-22] The concept of gap solitons was introduced by Chen and Mills when they investigated the nonlinear optical response of superlattices.[23] For a diatomic lattice, the phonon spectrum of the system consists of two branches (acoustic and optical). If nonlinearity is introduced, the gap solitons may appear as localized excitations when the nonlinear frequency is shifted into the linear-spectrum gap induced by the mass or force-constant difference of two kinds of atoms.

There are several theoretical methods to study the nonlinear excitations in 1D diatomic lattices. The first one proposed by Büttner and Bilz[4] is using the so-called "decoupling ansatz" plus a continuum approximation for the motion of the two different sublattices. Because this ansatz is based on some relations previously assumed between the displacement of light and heavy atoms, it is not satisfactory in theory. The second method was introduced by Yajima and Satsuma.[5] They discussed the dynamics of the lattices in terms of normal-mode coordinates whose relation with the actual displacements, as pointed out by Dash and Patnaik,[6] is very complicated and it is difficult to visualize the solitonlike behavior of the displacements. The third one is the so-called "semicontinuum approximation" employed by Collins.[9] In this treatment the decoupling ansatz has also been used [see Eq. (3.19) in Ref. 9], and the method can only be applied to acoustic excitations. The fourth method is due to Kivshar and Flytzanis.[20] They considered nonlinear coupled modes in a Klein-Gordon-type diatomic lattice, analyzing soliton solutions in the vicinity of the gap of the linear spectrum. In the above approaches, the first three methods were used by those authors to investigate the soliton excitations at $q \simeq 0$ (q is the wave number of the carrier waves) and the fourth one is only valid at $q \simeq q_B$ [where q_B is the edge of the Brillouin zone (BZ) of linear spectrum] and small mass difference.[21] Pnevmatikos, Flytzanis, and Romoissenet considered the soliton dynamics in nonlinear diatomic lattices in the quasi-discrete approximation (see Sec. IV in Ref. 8), but the decoupling ansatz was also used and the results obtained are divergent when q is near q_B [see Eqs. (4.5), (4.6), and (A5)–(A8) in the Appendix of Ref. 8].

Recently, some interesting gap soliton patterns have been observed[24] in a nonlinear diatomic pendulum lattice based on the experiment of Denardo.[25] These excitations are localized in the lattice in which the heavy atoms are at rest and the light ones form a nonpropagating envelope soliton (or kink) with opposite phase phase between the nearest neighbors. The lattice vibratory patterns are shown in Fig. 1. They cannot be explained by previous theoretical approaches. In this paper we try to introduce

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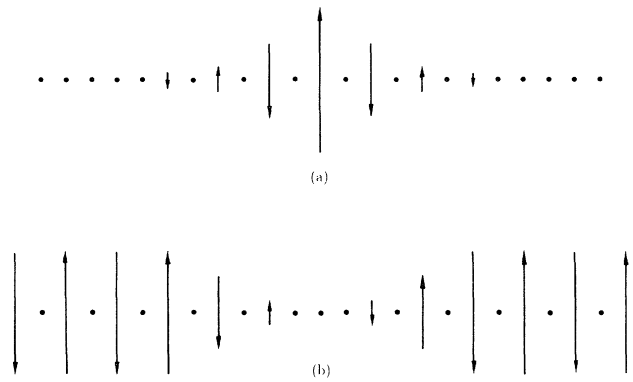

FIG. 1. The lattice patterns of (a) the gap soliton and (b) the resonant kink observed recently in a diatomic pendulum chain (Ref. 24).

a systematic method to study the nonlinear excitations in nonlinear diatomic lattices under a quasidiscreteness approximation. We show that the decoupling ansatz widely used in the literature is unnecessary and can be derived naturally by our approach. Some new types of gap solitons and kinks are proposed and when $q=q_B$ the results coincide with that of Kivshar and Flytzanis if the difference of mass of the two kinds of atoms becomes small. Our method is valid in the whole BZ and without any divergence. It can be used to explain the recent experimental observation about the gap solitons and kinks in the nonlinear diatomic pendulum lattice.[24] A simple result for the nonlinear on-site potential has been obtained recently.[26] The paper is organized as follows. In Sec. II we present our model and its asymptotic expansion. In Sec. III we discuss the acoustic-mode excitations and in Sec. IV the optical-mode excitations. A long-wave approximation is given in Sec. V. Section VI presents the gap solitons. A discussion and summary is given in the last section.

II. MODEL AND ASYMPTOTIC EXPANSION

The Hamiltonian of 1D nonlinear lattices of atoms with nearest-neighbor interactions and on-site potential is given by

$$H=\sum_i \left[\tfrac{1}{2}m_i \left[\frac{du_i}{dt} \right]^2 + \tfrac{1}{2}K_2(u_{i+1}-u_i)^2 + \tfrac{1}{4}K_4(u_{i+1}-u_i)^4 + \tfrac{1}{2}m_i\omega_0^2 u_i^2 - \tfrac{1}{4}\alpha u_i^4 \right] , \quad (1)$$

where $u_i=u_i(t)$ is the displacement of the ith particle with mass m_i from its equilibrium position. K_2 and K_4 are harmonic and quartic force constants, respectively. ω_0 and α are on-site potential parameters. The equation of motion satisfied by the u_j's is given by

$$m_j \frac{d^2}{dt^2}u_j - K_2(u_{j+1}+u_{j-1}-2u_j) - K_4[(u_{j+1}-u_j)^3+(u_{j-1}-u_j)^3] + \omega_0^2 m_j u_j - m_j \alpha u_j^3 = 0 . \quad (2)$$

For a diatomic lattice we can assume that $u_{2k}=v_n$ and $m_{2k}=m$ for $j=2k$ (even particles) and $u_{2k+1}=w_n$ and $m_{2k+1}=M$ $(M>m)$ for $j=2k+1$ (odd particles). n is the index of the nth unit cell with a spacing of $a=2a_0$ (see Fig. 2). By these notations the equations of motion for the even and the odd particles can be written separately as

$$\frac{d^2}{dt^2}v_n - I_2(w_n+w_{n-1}-2v_n) + \omega_0^2 v_n - \alpha v_n^3 - I_4[(w_n-v_n)^3+(w_{n-1}-v_n)^3] = 0 , \quad (3)$$

$$\frac{d^2}{dt^2}w_n - J_2(v_n+v_{n+1}-2w_n) + \omega_0^2 w_n - \alpha w_n^3 - J_4[(v_n-w_n)^3+(v_{n+1}-w_n)^3] = 0 , \quad (4)$$

where $I_i=K_i/m$ and $J_i=K_i/M$ $(i=2,4)$. In order to include the effects of anharmonicity and discreteness of the system, we employ the method of multiple scales combined with a quasidiscreteness approximation introduced by Tsuyui[27] and developed and simplified recently in Refs. 17 and 28. In this treatment one sets

$$u_n(t) = \epsilon u^{(1)}(\xi_n,\tau;\phi_n) + \epsilon^2 u^{(2)}(\xi_n,\tau;\phi_n) + \epsilon^3 u^{(3)}(\xi_n,\tau;\phi_n) + \cdots = \sum_{\nu=1}^{\infty} \epsilon^\nu u_{n,n}^{(\nu)} , \quad (5)$$

where ϵ is a small but finite parameter denoting the relative amplitude of the excitations and $u_{n,n}^{(\nu)} \equiv u^{(\nu)}(\xi_n,\tau;\phi_n)$, i.e., the first (second) subscript n represents the variable $\xi_n(\phi_n)$. ξ_n and τ are "slow" variables defined by $\xi_n=\epsilon(na-\lambda t)$ and $\tau=\epsilon^2 t$, respectively. They are called the multiple-scales variables. λ is a parameter to be determined by a solvability condition. The "fast" variable, $\phi_n=qna-\omega t$, representing the phase of the carrier wave, is taken to be completely discrete. Here q and ω are the wave number and frequency of the carrier wave, respectively. In terms of these notations, by substituting (5) into (3) and (4) and comparing the powers of ϵ, we can obtain the following equations:

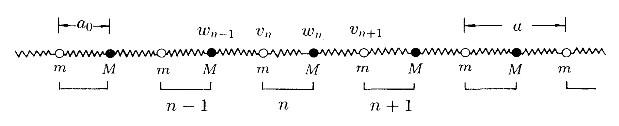

FIG. 2. A diatomic lattice chain in which $u_{2k}=v_n$ and $m_{2k}=m$ for even particles and $u_{2k+1}=w_n$ and $m_{2k+1}=M$ for odd particles. n is the index of the unit cell, $a=2a_0$ is the spacing of the unit cell, and a_0 is the spacing between two nearest-neighbor atoms.

$$\left[\frac{\partial^2}{\partial t^2}+\omega_0^2+2I_2\right]v_{n,n}^{(j)}-I_2(w_{n,n}^{(j)}+w_{n,n-1}^{(j)})=M_{n,n}^{(j)},\quad j=1,2,3\ldots \tag{6}$$

with

$$M_{n,n}^{(1)}=0\ , \tag{7}$$

$$M_{n,n}^{(2)}=2\lambda\frac{\partial^2}{\partial t\partial\xi_n}v_{n,n}^{(1)}-I_2a\frac{\partial}{\partial\xi_n}w_{n,n-1}^{(1)}\ , \tag{8}$$

$$M_{n,n}^{(3)}=2\lambda\frac{\partial^2}{\partial t\partial\xi_n}v_{n,n}^{(2)}-\left[2\frac{\partial^2}{\partial t\partial\tau}+\lambda^2\frac{\partial^2}{\partial\xi_n^2}\right]v_{n,n}^{(1)}+I_2\left[-a\frac{\partial}{\partial\xi_n}w_{n,n-1}^{(2)}+\frac{a^2}{2}\frac{\partial^2}{\partial\xi_n^2}w_{n,n-1}^{(1)}\right]$$
$$+\alpha(v_{n,n}^{(1)})^3+I_4[(w_{n,n}^{(1)}-v_{n,n}^{(1)})^3+(w_{n,n-1}^{(1)}-v_{n,n}^{(1)})^3]\ , \tag{9}$$

