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Soliton Solutions in a Diatomic Lattice System

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Abstract

A continuum limit is considered for a diatomic lattice system with a cubic nonlinearity. A long wave equation describing the interaction of acoustic and optical modes is obtained. It reduces, in certain approximations, to equations having coupled wave solutions. The solutions exhibit trapping of an optical mode by an acoustic soliton. The form of the trapped optical wave depends on the mass ratio of adjacent particles in the diatomic lattice.

§1. Introduction

Since Fermi, Pasta and Ulam[1)] discovered the famous recurrence phenomenon of the lattice system with cubic interaction potential, considerable effort has been made to account for the result. Especially Zabusky and Kruskal[2)] showed that a continuum limit of the system reduces to the Korteweg-deVries equation which arises in a broad class of nonlinear dispersive systems. The numerical study of the equation revealed that solitons, which preserve their identities through mutual interactions, play an important role in the development of solutions. The realization of recurrence in the lattice system is closely related to the fact that the solitons are quite stable entities.

The Toda lattice, a one-dimensional lattice with exponential potential between the nearest neighbors, is an excellent model to study nonlinear lattice wave propagations analytically.[3)] A remarkable point is that the equation of motion can be solved exactly. The equation admits the lattice soliton solution. The lattice soliton behaves stably in a similar fashion as the soliton of the Korteweg-deVries equation. The analytical methods such as the inverse scattering transform and Hirota's method clarify the underlying properties of soliton phenomena.[4)]

Several attempts have been performed both numerically and analytically to make clear the question how inhomogeneities affect the nonlinear wave propagations, especially the behavior of solitons; scattering of solitons from a mass interface in the lattice with the potential including cubic and quartic nonlinearities,[5),6)] scattering of solitons from a mass impurity in the Toda lattice,[7)-9)] excitation of localized mode caused by the incidence of soliton to an impurity in the Toda lattice,[8)] and so on. Interesting subjects on the nonlinear wave modulation in lattice systems have also been treated by many authors.[10)]

As is well known, the linear diatomic lattice system has the optical mode as well as the acoustic mode. A nonlinear interaction between them is expected to cause the formation of a coupled soliton.

In this paper, we investigate a one-dimensional diatomic lattice with the interaction potential including cubic nonlinearity. In §2, we present the model lattice system and, considering the continuum limit, obtain a long wave equation. Its linear dispersion relation, of course, includes an optical mode as well as an acoustic mode. We rewrite the long wave equation in terms of the normal mode coordinates. The equation so obtained is reduced to two sets of coupled wave equations according as the degree of approximations. Steady solutions of the coupled wave equations are examined in §3. The solusions exhibit coupled soliton solutions of acoustic and optical waves. If nonlinear and dispersion effects on the acoustic waves can not be neglected, the wave form of the optical soliton depends upon the mass ratio of adjacent particles in the diatomic lattice. Concluding remarks are given in §4.

§2 Continuum limit of a diatomic lattice

We start with a one-dimensional infinite diatomic lattice whose equaiton of motion is written by

$$\mu_n y_{n,tt} = \gamma(y_{n+1} - 2y_n + y_{n-1})\{1 - \alpha(y_{n+1} - y_{n-1})\}, \qquad (1a)$$

$$\mu_n = m\delta_{n,2j} + M\delta_{n,2j+1}, \qquad (1b)$$

with an arbitrary integer j, where y_n and μ_n are the displacement and the mass of the n-th particle, γ the force constant, and α the parameter related to the strength of nonlinearity. The mass m is assigned to the even lattice points and M to the odd points.

We take a continuum limit of Eq.(1a) to suppose a long wavelength disturbance of the system. We denote the displacement y_n by $q(x,t)\delta_{n,2j} + Q(x,t)\delta_{n,2j+1}$, where x = na and a is a lattice constant. Assuming that a is very smaller than the wavelength, Taylor-expanding q ang Q, and neglecting the terms of order a^5, we obtain from Eq.(1a),

$$q_{tt} = \omega_1^2[2(Q - q) + a^2Q_{xx} + a^4Q_{xxxx}/12 - 4\alpha a(Q - q)Q_x - 2\alpha a^3(Q - q)Q_{xxx}/3 - 2\alpha a^3Q_xQ_{xx}], \quad (2a)$$