$\vdots\ \vdots$

and

$$\left[\frac{\partial^2}{\partial t^2}+\omega_0^2+2J_2\right]w_{n,n}^{(j)}-J_2(v_{n,n}^{(j)}+v_{n,n+1}^{(j)})=N_{n,n}^{(j)},\quad j=1,2,3\ldots \tag{10}$$

with

$$N_{n,n}^{(1)}=0\ , \tag{11}$$

$$N_{n,n}^{(2)}=2\lambda\frac{\partial^2}{\partial t\partial\xi_n}w_{n,n}^{(1)}+J_2a\frac{\partial}{\partial\xi_n}v_{n,n+1}^{(1)}\ , \tag{12}$$

$$N_{n,n}^{(3)}=2\lambda\frac{\partial^2}{\partial t\partial\xi_n}w_{n,n}^{(2)}-\left[2\frac{\partial^2}{\partial t\partial\tau}+\lambda^2\frac{\partial^2}{\partial\xi_n^2}\right]w_{n,n}^{(1)}+J_2\left[a\frac{\partial}{\partial\xi_n}v_{n,n+1}^{(1)}+\frac{a^2}{2}\frac{\partial^2}{\partial\xi_n^2}v_{n,n+1}^{(1)}\right]$$
$$+\alpha(w_{n,n}^{(1)})^3+J_4[(v_{n,n}^{(1)}-w_{n,n}^{(1)})^3+(v_{n,n+1}^{(1)}-w_{n,n}^{(1)})^3]\ , \tag{13}$$

$\vdots\ \vdots\ .$

In deriving the above equations we have used the Taylor expansion[17,27,28]

$$u_{n\pm1}(t)=\sum_{\nu=1}^{\infty}\epsilon^\nu u^{(\nu)}(\xi_n\pm\epsilon a,\tau,\phi_{n\pm1})$$
$$=\sum_{\nu=1}^{\infty}\epsilon^\nu\left[\sum_{\mu=0}^{\infty}\frac{1}{\mu}\left[\pm a\epsilon\frac{\partial}{\partial\xi_n}\right]^\mu u_{n,n\pm1}^{(\nu)}\right]. \tag{14}$$

The asymptotic expansions (6)–(13) for controlling Eqs. (3) and (4) have some symmetries which can be used to simplify the calculation in each order approximation.

III. ACOUSTIC-MODE EXCITATIONS

First we investigate the low-frequency ("acoustic") mode excitations of the system. In this case we rewrite (6) and (10) into the form

$$\left[\frac{\partial^2}{\partial t^2}+\omega_1^2\right]\left[\frac{\partial^2}{\partial t^2}+\omega_2^2\right]w_{n,n}^{(j)}-I_2J_2(w_{n,n-1}^{(j)}+w_{n,n+1}^{(j)}+2w_{n,n}^{(j)})$$
$$=J_2(M_{n,n}^{(j)}+M_{n,n+1}^{(j)})+\left[\frac{\partial^2}{\partial t^2}+\omega_2^2\right]N_{n,n}^{(j)}\ , \tag{15}$$

$$\left[\frac{\partial^2}{\partial t^2}+\omega_2^2\right]v_{n,n}^{(j)}=I_2(w_{n,n}^{(j)}+w_{n,n-1}^{(j)})+M_{n,n}^{(j)} \tag{16}$$

with $j=1,2,3\ldots$, and $\omega_1^2=\omega_0^2+2J_2$, $\omega_2^2=\omega_0^2+2I_2$. We can solve the displacement of the heavy atoms, $w_{n,n}^{(j)}$, from (15) and then get the displacement of light atoms, $v_{n,n}^{(j)}$ from (16) step by step.

(1) Let $j=1$. Since $M_{n,n}^{(1)}=N_{n,n}^{(1)}=0$ we have the linear wave equations

$$\left[\frac{\partial^2}{\partial t^2}+\omega_1^2\right]\left[\frac{\partial^2}{\partial t^2}+\omega_2^2\right]w_{n,n}^{(1)}-I_2J_2(w_{n,n-1}^{(1)}+w_{n,n+1}^{(1)}+2w_{n,n}^{(1)})=0\ , \tag{17}$$

$$\left[\frac{\partial^2}{\partial t^2}+\omega_2^2\right]v_{n,n}^{(1)}=I_2(w_{n,n}^{(1)}+w_{n,n-1}^{(1)})\ . \tag{18}$$

From (17) it is easy to get the solution

$$w_{n,n}^{(1)}=A_-(\xi_n,\tau)\exp(i\phi_n)+\text{c.c.}\ ,$$

where $A_-(\xi_n,\tau)$ is an envelope function to be determined later, and

$$(\omega^2-\omega_1^2)(\omega^2-\omega_2^2)-2I_2J_2[1+\cos(qa)]=0\ , \tag{19}$$

or

$$\omega^2=(\omega_\pm)^2 =\omega_0^2+I_2+J_2 \pm\left[(I_2+J_2)^2-4I_2J_2\sin^2\left[\frac{qa}{2}\right]\right]^{1/2} . \quad (20)$$

For the acoustic mode we should take $\omega=\omega_-(q)$.[29] Solving (18) to get $v_{n,n}^{(1)}$, we have

$$w_{n,n}^{(1)}=A_-(\xi_n,\tau)e^{i\phi_n^-}+\text{c.c.} , \quad (21)$$

$$v_{n,n}^{(1)}=-\frac{I_2(1+e^{-iqa})}{\omega_-^2-\omega_2^2}A_-(\xi_n,\tau)e^{i\phi_n^-}+\text{c.c.} , \quad (22)$$

with $\phi_n^-=qna-\omega_-(q)t$.

(2) By letting $j=2$ in (15) and (16) we have the second-order approximation equations

$$\left[\frac{\partial^2}{\partial t^2}+\omega_1^2\right]\left[\frac{\partial^2}{\partial t^2}+\omega_2^2\right]w_{n,n}^{(2)} -I_2J_2(w_{n,n-1}^{(2)}+w_{n,n+1}^{(2)}+2w_{n,n}^{(2)}) =J_2(M_{n,n}^{(2)}+M_{n,n+1}^{(2)})+\left[\frac{\partial^2}{\partial t^2}+\omega_2^2\right]N_{n,n}^{(2)} , \quad (23)$$

$$\left[\frac{\partial^2}{\partial t^2}+\omega_2^2\right]v_{n,n}^{(2)}=I_2(w_{n,n}^{(2)}+w_{n,n-1}^{(2)})+M_{n,n}^{(2)} . \quad (24)$$

Using (21) and (22) we can calculate $M_{n,n}^{(2)}$, $M_{n,n+1}^{(2)}$, and $N_{n,n}^{(2)}$. Then (23) and (24) become

$$\hat{L}w_{n,n}^{(2)}=2i\left\{\lambda\omega_-\left[\frac{2I_2J_2[1+\cos(qa)]}{\omega_-^2-\omega_2^2}+\omega_-^2-\omega_2^2\right] +I_2J_2a\sin(qa)\right\}\frac{\partial A_-}{\partial\xi_n}e^{i\phi_n^-}+\text{c.c.} , \quad (25)$$

$$\left[\frac{\partial^2}{\partial t^2}+\omega_2^2\right]v_{n,n}^{(2)}=I_2(w_{n,n}^{(2)}+w_{n,n-1}^{(2)}) +\left[2i\lambda\omega_-\frac{J_2(1+e^{-iqa})}{\omega_-^2-\omega_2^2} -J_2ae^{-iqa}\right]\frac{\partial A_-}{\partial\xi_n}e^{i\phi_n^-}+\text{c.c.} , \quad (26)$$

where c.c. represents complex conjugate. The operator $\hat{L}$ in (25) is defined by

$$\hat{L}u_{n,n}^{(j)}=\left[\frac{\partial^2}{\partial t^2}+\omega_1^2\right]\left[\frac{\partial^2}{\partial t^2}+\omega_2^2\right]u_{n,n}^{(j)} -I_2J_2(u_{n,n-1}^{(j)}+u_{n,n+1}^{(j)}+2u_{n,n}^{(j)}) , \quad (27)$$

where $u_{n,n}^{(j)}$ $(j=1,2,3,\dots)$ is a set of arbitrary functions.

We note that the term proportional to $\exp(i\phi_n^-)$ on the right-hand side of (25) is a *secular term* that must be eliminated in order for the theory to be valid *(solvability condition)*.[30] Hence we must set

$$\lambda\omega_-\left[\frac{2I_2J_2(1+\cos qa)}{\omega_-^2-\omega_2^2}+\omega_-^2-\omega_2^2\right] +I_2J_2\sin(qa)=0 . \quad (28)$$

From (19) (for $\omega=\omega_-$) it is easy to show that the above condition means that

$$\lambda=V_g^-=\frac{d\omega_-}{dq}=\frac{I_2J_2a\sin(qa)}{\omega_-(\omega_1^2+\omega_2^2-2\omega_-^2)} , \quad (29)$$

i.e., the parameter λ $(=V_g^-)$ is the group velocity of carrier waves of the acoustic mode. In the following we write $\xi_n=\xi_n^-$.

Solving (25) and (26) we obtain

$$w_{n,n}^{(2)}=B_-(\xi_n,\tau)e^{i\phi_n^-}+\text{c.c.} \quad (30)$$

$$v_{n,n}^{(2)}=-\frac{1}{\omega_-^2-\omega_2^2}\left\{I_2(1+e^{-iqa})B_- +\left[2iV_g^-\omega_-\frac{I_2(1+e^{-iqa})}{\omega_-^2-\omega_2^2} -I_2ae^{-iqa}\right]\frac{\partial A_-}{\partial\xi_n^-}\right\}e^{i\phi_n^-}+\text{c.c.} , \quad (31)$$

where $B_-(\xi_n^-,\tau)$ is another undetermined function. In fact we can let $B_-=0$ because it can be transferred to the lowest-order solution (21) and (22) and the transferred quantity can then be regarded as a new quantity for $A_-(\xi_n,\tau)$.[30] So one has

$$w_{n,n}^{(2)}=0 , \quad (32)$$

$$v_{n,n}^{(2)}=-\frac{1}{\omega_-^2-\omega_2^2}\left[2iV_g^-\omega_-\frac{I_2(1+e^{-iqa})}{\omega_-^2-\omega_2^2}-I_2ae^{-iqa}\right] \times\frac{\partial A_-}{\partial\xi_n^-}e^{i\phi_n^-}+\text{c.c.} \quad (33)$$

(3) When $j=3$ we have the third-order approximation equations

$$\hat{L}w_{n,n}^{(3)}=J_2(M_{n,n}^{(3)}+M_{n,n+1}^{(3)})+\left[\frac{\partial^2}{\partial t^2}+\omega_2^2\right]N_{n,n}^{(3)} , \quad (34)$$

$$\left[\frac{\partial^2}{\partial t^2}+\omega_2^2\right]v_{n,n}^{(3)}=I_2(w_{n,n}^{(3)}+w_{n,n-1}^{(3)})+M_{n,n}^{(3)} . \quad (35)$$

Using (21), (22), (32), and (33), we can obtain $M_{n,n}^{(3)}$, $M_{n,n+1}^{(3)}$, and $N_{n,n}^{(3)}$. By a detailed calculation we get

$$\hat{L}w_{n,n}^{(3)}=2\omega_-(\omega_1^2+\omega_2^2-2\omega_-^2)\left[i\frac{\partial A_-}{\partial\tau}+\frac{1}{2}\Gamma_-\frac{\partial}{\partial\xi_n^-}\frac{\partial}{\partial\xi_n^-}A_-+\Delta_-|A_-|^2A_-\right]e^{i\phi_n^-}+\text{c.c.}\ +\ \text{higher harmonics} , \quad (36)$$

where

$$\Gamma_- = \frac{d^2\omega_-}{dq^2} = \frac{2(\omega_1^2+\omega_2^2-4\omega_-^2)(V_g^-)^2 - a^2[(\omega_-^2-\omega_1^2)(\omega_-^2-\omega_2^2)-2I_2J_2]}{2\omega_-(2\omega_-^2-\omega_1^2-\omega_2^2)}, \tag{37}$$

$$\Delta_- = \frac{1}{2\omega_-(2\omega_-^2-\omega_1^2-\omega_2^2)}\left\{3\alpha(\omega_-^2-\omega_2^2)\left[1+\frac{I_2}{J_2}\left[\frac{\omega_-^2-\omega_1^2}{\omega_-^2-\omega_2^2}\right]^2\right]\right.$$
$$-6J_4(\omega_-^2-\omega_2^2)\left[1+\frac{\omega_-^2-\omega_1^2}{2J_2}\right]\left[1+\frac{\omega_-^2-\omega_1^2}{J_2}\left[1+\frac{I_2}{\omega_-^2-\omega_2^2}\right]\right]$$
$$\left.-6I_4(\omega_-^2-\omega_1^2)\left[1+\frac{\omega_-^2-\omega_2^2}{2I_2}\right]\left[1+\frac{\omega_-^2-\omega_1^2}{J_2}\left[1+\frac{I_2}{\omega_-^2-\omega_2^2}\right]\right]\right\}. \tag{38}$$

In order to simplify the expressions of Γ_- and Δ_-, (19) (for $\omega=\omega_-$) has been used. Again, for eliminating the secular term in $w_{n,n}^{(3)}$, we must require that the coefficient proportional to $\exp(i\phi_n^-)$ on the right-hand side of (36) vanishes. This then gives the closed equation for $A_-(\xi_n,\tau)$

$$i\frac{\partial A_-}{\partial\tau}+\tfrac{1}{2}\Gamma_-\frac{\partial}{\partial\xi_n^-}\frac{\partial}{\partial\xi_n^-}A_-+\Delta_-|A_-|^2A_-=0\ . \tag{39}$$

The solutions of (39) will be given in later sections.

IV. OPTICAL-MODE EXCITATIONS

For the higher-frequency optical-mode excitations we recast (6) and (10) into the form

$$\hat{L}v_{n,n}^{(j)}=I_2(N_{n,n}^{(j)}+N_{n,n-1}^{(j)})+\left[\frac{\partial^2}{\partial t^2}+\omega_1^2\right]M_{n,n}^{(j)}\ , \tag{40}$$

$$\left[\frac{\partial^2}{\partial t^2}+\omega_1^2\right]w_{n,n}^{(j)}=J_2(v_{n,n}^{(j)}+v_{n,n+1}^{(j)})+N_{n,n}^{(j)} \tag{41}$$

with $j=1,2,3,\ldots$. We can solve them order by order by the procedure used in solving the acoustic mode in the last section. However, we should notice that there is useful symmetry between (7)–(10) and (11)–(14). In fact, if we let

$$a\to -a\ ,$$
$$I_2\rightleftharpoons J_2,\quad I_4\rightleftharpoons J_4\ , \tag{42}$$
$$w_{n,n}\rightleftharpoons v_{n,n}^{(j)},\quad w_{n,n\pm1}^{(j)}\to v_{n,n\mp1}^{(j)}\ ,$$

then (7)–(10) transform into (11)–(14) [under (42), $M_{n,n}^{(j)}\to N_{n,n}^{(j)}$, $N_{n,n}^{(j)}\to M_{n,n}^{(j)}$, and $M_{n,n+1}^{(j)}\to N_{n,n-1}^{(j)}$]. This property results from the symmetry between (3) and (4). By use of this and the results obtained for the acoustic mode in the last section, we can immediately write the solution of $w_{n,n}^{(j)}$ and $v_{n,n}^{(j)}$ $(j=1,2,3,\ldots)$ in the optical mode as the following:

(1) $j=1$. We have

$$v_{n,n}^{(1)}=A_+(\xi_n,\tau)e^{i\phi_n^+}+\text{c.c.}\ , \tag{43}$$

$$w_{n,n}^{(1)}=-\frac{J_2(1+e^{iqa})}{\omega_+^2-\omega_1^2}A_+(\xi_n,\tau)e^{i\phi_n^+}+\text{c.c.}\ , \tag{44}$$

where $\phi_n^+=qna-\omega_+(q)t$ and $A_+(\xi_n,\tau)$ is an envelope function to be determined in later approximations. $\omega_+(q)$ is the linear dispersion relation of the optical mode defined by

$$\omega_+^2(q)=\omega_0^2+I_2+J_2+\sqrt{(I_2+J_2)^2-4I_2J_2\sin^2(qa/2)}\ . \tag{45}$$

A diagrammatic representation for $\omega_-(q)$ and $\omega_+(q)$ is shown in Fig. 3(a). There exist frequency gaps at $q=0$ and $\pm\pi/a$.

(2) $j=2$. The condition for eliminating the secular term in $v_{n,n}^{(2)}$ gives

$$\lambda=V_g^+=\frac{d\omega_+}{dq}=\frac{I_2J_2a\sin(qa)}{\omega_+(\omega_1^2+\omega_2^2-2\omega_+^2)}\ , \tag{46}$$

i.e., $\lambda=V_g^+$ is the group velocity of the carrier waves of the optical mode. Thus in this case we have

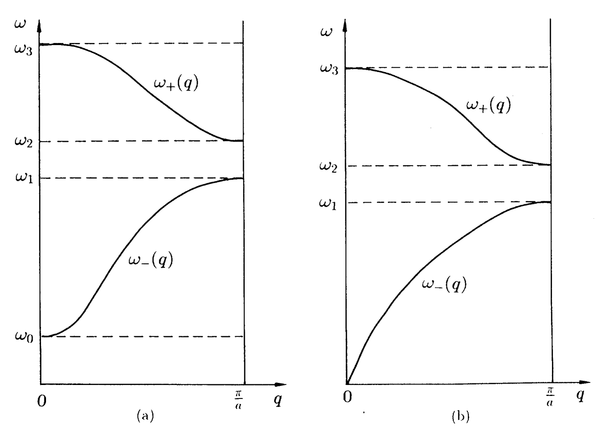

FIG. 3. The linear dispersion curves of the diatomic lattice. $\omega_-(q)$ and $\omega_+(q)$ represent the "acoustic" (the lower branch) and "optical" (the upper branch) modes, respectively. (a) $\omega_0=0$; (b) $\omega_0\neq 0$.

$\xi_n = \xi_n^+ = \epsilon(na - V_g^+ t)$. The solution in this order is

$$v_{n,n}^{(2)} = B_+(\xi_n^+,\tau)e^{i\phi_n^+} + \text{c.c.} , \tag{47}$$

$$w_{n,n}^{(2)} = -\frac{1}{\omega_+^2-\omega_1^2}\left\{ J_2(1+e^{iqa})B_+ + \left[2iV_g^+\omega_+ \frac{J_2(1+e^{iqa})}{\omega_+^2-\omega_1^2} + J_2 a e^{iqa} \right] \frac{\partial A_+}{\partial \xi_n^+} \right\} e^{i\phi_n^+} + \text{c.c.} , \tag{48}$$

where $B_+(\xi_n^+,\tau)$ is another undetermined function. By the same reason stated in the last section, we can set $B_+=0$. Hence we have

$$v_{n,n}^{(2)} = 0 , \tag{49}$$

$$w_{n,n}^{(2)} = -\frac{1}{\omega_+^2-\omega_1^2}\left[2iV_g^+\omega_+ \frac{J_2(1+e^{iqa})}{\omega_+^2-\omega_1^2} + J_2 a e^{iqa} \right] \times \frac{\partial A_+}{\partial \xi_n^+} e^{i\phi_n^+} + \text{c.c.} \tag{50}$$

(3) $j=3$. The solvability condition for $v_{n,n}^{(3)}$ yields the controlling equation for A_+:

$$i\frac{\partial A_+}{\partial \tau} + \tfrac{1}{2}\Gamma_+ \frac{\partial}{\partial \xi_n^+}\frac{\partial}{\partial \xi_n^+}A_+ + \Delta_+|A_+|^2A_+ = 0 \tag{51}$$

with

$$\Gamma_+ = \frac{d^2\omega_+}{dq^2} = \frac{2(\omega_1^2+\omega_2^2-4\omega_+^2)(V_g^+)^2 - a^2[(\omega_+^2-\omega_1^2)(\omega_+^2-\omega_2^2) - 2I_2J_2]}{2\omega_+(2\omega_+^2-\omega_1^2-\omega_2^2)} , \tag{52}$$

$$\begin{aligned}\Delta_+ = \frac{1}{2\omega_+(2\omega_+^2-\omega_1^2-\omega_2^2)} \Bigg\{ & 3\alpha(\omega_+^2-\omega_1^2)\left[1+\frac{J_2}{I_2}\left[\frac{\omega_+^2-\omega_2^2}{\omega_+^2-\omega_1^2}\right]^2\right] \\ & -6I_4(\omega_+^2-\omega_1^2)\left[1+\frac{\omega_+^2-\omega_2^2}{2I_2}\right]\left[1+\frac{\omega_+^2-\omega_2^2}{I_2}\left[1+\frac{J_2}{\omega_+^2-\omega_1^2}\right]\right] \\ & -6J_4(\omega_+^2-\omega_2^2)\left[1+\frac{\omega_+^2-\omega_1^2}{2I_2}\right]\left[1+\frac{\omega_+^2-\omega_2^2}{I_2}\left[1+\frac{J_2}{\omega_+^2-\omega_1^2}\right]\right]\Bigg\} .\end{aligned} \tag{53}$$

The correctness of the above equations can be checked by solving (40) and (41) directly.