$$Q_{tt} = \omega_2^2[2(q - Q) + a^2q_{xx} + a^4q_{xxxx}/12 - 4\alpha a(q - Q)q_x - 2\alpha a^3(q - Q)q_{xxx}/3 - 2\alpha a^3q_xq_{xx}], \quad (2b)$$

where $\omega_1^2 = \gamma/m$, $\omega_2^2 = \gamma/M$ and the subscripts x and t stand for partial differentiations with respect to the corresponding variables. A characteristic feature of diatomic lattice systems is that they have optical vibration modes as well as acoustic modes. The linearized version of Eqs.(2a) and (2b) is expressed as

$$\omega^2\begin{pmatrix}\bar{q}\\ \bar{Q}\end{pmatrix} - 2\begin{pmatrix}\omega_1^2 & -\omega_1^2f(ka)\\ -\omega_2^2f(ka) & \omega_2^2\end{pmatrix}\begin{pmatrix}\bar{q}\\ \bar{Q}\end{pmatrix} = 0, \quad (3)$$

where $\bar{q}$ and $\bar{Q}$ are the Fourier amplitudes of q and Q with the frequency ω and the wavenumber k, and

$$f(x) = 1 - x^2/2 + x^4/24. \quad (4)$$

Equation (3) gives the linear dispersion relation,

$$\omega^2 = (\omega_1^2 + \omega_2^2)[1 \pm \sqrt{1 - A\{1 - f^2(ka)\}}], \tag{5}$$

$$A = 4\omega_1^2\omega_2^2/(\omega_1^2 + \omega_2^2)^2 = 4mM/(m + M)^2. \tag{6}$$

We note here that Eq.(5) corresponds to the wellknown dispersion equation without the long wave approximations if $f(x)=\cos x$. The upper sign in Eq.(5) corresponds to the optical mode, $\omega=\omega_h$, and the lower sign to the acoustic mode, $\omega=\omega_\ell$. Under the approximation we are considering, they may be expressed as

$$\omega_h^2 = 2(\omega_1^2 + \omega_2^2)\{1 - Ak^2a^2/4 + A(1 - 3A/4)k^4a^4/12\}, \tag{7a}$$

$$\omega_\ell^2 = 2\,\frac{\gamma}{m+M}\,k^2a^2\{1 - (1 - 3A/4)k^2a^2/3\}. \tag{7b}$$

In order to investigate the wave propagation of our system, it is convenient to introduce the normal mode coordinates $\bar{r}$ and $\bar{R}$, instead of $\bar{q}$ and $\bar{Q}$, through

$$\begin{pmatrix} \bar{R} \\ \bar{r} \end{pmatrix} = \begin{pmatrix} \frac{m}{m+M} - \frac{A}{4}\,k^2a^2 + \frac{A}{12}(1-\frac{3}{4}A)k^4a^4 & \frac{M}{m+M}\,f(ka) \\ 1 - \frac{m+M}{4M}\,Ak^2a^2 + \frac{m+M}{12M}\,A(1-\frac{3}{4}A)k^4a^4 & -f(ka) \end{pmatrix} \begin{pmatrix} \bar{q} \\ \bar{Q} \end{pmatrix}. \tag{8}$$

It is shown directly that Eq.(3) is diagonalized by means of this transformation. We carry out the Fourier transform of Eq.(8) to obtain

$$R = \frac{mq+MQ}{m+M} + \frac{1}{4}\,Aa^2q_{xx} + \frac{M}{2(m+M)}\,a^2Q_{xx}$$
$$+ \frac{1}{12}\,A(1-\frac{3}{4}A)a^4q_{xxxx} + \frac{M}{24(m+M)}\,a^4Q_{xxxx}, \tag{9a}$$

$$r = q - Q + \frac{m+M}{4M} \Lambda a^2 q_{xx} - \frac{1}{2} a^2 Q_{xx}$$

$$+ \frac{m+M}{12M} \Lambda(1 - \frac{3}{4}\Lambda) a^4 q_{xxxx} - \frac{1}{24} a^4 Q_{xxxx}. \quad (9b)$$

The coordinates R and r describe the low and high frequency modes, tending in the long wavelength limit to the center of mass coordinate of two adjacent particles and their relative coordinate, respectively.