From (39) and (51) we can see that the envelope functions $A_-(\xi_n^-,\tau)$ (for the acoustic mode) and $A_+(\xi_n^+,\tau)$ (for the optical mode) evolve according to the nonlinear Schrödinger (NLS) equation in a unified form

$$i\frac{\partial A_\pm}{\partial \tau} + \tfrac{1}{2}\Gamma_\pm \frac{\partial}{\partial \xi_n^\pm}\frac{\partial}{\partial \xi_n^\pm}A_\pm + \Delta_\pm|A_\pm|^2A_\pm = 0 . \tag{54}$$

The NLS equation is a completely integrable system and can be solved exactly by the inverse scattering transform (IST).[31] In order to return to the original variables we let $A_\pm(\xi_n^\pm,\tau) = (1/\epsilon)F_\pm(x_n^\pm,t)$ and noting that $\xi_n^\pm = \epsilon(na - V_g^\pm t) = \epsilon x_n^\pm$ and $\tau = \epsilon^2 t$ we have

$$i\frac{\partial F_\pm}{\partial t} + \tfrac{1}{2}\Gamma_\pm \frac{\partial}{\partial x_n^\pm}\frac{\partial}{\partial x_n^\pm}F_\pm + \Delta_\pm|F_\pm|^2F_\pm = 0 . \tag{55}$$

Whether the solution is soliton or kink ("dark" soliton) depends on the sign of $\Gamma_\pm\Delta_\pm$. For $\text{sgn}(\Gamma_\pm\Delta_\pm) > 0$, we have the single-soliton solution

$$F_\pm = \left[\frac{\Gamma_\pm}{\Delta_\pm}\right]^{1/2} \eta_\pm \text{sech}\{\eta_\pm[x_n^\pm - \sigma_\pm\Gamma_\pm t - x_{n_0}^\pm]\} \times \exp\{i\sigma_\pm x_n^\pm - i\tfrac{1}{2}(\sigma_\pm^2-\eta_\pm^2)\Gamma_\pm t - i\phi_{n_0}^\pm\} , \tag{56}$$

where $\eta_\pm$, $\sigma_\pm$, $x_{n_0}^\pm$, and $\phi_{n0}^\pm$ are constants. If $V_g^\pm + \sigma_\pm\Gamma_\pm = 0$, it is a nonpropagating localized solution. The two-soliton bound state can be given as[32]

$$F_\pm = \left[\frac{\Gamma_\pm}{\Delta_\pm}\right]^{1/2} \frac{(\eta_2^\pm)^2-(\eta_1^\pm)^2}{Q} \times \{\eta_1^\pm \text{sech}[\eta_1^\pm(x_n^\pm + x_{n_0}^\pm)]\exp(i\tfrac{1}{2}(\eta_1^\pm)^2\Gamma_\pm t] + \eta_2^\pm \text{sech}[\eta_2^\pm(x_n^\pm - x_{n_0}^\pm)]\exp[i\tfrac{1}{2}(\eta_2^\pm)^2\Gamma_\pm t]\} , \tag{57}$$

with

$$\begin{aligned} Q = {} & (\eta_2^\pm)^2 - (\eta_1^\pm)^2 \\ & -2\eta_1^\pm\eta_2^\pm\{\tanh[\eta_1^\pm(x_n^\pm + x_{n_0}^\pm)]\tanh[\eta_2^\pm(x_n^\pm - x_{n_0}^\pm)] \\ & -\text{sech}[\eta_1^\pm(x_n^\pm + x_{n_0}^\pm)]\text{sech}[\eta_2^\pm(x_n^\pm - x_{n_0}^\pm)] \\ & \times\cos(\tfrac{1}{2}[(\eta_2^\pm)^2 - (\eta_1^\pm)^2]\Gamma_\pm t)\} , \end{aligned} \tag{58}$$

where $\eta_1^\pm$, $\eta_2^\pm$, and $x_{n_0}^\pm$ are constants.

For $\text{sgn}(\Gamma_\pm\Delta_\pm) < 0$, one has the kink ("dark" soliton) solution:

$$F_{\pm}=\left[\frac{-\Gamma_{\pm}}{\Delta_{\pm}}\right]^{1/2}\eta_{\pm}\tanh\{\eta_{\pm}[x_n^{\pm}-\sigma_{\pm}\Gamma_{\pm}t-x_{n_0}^{\pm}]\}$$
$$\times\exp\{i\sigma_{\pm}x_n^{\pm}-i\tfrac{1}{2}(\sigma_{\pm}^2+2\eta_{\pm}^2)\Gamma_{\pm}t-i\phi_{n_0}^{\pm}\} . \quad (59)$$

The multikink solutions also can obtained by the IST.

We must point out that the approach developed above has many advantages. It is valid in the whole BZ if $\omega_0\neq 0$ (the case $\omega_0=0$ will be treated in the next section). The method is systematic and without any divergence in each order approximation. Also it allows us to use the symmetry between the acoustic and the optical modes which may simplify the calculations considerably.

V. LONG-WAVE APPROXIMATION

From (20) we can see that the frequency of the acoustic mode, $\omega_-(q)$, will be zero at $q=0$ for the nearest-neighbor potential ($\omega_0=0$ and $\alpha=0$). Because in this case Γ_- and Δ_- are divergent [see (37) and (38) in Sec. III], the nonlinear modulational equation for $A_-(\xi_n^-,\tau)$, the NLS equation (39), is invalid. In fact, when $\omega_0=0$, the linear dispersion curve of the system will change from Fig. 3(a) into Fig. 3(b). $q=0$ corresponds to the acoustic mode with long wavelength. We should apply the so-called long-wave approximation to study the nonlinear excitations of the system.[30]

For the nearest-neighbor potential, the acoustic mode of long wavelength represents the motion of the mass center of unit cells of the lattice. The excitation is a pure "direct current," i.e., it is independent of the fast variables $\phi_n(t)$ [$=qna-\omega_-(q)t$]. This may be best seen from the general expression for the displacement of the nth atom

$$u_n(t)=\sum_{\nu=0}^{\infty}\epsilon^{\nu}\sum_{l=-\infty}^{\infty}u^{(\nu,l)}(\xi_n,\tau)\times\exp\{il[qna-\omega(q)t]\} , \quad (60)$$

where $u^{(\nu,-l)}=(u^{(\nu,l)})^*$. For the acoustic mode at $q=0$ we have $\omega=\omega_-(0)=0$ when $\omega_0=0$. Thus the phase $\phi_n(t)=qna-\omega_-(q)t=0$ in this case. Then (60) becomes

$$u_n(t)=\sum_{\nu=0}^{\infty}\epsilon^{\nu}\sum_{l=-\infty}^{\infty}u^{(\nu,l)}(\xi_n,\tau)=\sum_{\nu=0}^{\infty}\epsilon^{\nu}u^{(\nu)}(\xi_n,\tau) , \quad (61)$$

where

$$u^{(\nu)}(\xi_n,\tau)\equiv\sum_{l}u^{(\nu,l)}(\xi_n,\tau) .$$

Obviously (61) is a "direct current" type excitation being independent of the "fast" variables $\phi_n(t)$.

In the following we consider the nonlinear excitations in the acoustic mode for the nearest-neighbor potential at $q=0$ by using a "discrete" long-wave approximation. We choose the slow variables $\xi_n=\epsilon(na-ct)$ and $\tau=\epsilon^3t$, where c is a constant to be determined later, and use the Taylor expansion

$$u_{n\pm1}(t)=\sum_{\nu=0}^{\infty}\epsilon^{\nu}u^{(\nu)}(\xi_{n\pm1},\tau)$$
$$=\sum_{\nu=0}^{\infty}\epsilon^{\nu}u^{(\nu)}(\xi_n\pm\epsilon a,\tau)$$
$$=\sum_{\nu=0}^{\infty}\sum_{\mu=0}^{\nu}\frac{1}{\mu}\left[\pm a\frac{\partial}{\partial\xi_n}\right]^{\nu}u^{(\nu-\mu)}(\xi_n,\tau) . \quad (62)$$

The Eqs. (3) and (4) for $\omega_0=\alpha=0$, by comparing the powers of ϵ, can be expanded as

$$w^{(j)}-v^{(j)}=M^{(j)} , \quad (63)$$

with $j=1,2,3,\dots$, and

$$M^{(0)}=0 , \quad (64)$$

$$M^{(1)}=\frac{a}{2}\frac{\partial}{\partial\xi_n}w^{(0)} , \quad (65)$$

$$M^{(2)}=\frac{a}{2}\frac{\partial}{\partial\xi_n}w^{(1)}+\frac{c^2}{2I_2}\frac{\partial^2}{\partial\xi_n^2}v^{(0)}-\frac{a^2}{4}\frac{\partial^2}{\partial\xi_n^2}w^{(0)} , \quad (66)$$

$$M^{(3)}=\frac{a}{2}\frac{\partial}{\partial\xi_n}w^{(2)}+\frac{c^2}{2I_2}\frac{\partial^2}{\partial\xi_n^2}v^{(1)}-\frac{a^2}{4}\frac{\partial^2}{\partial\xi_n^2}w^{(1)}+\frac{a^3}{12}\frac{\partial^3}{\partial\xi_n^3}w^{(0)}-\frac{I_4}{I_2}\left[(w^{(1)}-v^{(1)})^3+\left[w^{(1)}-v^{(1)}-a\frac{\partial}{\partial\xi_n}w^{(0)}\right]^3\right] , \quad (67)$$

$$M^{(4)}=\frac{a}{2}\frac{\partial}{\partial\xi_n}w^{(3)}+\frac{c^2}{2I_2}\frac{\partial^2}{\partial\xi_n^2}v^{(2)}-\frac{a^2}{4}\frac{\partial^2}{\partial\xi_n^2}w^{(2)}+\frac{a^3}{12}\frac{\partial^3}{\partial\xi_n^3}w^{(1)}-\frac{a^4}{48}\frac{\partial^4}{\partial\xi_n^4}w^{(0)}-\frac{c}{I_2}\frac{\partial^2}{\partial\xi_n\partial\tau}v^{(0)}$$
$$-\frac{3I_4}{2I_2}\left[(w^{(1)}-v^{(1)})^2(w^{(2)}-v^{(2)})+\left[w^{(1)}-v^{(1)}-a\frac{\partial}{\partial\xi_n}w^{(0)}\right]^2\left[w^{(2)}-v^{(2)}-a\frac{\partial}{\partial\xi_n}w^{(1)}+\frac{a^2}{2}\frac{\partial^2}{\partial\xi_n^2}w^{(0)}\right]\right] , \quad (68)$$

$\vdots \quad \vdots$

and

$$v^{(j)}-w^{(j)}=N^{(j)} , \tag{69}$$

with $j=1,2,3,\ldots$, and

$$N^{(0)}=0 , \tag{70}$$

$$N^{(1)}=-\frac{a}{2}\frac{\partial}{\partial\xi_n}v^{(0)} , \tag{71}$$

$$N^{(2)}=-\frac{a}{2}\frac{\partial}{\partial\xi_n}v^{(1)}+\frac{c^2}{2J_2}\frac{\partial^2}{\partial\xi_n^2}w^{(0)}-\frac{a^2}{4}\frac{\partial^2}{\partial\xi_n^2}v^{(0)} , \tag{72}$$

$$N^{(3)}=-\frac{a}{2}\frac{\partial}{\partial\xi_n}v^{(2)}+\frac{c^2}{2J_2}\frac{\partial^2}{\partial\xi_n^2}w^{(1)}-\frac{a^2}{4}\frac{\partial^2}{\partial\xi_n^2}v^{(1)}-\frac{a^3}{12}\frac{\partial^3}{\partial\xi_n^3}v^{(0)}-\frac{J_4}{J_2}\left[(v^{(1)}-w^{(1)})^3+\left[v^{(1)}-w^{(1)}+a\frac{\partial}{\partial\xi_n}v^{(0)}\right]^3\right] , \tag{73}$$

$$N^{(4)}=-\frac{a}{2}\frac{\partial}{\partial\xi_n}v^{(3)}+\frac{c^2}{2J_2}\frac{\partial^2}{\partial\xi_n^2}w^{(2)}-\frac{a^2}{4}\frac{\partial^2}{\partial\xi_n^2}v^{(2)}-\frac{a^3}{12}\frac{\partial^3}{\partial\xi_n^3}v^{(1)}-\frac{a^4}{48}\frac{\partial^4}{\partial\xi_n^4}v^{(0)}-\frac{c}{J_2}\frac{\partial^2}{\partial\xi_n\partial\tau}w^{(0)}$$
$$-\frac{3J_4}{2J_2}\left[(v^{(1)}-w^{(1)})^2(v^{(2)}-w^{(2)})+\left[v^{(1)}-w^{(1)}+a\frac{\partial}{\partial\xi_n}v^{(0)}\right]^2\left[v^{(2)}-w^{(2)}-a\frac{\partial}{\partial\xi_n}v^{(1)}+\frac{a^2}{2}\frac{\partial^2}{\partial\xi_n^2}v^{(0)}\right]\right] , \tag{74}$$

$\vdots \quad \vdots .$

Also there is a symmetry between (63)–(68) and (69)–(74). In fact, if we let $w^{(j)}\rightleftharpoons v^{(j)}$ ($j=1,2,3,4,\ldots$), $a\to -a$, $I_2\rightleftharpoons J_2$, and $I_4\rightleftharpoons J_4$, then (63)–(68) transform into (69)–(74). We recast (63) and (69) into

$$M^{(j)}+N^{(j)}=0 , \tag{75}$$

$$w^{(j)}=v^{(j)}+M^{(j)} , \tag{76}$$

$j=1,2,3,\ldots$. Then one can solve them order by order.

(1) Let $j=0$ in (75) and (76); we get

$$v^{(0)}=w^{(0)}=A_0(\xi_n,\tau) , \tag{77}$$

where A_0 is an arbitrary function to be determined later.

(2) If setting $j=1$ in (75) and (76), one can obtain $v^{(1)}=B_0(\xi_n,\tau)$ and $w^{(1)}=B_0+(a/2)(\partial/\partial\xi_n)A_0$. In fact we can let $B_0=0$ because it can be incorporated into the lowest-order solution (77) by defining A_0.[30] Thus one has

$$v^{(1)}=0 , \tag{78}$$

$$w^{(1)}=\frac{a}{2}\frac{\partial A_0}{\partial\xi_n} . \tag{79}$$

(3) When $j=2$, we have

$$M^{(2)}+N^{(2)}=0 , \tag{80}$$

$$w^{(2)}=v^{(2)}+M^{(2)} . \tag{81}$$

By using (77)–(79) we can calculate $M^{(2)}$ and $N^{(2)}$. Then (78) gives the equation determining the parameters c (the speed of sound) as

$$c^2=\frac{a^2}{2}\frac{I_2J_2}{I_2+J_2}=\frac{a^2}{4}\frac{2K_2}{m+M} . \tag{82}$$

And by (81) one can get the solution $v^{(2)}=C_0(\xi_n,\tau)$ and

$$w^{(2)}=C_0+\frac{c^2}{2I_2}\frac{\partial^2}{\partial\xi_n^2}A_0 .$$

In fact we can set $C_0=0$ because it can be incorporated into the lowest-order solution A_0.[30] So one has

$$v^{(2)}=0 , \tag{83}$$

$$w^{(2)}=\frac{c^2}{2I_2}\frac{\partial^2 A_0}{\partial\xi_n^2} . \tag{84}$$

(4) By letting $j=3$ we have the third-order approximation equation

$$M^{(3)}+N^{(3)}=0 , \tag{85}$$

$$w^{(3)}=v^{(3)}+M^{(3)} . \tag{86}$$

In terms of the lower-order solutions we can calculate $M^{(3)}$ and $N^{(3)}$. Substituting them into (85) still yields (82). By (86) we obtain the solution $v^{(3)}=D_0(\xi_n,\tau)$,

$$w^{(3)}=D_0+\frac{a}{4}\left[\frac{c^2}{I_2}-\frac{a^2}{6}\right]\frac{\partial^3}{\partial\xi_n^3}A_0 ,$$

where D_0 is an arbitrary function. Again by letting $D_0=0$ we have

$$v^{(3)}=0 , \tag{87}$$

$$w^{(3)}=\frac{a}{4}\left[\frac{c^2}{I_2}-\frac{a^2}{6}\right]\frac{\partial^3}{\partial\xi_n^3}A_0 . \tag{88}$$

(5) In the fourth-order approximation we have the equations

$$M^{(4)}+N^{(4)}=0 , \tag{89}$$

$$w^{(4)}=v^{(4)}+M^{(4)} \ . \tag{90}$$

Using the lower-order solutions we can obtain $M^{(4)}$ and $N^{(4)}$. By (89) we get the equation for $A_0(\xi_n,\tau)$

$$\frac{\partial^2}{\partial\tau\partial\xi_n}A_0+q\left[\frac{\partial A_0}{\partial\xi_n}\right]^2\frac{\partial^2 A_0}{\partial\xi_n^2}+h\frac{\partial^4 A_0}{\partial\xi_n^4}=0 \ , \tag{91}$$

with

$$q=\frac{3a^4I_2J_4}{16c(I_2+J_2)}=\frac{3a^3}{16}\frac{K_4}{K_2}\left[\frac{2K_2}{M+m}\right]^{1/2} , \tag{92}$$

$$h=\frac{a^3}{16}\left[\frac{2I_2J_2}{I_2+J_2}\right]^{1/2}\left[\frac{1}{3}-\frac{I_2J_2}{(I_2+J_2)^2}\right]$$
$$=\frac{a^3}{16}\left[\frac{2K_2}{M+m}\right]^{1/2}\left[\frac{1}{3}-\frac{mM}{(M+m)^2}\right] . \tag{93}$$

From (90) we can obtain

$$v^{(4)}=E_0 \ , \tag{94}$$

$$w^{(4)}=E_0-\frac{c}{I_2}\frac{\partial}{\partial\xi_n}\left[\frac{\partial A_0}{\partial\tau}+\frac{1}{8}\frac{I_4a^2c}{I_2}\left[\frac{\partial A_0}{\partial\xi_n}\right]^3\right] . \tag{95}$$

Again by setting $E_0=0$ and using (91) they can be simplified into

$$v^{(4)}=0 \ , \tag{96}$$

$$w^{(4)}=-\frac{c}{I_2}h\frac{\partial^4 A_0}{\partial\xi_n^4} \ . \tag{97}$$

Making the transformation $u=\epsilon\partial A_0/\partial\xi_n=\partial A_0/\partial x_n$ and noting that $\xi_n=\epsilon(na-\omega t)=\epsilon x_n$ and $\tau=\epsilon^3 t$, we can recast (91) into

$$\frac{\partial u}{\partial t}+qu^2\frac{\partial u}{\partial x_n}+h\frac{\partial^3 u}{\partial x_n^3}=0 \ , \tag{98}$$

with $x_n=na-ct$. (94) is the modified Korteweg–de Vries (MKdV) equation, also being a completely integral system and can be solved exactly by the IST.[31] The single-soliton solution is given by

$$u(x_n,t)=\pm\left[\frac{6h}{q}\right]^{1/2}2\kappa\,\mathrm{sech}\left\{2\kappa\left[x_n-\frac{4\kappa^2}{h}t-x_n^0\right]\right\} , \tag{99}$$

where κ and x_n^0 are constants. Thus we have the kink solution for A_0

$$A_0=\int u(x_n,t)dx_n$$
$$=\pm\left[\frac{6h}{q}\right]^{1/2}\sin^{-1}\left\{\tanh\left[2\kappa\left[x_n-\frac{4\kappa^2}{h}t-x_n^0\right]\right]\right\} . \tag{100}$$

The integration constant has been suppressed. (100) also can be rewritten as

$$A_0=\pm\left[\frac{6h}{q}\right]^{1/2}\tan^{-1}\left\{\sinh\left[2\kappa\left[x_n-\frac{4\kappa^2}{h}t-x_n^0\right]\right]\right\} . \tag{101}$$

Equation (98) also admits the breather solution

$$u=\pm 2\left[\frac{6h}{q}\right]^{1/2}$$
$$\times\frac{\partial}{\partial x_n}\left\{\tan^{-1}\left[\frac{\beta}{\alpha}\frac{\sin[2\alpha x_n+(\delta/h)t-\phi_0]}{\alpha\cosh[2\beta x_n+(\gamma/h)t+\psi_0]}\right]\right\} , \tag{102}$$

with $\gamma=8\beta(3\alpha^2-\beta^2)$ and $\delta=8\alpha(\alpha^2-3\beta^2)$, where α, β ϕ_0, and ψ_0 are constants. Hence one has

$$A_0=\pm 2\left[\frac{6h}{q}\right]^{1/2}$$
$$\times\tan^{-1}\left[\frac{\beta}{\alpha}\frac{\sin[2\alpha x_n+(\delta/h)t-\phi_0]}{\cosh[2\beta x_n+(\gamma/h)t+\psi_0]}\right] . \tag{103}$$

Obviously it becomes an envelope soliton of the NLS equation when (β/α) is small. Unlike the single-kink solution (101), the breather can be localized at some lattice sites when $2\beta c=\delta/h$, and has an internal vibration with the frequency $c-\delta/(2\alpha h)$.

VI. GAP SOLITONS, RESONANT KINKS, AND INTRINSIC LOCALIZED MODES

For a diatomic lattice, the phonon spectrum of the system consists of two parts—the acoustic $[\omega_-(q)]$ and optical $[\omega_+(q)]$ branches. In addition to the bottom gap (the width $\Delta\omega=\omega_0$) below the dispersion curve of the acoustic mode (when $\omega_0\neq 0$), there exists a frequency gap $(\Delta\omega=\omega_2-\omega_1)$ between the acoustic and the optical branches. The system also has an upper cutoff frequency ω_3 $[=\omega_+(q=0)]$. In the linear case, a spectrum gap or a cutoff means that waves of certain wavelengths are forbidden. However, for the nonlinear lattice one may allow such waves to exist in the form of gap solitons[23,19] or so-called intrinsic localized modes.[13] Since the results obtained in the previous sections are valid in the whole BZ, they can give the solutions of the gap solitons and the intrinsic localized modes of the system in a simple way. These solutions may be obtained by solving (55) at $q=0$ or $\pm\pi/a$. In the following, without loss of generality, we only write down the explicit expressions of nonpropagating solutions for $\alpha>0$ and $K_4>0$ in the first-order approximation.

(1) For the acoustic mode at $q=0$, we have $\omega_-=\omega_0$, $V_g^-=0$, $x_n^-=na\equiv x_n$, $\Gamma_-=K_2a^2/[\omega_0(M+m)]$, and $\Delta_-=3\alpha/(2\omega_0)$. Equation (55) for F_- gives the single-soliton solution

$$F_-(x_n,t)=(\Gamma_-/\Delta_-)^{1/2}\eta_0\mathrm{sech}[\eta_0(x_n-x_n^0)]$$
$$\times\exp[i(\tfrac{1}{2}\Gamma_-\eta_0^2t-\phi_0)] \ , \tag{104}$$

where η_0, x_n^0, and ϕ_0 are constants. Thus we have the lattice configuration

$$w_n(t)\approx 2(\Gamma_-/\Delta_-)^{1/2}\eta_0\mathrm{sech}[\eta_0(n-n_0)a] \times\cos(\Omega_0 t-\phi_0)\ , \quad (105)$$

$$v_n(t)\approx 2(\Gamma_-/\Delta_-)^{1/2}\eta_0\mathrm{sech}[\eta_0(n-n_0)a] \times\cos(\Omega_0 t-\phi_0)=w_n(t)\ , \quad (106)$$

where n_0 is an arbitrary integer, and

$$\Omega_0=\omega_0-\tfrac{1}{2}\Gamma_-\eta_0^2\ , \quad (107)$$

being within the bottom gap of the dispersion curve of the acoustic mode. Hence this type of excitation may be called a *bottom gap soliton* of the system. The wave pattern in the lattice is shown in Fig. 4. (105) and (106) show that the heavy atoms and the light ones vibrate in phase. We should note that the nearest-neighbor interaction has no contribution to the formation of the bottom gap soliton because in this case Δ_- is independent of K_4.

(2) In the case of the acoustic mode at $q=\pm\pi/a$, one has $\omega_-=\omega_1$, $V_g^-=0$, $\Gamma_-=-K_2a^2/[2\omega_1(M-m)]$, and

$$\Delta_-=\frac{3}{2\omega_1}(\alpha-2J_4)=\frac{3\alpha}{2M\omega_1}(M-m_c)\ , \quad (108)$$

where $m_c=2K_4/\alpha$. Because Δ_- changes its sign at $M=m_c$, the solution of (55) for F_- will occur as a "phase transition" from soliton to kink. Thus m_c plays the role of a "critical mass." When $M<m_c$, we have the soliton solution

$$F_-(x_n,t)=(|\Gamma_-|/|\Delta_-|)^{1/2}\eta_0\mathrm{sech}[\eta_0(x_n-x_n^0)] \times\exp[i(\tfrac{1}{2}|\Gamma_-|\eta_0^2t-\phi_0)]\ . \quad (109)$$

The lattice configuration has the form

$$w_n(t)\approx(-1)^n 2(|\Gamma_-|/|\Delta_-|)^{1/2}\eta_0\mathrm{sech}[\eta_0(n-n_0)a] \times\cos(\Omega_1^s t-\phi_0)\ , \quad (110)$$

$$v_n(t)\approx 0\ , \quad (111)$$

with the vibratory frequency

$$\Omega_1^s=\omega_1+\tfrac{1}{2}|\Gamma_-|\eta_0^2\ , \quad (112)$$

being within the frequency gap between the dispersion curves of the acoustic and optical modes. The lattice pattern is like Fig. 1(a) but in this case all the light particles are at rest and the heavy ones oscillate with opposite phase between their nearest neighbors, forming a nonpropagating *gap soliton*.

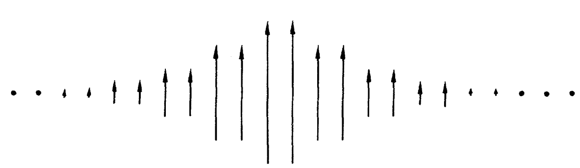

FIG. 4. The bottom gap soliton pattern for the acoustic mode at $q=0$.

For $M>m_c$, (55) for F_- has the kink solution

$$F_-(x_n,t)=(|\Gamma_-|/\Delta_-)^{1/2}\eta_0\tanh[\eta_0(x_n-x_n^0)] \times\exp[i(|\Gamma_-|\eta_0^2t-\phi_0)]\ . \quad (113)$$

Then the system has the configuration

$$w_n(t)\approx(-1)^n 2(|\Gamma_-|/\Delta_-)^{1/2}\eta_0\tanh[\eta_0(n-n_0)a] \times\cos(\Omega_1^k t-\phi_0)\ , \quad (114)$$

$$v_n(t)\approx 0\ , \quad (115)$$

with

$$\Omega_1^k=\omega_1-|\Gamma_-|\eta_0^2\ , \quad (116)$$

being within the frequency band of the acoustic mode. So it is a *resonant kink* of the system. The lattice pattern is like Fig. 1(b) but in the present case all the light atoms are at rest.

(3) For the optical mode at $q=\pm\pi/a$, we have $\omega_+=\omega_2$, $V_g^+=0$, $\Gamma_+=K_2a^2/[2\omega_2(M-m)]$, and

$$\Delta_+=\frac{3}{2\omega_2}(\alpha-2I_4)=\frac{3\alpha}{2m\omega_2}(m-m_c)\ , \quad (117)$$

i.e., Δ_+ also will change its sign at $m=m_c$. For $m>m_c$, Eq. (55) for F_+ in this case has the single-soliton solution

$$F_+(x_n,t)=(\Gamma_+/\Delta_+)^{1/2}\eta_0\mathrm{sech}[\eta_0(x_n-x_n^0)] \times\exp[i(\tfrac{1}{2}\Gamma_+\eta_0^2t-\phi_0)]\ . \quad (118)$$

The lattice displacement has the form

$$v_n(t)\approx(-1)^n 2(\Gamma_+/\Delta_+)^{1/2}\eta_0\mathrm{sech}[\eta_0(n-n_0)a] \times\cos(\Omega_2^s t-\phi_0)\ , \quad (119)$$

$$w_n(t)\approx 0\ , \quad (120)$$

with the vibratory frequency

$$\Omega_2^s=\omega_2-\tfrac{1}{2}\Gamma_+\eta_0^2\ , \quad (121)$$

being within the frequency gap between the acoustic and optical modes. It is a typical gap soliton in which all the heavy atoms are at rest and the light ones oscillate with opposite phase between their nearest neighbors. The vibrating pattern of the lattice is just as that shown in Fig. 1(a), which has been observed recently in a diatomic pendulum lattice experiment by Lou *et al.*[24] It is easy to show that Eqs. (3) and (4) can be used to describe the dynamics of the diatomic pendulum lattice in Ref. 24, where v_n (w_n) represents the displacement of the light (heavy) particles at the nth unit cell, ω_0 is the linear frequency of an uncoupled pendulum, α is the nonlinear coefficient resulting from the gravitational potential, and K_4 is the anharmonic force constant by the nearest-neighbor interaction.

When $m<m_c$, the system will undergo a transition from soliton to kink. Equation (55) for F_+ in this case yields the kink solution

$$F_+(x_n,t)=(\Gamma_+/|\Delta_+|)^{1/2}\eta_0\tanh[\eta_0(x_n-x_n^0)]\times\exp[-i(\Gamma_+\eta_0^2t-\phi_0)] \ . \tag{122}$$

The lattice displacement is

$$v_n(t)\approx(-1)^n 2(\Gamma_+/|\Delta_+|)^{1/2}\eta_0\tanh[\eta_0(n-n_0)a]\times\cos(\Omega_2^k t-\phi_0) \ , \tag{123}$$

$$w_n(t)\approx 0 \ , \tag{124}$$

with

$$\Omega_2^k=\omega_2+\Gamma_+\eta_0^2 \ , \tag{125}$$

being within the frequency band of the optical mode. Thus (123) and (124) is a *resonant kink,* in which all the heavy atoms are at rest and the light ones oscillate with opposite phase. The vibrating pattern of the lattice is just as that shown in Fig. 1(b), which also has been observed experimentally. So in our approach the experimental results of Ref. 24 about the gap solitons and the resonant kinks can be well explained qualitatively.

(4) For the optical mode at $q=0$, one has $\omega_+=\omega_3\equiv\sqrt{\omega_0^2+2(I_2+J_2)}$, $V_g^+=0$, $\Gamma_+=-K_2a^2/[2\omega_3(M+m)]$, and

$$\Delta_+=\frac{3}{2\omega_3}\left[\left[1-\frac{m}{M}\right]^2+\frac{m}{M}\right](\alpha-\delta) \ , \tag{126}$$

$$\delta=\frac{2K_4}{m[(1-m/M)^2+m/M]}\left[\left[1+\frac{m}{M}\right]^2+\frac{m}{M}\left[3+\frac{m}{M}\right]\right] . \tag{127}$$

For $\alpha>\delta$, $\Delta_+>0$, Eq. (55) for F_+ has the kink solution

$$F_+(x_n,t)=(|\Gamma_+|/\Delta_+)^{1/2}\eta_0\tanh[\eta_0(x_n-x_n^0)]\times\exp[i(|\Gamma_+|\eta_0^2t-\phi_0)] \ . \tag{128}$$

The lattice displacement in this case is

$$v_n(t)\approx 2(|\Gamma_+|/\Delta_+)^{1/2}\eta_0\tanh[\eta_0(n-n_0)a]\times\cos(\Omega_3^k t-\phi_0) \ , \tag{129}$$

$$w_n(t)\approx-\frac{m}{M}2(|\Gamma_+|/\Delta_+)^{1/2}\eta_0\tanh[\eta_0(n-n_0)a]\times\cos(\Omega_3^k t-\phi_0)=-\frac{m}{M}v_n(t) \ , \tag{130}$$

with

$$\Omega_3^k=\omega_3-|\Gamma_+|\eta_0^2 \ , \tag{131}$$

being within the frequency band of the optical mode. Thus (129) and (130) is also a resonant kink in which the light atoms and heavy ones vibrate with opposite phase, satisfying $mv_n(t)+Mw_n(t)\simeq 0$. The lattice pattern is shown in Fig. 5(a).

When $\alpha<\delta$, $\Delta_+<0$, a transition from kink to soliton occurs. Equation (55) for F_+ admits the soliton solution

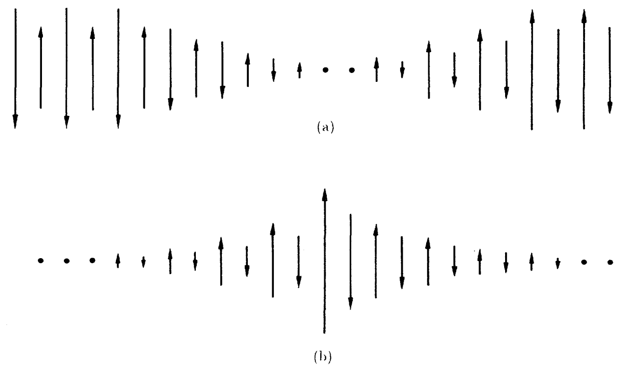

FIG. 5. The lattice patterns of (a) the resonant kink and (b) the intrinsic localized mode for the optical mode at $q=0$.

$$F_+(x_n,t)=(|\Gamma_+|/|\Delta_+|)^{1/2}\eta_0\,\text{sech}[\eta_0(x_n-x_n^0)]\times\exp[-i(\tfrac{1}{2}|\Gamma_+|\eta_0^2t+\phi_0)] \ . \tag{132}$$

The lattice configuration yields

$$v_n(t)\approx 2(|\Gamma_+|/|\Delta_+|)^{1/2}\eta_0\,\text{sech}[\eta_0(n-n_0)a]\times\cos(\Omega_3^s t-\phi_0) \ , \tag{133}$$

$$w_n(t)\approx-\frac{m}{M}2(|\Gamma_+|/|\Delta_+|)^{1/2}\eta_0\,\text{sech}[\eta_0(n-n_0)a]\times\cos(\Omega_3^s t-\phi_0)=-\frac{m}{M}v_n(t) \ , \tag{134}$$

with the vibrating frequency

$$\Omega_3^s=\omega_3+\tfrac{1}{2}|\Gamma_+|\eta_0^2 \ , \tag{135}$$

being above the frequency band of the optical mode. So (133) and (134) is an *intrinsic localized mode* of the system. The lattice pattern is shown in Fig. 5(b).

VII. DECOUPLING ANSATZ AND THE GAP SOLITON THEORY OF KF

A. Decoupling ansatz

For a nonlinear diatomic lattice, the displacements of the light and heavy atoms are controlled by two coupling nonlinear equations. The theoretical approach to this set of equations, even though in the weak nonlinear approximation, is not tractable. In their study of the soliton excitations in a diatomic lattice for quartic nearest-neighbor anharmonicity (i.e., $\omega_0=\alpha=0$), Büttner and Bilz[4] introduced a *decoupling ansatz* in the continuum limit (i.e., at $q=0$) for relating the displacement of the light atoms to that of the heavy atoms, which in our notation has the form

$$w_n=\lambda_i\left[v_n+b_{i,1}a_0\frac{\partial}{\partial x_n}v_n+b_{i,2}\frac{a_0^2}{2}\frac{\partial^2}{\partial x_n^2}v_n+b_{i,3}\frac{a_0^3}{6}\frac{\partial^3}{\partial x_n^3}v_n+b_{i,4}\frac{a_0^4}{24}\frac{\partial^4}{\partial x_n^4}v_n+\cdots\right] , \tag{136}$$

where $x_n = na$ and constants λ_i and $b_{i,j}$ ($j=1,2,3,4,\ldots$) are determined so that the two equations satisfied by the light and heavy atoms are identical. The index i means the acoustic mode (for $i=1$) or the optical mode (for $i=2$). Later this ansatz was widely used by Dash and Patnaik,[6] Pnevmatikos and co-workers,[7,8] and Collins[9] among others in the continuum approximation. Obviously, the use of the decoupling ansatz cannot avoid some guesses in solving the equations of motion. In this section we show that this ansatz may be derived naturally by our approach at $q=0$. In the following we let $\omega_0=\alpha=0$ in order to compare our results with that under the decoupling ansatz.

(1) For the acoustic mode at $q=0$, from Sec. V we have

$$v_n = v^{(0)} = A_0 , \tag{137}$$

$$\begin{aligned} w_n &= w^{(0)} + \epsilon w^{(1)} + \epsilon^2 w^{(2)} + \epsilon^3 w^{(3)} + \epsilon^4 w^{(4)} + \cdots \\ &= A_0 + \epsilon \frac{a}{2}\frac{\partial}{\partial \xi_n} A_0 + \epsilon^2 \frac{c^2}{2I_2}\frac{\partial^2}{\partial \xi_n^2} A_0 \\ &\quad + \epsilon^3 \frac{a}{4}\left[\frac{c^2}{I_2} - \frac{a^2}{6}\right]\frac{\partial^3}{\partial \xi_n^3} A_0 \\ &\quad + \epsilon^4 \frac{c}{I_2} h \frac{\partial^4}{\partial \xi_n^4} A_0 + \cdots . \end{aligned} \tag{138}$$

Since $\xi_n = \epsilon(na - ct)$, one has $\epsilon \partial/\partial \xi_n = \partial/\partial x_n$. Thus from (137) and (138) we have

$$\begin{aligned} w_n &= v_n + \frac{a}{2}\frac{\partial}{\partial x_n} v_n + \frac{c^2}{2I_2}\frac{\partial^2}{\partial x_n^2} v_n + \frac{a}{4}\left[\frac{c^2}{I_2} - \frac{a^2}{6}\right]\frac{\partial^3}{\partial x_n^3} v_n \\ &\quad + \frac{c}{I_2} h \frac{\partial^4}{\partial x_n^4} v_n + \cdots \\ &= \lambda_1 \left[v_n + b_{1,1} a_0 \frac{\partial}{\partial x_n} v_n + b_{1,2} \frac{a_0^2}{2}\frac{\partial^2}{\partial x_n^2} v_n \right. \\ &\quad \left. + b_{1,3}\frac{a_0^3}{6}\frac{\partial^3}{\partial x_n^3} v_n + b_{1,4}\frac{a_0^4}{24}\frac{\partial^4}{\partial x_n^4} v_n + \cdots \right] \end{aligned} \tag{139}$$

with

$$\begin{aligned} &\lambda_1 = 1, \quad b_{1,1} = 1, \quad b_{1,2} = \frac{2m}{M+m} , \\ &b_{1,3} = 2\frac{2m - M}{M+m} , \\ &b_{1,4} = \frac{m}{M+m}\left[\frac{1}{3} - \frac{Mm}{(M+m)^2}\right], \quad \ldots . \end{aligned} \tag{140}$$

This result is just the same as that of Refs. 4, 6, and 7 using the decoupling ansatz.

(2) For the optical mode at $q=0$, from Sec. IV we have

$$v_n = \epsilon v_{n,n}^{(1)} = \epsilon A_+(\xi_n, \tau) e^{i\phi_n^+} + \text{c.c.} = F_+(x_n, t) e^{-i\omega_3 t} + \text{c.c.} , \tag{141}$$

$$\begin{aligned} w_n &= \epsilon w_{n,n}^{(1)} + \epsilon^2 w_{n,n}^{(2)} + \epsilon^3 w_{n,n}^{(3)} + \cdots \\ &= \epsilon \left[\frac{-2J_2}{\omega_3^2 - \omega_1^2} A_+ e^{i\phi_n^+} + \text{c.c.} \right] + \epsilon^2 \left[\frac{-J_2 a}{\omega_3^2 - \omega_1^2}\frac{\partial}{\partial \xi_n^+} A_+ e^{i\phi_n^+} + \text{c.c.} \right] + \cdots \\ &= -\frac{m}{M}\left\{ [F_+ e^{-i\omega_3 t} + \text{c.c.}] + \frac{a}{2}\frac{\partial}{\partial x_n}[F_+ e^{-i\omega_3 t} + \text{c.c.}] + \cdots \right\} . \end{aligned} \tag{142}$$

So we have

$$w_n = \lambda_2 \left[v_n + b_{2,1} a_0 \frac{\partial}{\partial x_n} v_n + b_{2,2}\frac{a_0^2}{2}\frac{\partial^2}{\partial x_n^2} v_n + \cdots \right] \tag{143}$$

with

$$\lambda_2 = -\frac{m}{M}, \quad b_{2,1} = 1, \quad b_{2,2} = \frac{2M}{M+m}, \cdots , \tag{144}$$

where $b_{2,2}$ can be obtained from the third-order approximation solution of the optical mode at $q=0$. The relations (143) and (144) are also the same as the decoupling ansatz for the optical mode used in Refs. 4 and 7.

From (139) and (143) we conclude that the decoupling ansatz widely used in the literature is unnecessary and may be naturally derived by our present approach at $q=0$.[33]

B. Comparison with the gap soliton theory of Kivshar and Flytzanis

In 1992, a gap soliton theory for the nonlinear diatomic lattice in the case of $K_4=0$ and $q=\pi/2$ was proposed by Kivshar and Flytzanis (KF).[20] In the case of $M=m$, KF's theory can give a successful explanation for the self-induced gap solitons observed by Denardo *et al.*[25] It seems that there exist some relations between the approach of KF and ours given above. To see this we write down our solutions to the second-order approximation for $q=\pm\pi/a$ in the following (for comparison we set $K_4=0$).

(1) By using (21), (22), (32), (33), and (113), the lattice displacement for the acoustic mode at $q=\pm\pi/a$ may be written as

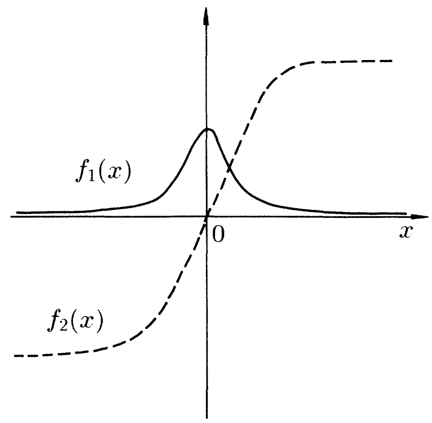

FIG. 6. A diagrammatic representation of $f_i(x)$ $(i=1,2)$ in (147) and (148).

$$v_n(t)=\epsilon v_{n,n}^{(1)}+\epsilon^2 v_{n,n}^{(2)} =(-1)^n 2 f_1(x_n)\cos(\Omega_1^k t-\phi_0) , \quad (145)$$

$$w_n(t)=\epsilon w_{n,n}^{(1)}+\epsilon^2 w_{n,n}^{(2)} =(-1)^n 2 f_2(x_n)\cos(\Omega_1^k t-\phi_0) , \quad (146)$$

with $x_n=na$ and

$$f_1(x)=\frac{Ma}{2(M-m)}\left[\frac{|\Gamma_-|}{\Delta_-}\right]^{1/2}\eta_0^2\text{sech}^2[\eta_0(x-x_0)] , \quad (147)$$

$$f_2(x)=\left[\frac{|\Gamma_-|}{\Delta_-}\right]^{1/2}\eta_0\tanh[\eta_0(x-x_0)] . \quad (148)$$

A diagrammatic representation of $f_1(x)$ and $f_2(x)$ is given in Fig. 6.

(2) For the optical mode at $q=\pm\pi/a$, using (43), (44), (49), (50), and (118), one has the lattice configuration

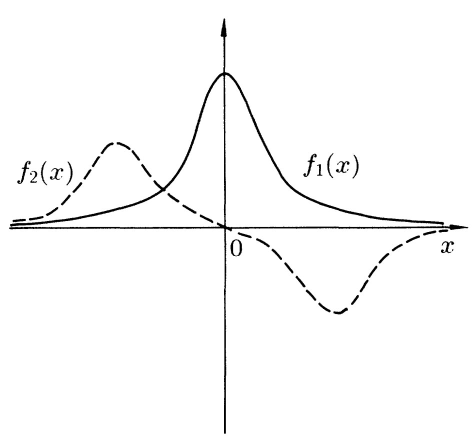

FIG. 7. A diagrammatic representation of $f_i(x)$ $(i=1,2)$ in (151) and (152).

$$v_n(t)=\epsilon v_{n,n}^{(1)}+\epsilon^2 v_{n,n}^{(2)} =(-1)^n 2 f_1(x_n)\cos(\Omega_2^s t-\phi_0) , \quad (149)$$

$$w_n(t)=\epsilon w_{n,n}^{(1)}+\epsilon^2 w_{n,n}^{(2)} =(-1)^n 2 f_2(x_n)\cos(\Omega_2^s t-\phi_0) , \quad (150)$$

with

$$f_1(x)=\left[\frac{\Gamma_+}{\Delta_+}\right]^{1/2}\eta_0\text{sech}[\eta_0(x-x_0)] , \quad (151)$$

$$f_2(x)=-\frac{Ma}{2(M-m)}\left[\frac{\Gamma_+}{\Delta_+}\right]^{1/2}\eta_0^2\text{sech}[\eta_0(x-x_0)] \times\tanh[\eta_0(x-x_0)] . \quad (152)$$

A diagrammatic representation of $f_1(x)$ and $f_2(x)$ is given in Fig. 7.

In (147), (148), (151), and (152), η_0 and x_0 are arbitrary constants. η_0 can be taken as the small expansion parameter used in (5), i.e., $\eta_0=O(\epsilon)$. We note that when

$$1-m/M=O(\epsilon) , \quad (153)$$

i.e., the mass difference of the atoms of different kind, $M-m$, has the same order as ϵ, the order of $f_1(x)$ in (147) and $f_2(x)$ in (152) will increase by 1. Thus $f_1(x)$ and $f_2(x)$ in (147), (148), (151), and (152) will have the same order under the condition (153). In this case, the diagrams of $f_1(x)$ and $f_2(x)$ shown in Figs. 7 and 6 qualitatively transform into Figs. 3 and 5 of Ref. 20. In fact, we can show that the solutions of KF, Eqs. (24) and (25) of Ref. 20, can have the form of (151) and (152) when the nonlinear shift of the soliton frequency is much smaller than the spectrum gap. Thus KF's theoretical approach and ours have different applicability regions at $g=\pm\pi/a$, which coincide provided the nonlinearity of the system is not too big and the mass difference between atoms becomes small.

VIII. SUMMARY AND CONCLUSIONS

In this paper we have investigated the nonlinear excitations in a 1D diatomic lattice model with a nonlinear onsite potential and a quartic anharmonicity between nearest neighbors. The method is systematic and has many advantages for the analysis of the soliton excitations in diatomic even multiatomic lattice systems in the whole BZ.

We first introduced an asymptotic expansion for the displacements of particles under a quasidiscreteness approximation. The original nonlinear controlling equations were transformed into a set of inhomogeneous linear equations, which can be solved order by order. The expansion procedure is quite general and can be applied to other nonlinear lattice systems.[34] In Secs. III and IV we have solved the acoustic and the optical modes, respectively. When $\omega_0\neq0$, the dynamics of the diatomic lattice was transformed into the NLS equation on $-\pi/a<q\leq\pi/a$. The symmetry between the acoustic- and the optical-mode equations allowed us to simplify the calculations considerably. In the case of the

nearest-neighbor interaction, we introduced a quasi-discrete long-wave approximation in Sec. V for the acoustic mode at $q=0$ and obtained the MKdV equation. The single soliton, kink, breather, and the two-soliton bound state can be readily written down, all of which are the typical nonlinear excitations of the system. We must point out that the results obtained in Secs. III–V are without any divergence for each order approximation solution.[33]

Gap solitons are interesting nonlinear excitations in diatomic lattice systems. Since the authors of Refs. 4–9 only studied the soliton dynamics in the continuum limit, i.e., the soliton excitations at $q=0$, the phenomenon of the gap solitons could not be considered. Because our approach is valid in the whole BZ, we can easily get the gap solitons as well as resonant kinks at $q=0$ or $\pm\pi/a$. Especially the gap soliton and the resonant kink observed recently are well explained qualitatively. In addition, bottom gap solitons, upper cutoff solitons (the intrinsic localized modes), and some resonant kinks are also predicted.

The decoupling ansatz is an assumption widely used for studying the soliton excitations in diatomic lattices. We have shown in Sec. VII that this ansatz is completely unnecessary and may be naturally derived in our approach. The gap soliton theory proposed by KF, which is successful for the explanation of the self-induced gap solitons, coincides with our treatment when $q=\pm\pi/a$ and the mass difference of the two kinds of atoms becomes small.

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