We now derive the equations governing R and r. From Eqs.(9a) and (9b), we find that q and Q are expressed accurately up to the order a^4 as

$$q = R + \frac{M}{m+M} r - \frac{1}{2} \Lambda a^2 (R_{xx} + \frac{M}{m+M} r_{xx}) - \frac{1}{6} \Lambda(1 - \frac{9}{4}\Lambda) a^4 (R_{xxxx} + \frac{M}{m+M} r_{xxxx}), \quad (10a)$$

$$Q = R - \frac{m}{m+M} r - \frac{1}{2} a^2 (R_{xx} - \frac{m}{m+M} r_{xx}) - \frac{M-m}{4M} \Lambda a^2 (R_{xx} + \frac{M}{m+M} r_{xx})$$

$$+ \frac{5}{24} a^4 (R_{xxxx} - \frac{m}{m+M} r_{xxxx}) + \frac{M-m}{24M} \Lambda(1 + \frac{9}{2}\Lambda) a^4 (R_{xxxx} + \frac{M}{m+M} r_{xxxx}). \quad (10b)$$

Differentiating Eqs.(9a) and (9b) twice with respect to t, substituting Eqs.(2) and (10), and neglecting the terms of order a^5, we obtain after a lengthy calculation,

$$R_{tt} - \frac{1}{4} \Omega^2 \Lambda a^2 R_{xx} - \frac{1}{12} \Omega^2 \Lambda(1 - \frac{3}{4}\Lambda) a^4 R_{xxxx} + \frac{1}{4} \alpha\Omega^2 \Lambda a^3 (R_x^2)_x$$

$$= - \frac{1}{4} \alpha\Omega^2 \Lambda a (r^2)_x + \frac{1}{6} \alpha\Omega^2 \frac{m-2M}{m+M} \Lambda a^3 (r r_{xx})_x - \frac{1}{12} \alpha\Omega^2 \frac{m^2+8mM+4M^2}{(m+M)^2} \Lambda a^3 (r_x^2)_x, \quad (11a)$$

$$r_{tt} + \Omega^2 r + \frac{1}{4} \Omega^2 \Lambda a^2 r_{xx} + \frac{1}{12} \Omega^2 \Lambda (1 - \frac{3}{4}\Lambda) a^4 r_{xxxx} + \alpha\Omega^2 \frac{m-M}{m+M} \Lambda a^3 r_x r_{xx}$$

$$= 2\alpha\Omega^2 a r R_x + \frac{2}{3} \alpha\Omega^2 \frac{2m-M}{m+M} a^3 r R_{xxx} + 2\alpha\Omega^2 (1 + \frac{m}{4M}) \Lambda a^3 r_x R_{xx}$$

$$+ \frac{1}{2} \alpha\Omega^2 \Lambda a^3 r_{xx} R_x, \tag{11b}$$

where Ω^2 is defined by

$$\Omega^2 = 2(\omega_1^2 + \omega_2^2). \tag{12}$$

These equations describe a coupling motion of acoustic and optical waves.

As is seen from Eqs.(11a) and (11b), the wave motion of the optical mode induces the acoustic waves. However, if the contribution from the optical mode is neglected in Eq.(11a), we obtain the equation of free acoustic wave,

$$n_{tt} - \frac{1}{4} \Omega^2 \Lambda a^2 n_{xx} - \frac{1}{12} \Omega^2 \Lambda (1 - \frac{3}{4}\Lambda) a^4 n_{xxxx} - \frac{1}{4} \alpha\Omega^2 \Lambda a^4 (n^2)_{xx} = 0, \tag{13}$$

where we have introduced

$$n = -R_x/a. \tag{14}$$

Equation (13) with m = M is equivalent to the equation which Zabusky derived as a continuum limit of the Fermi-Pasta-Ulam system.[11)] This equation is known to have an N-soliton solution describing a multiple collision of solitons.[12)] Each acoustic soliton is expressed as

$$n = N \operatorname{sech}^2\{(x - \lambda t)/\Delta\}, \tag{15}$$

where

$$\lambda = (\sqrt{A}\Omega a/2)(1 + 2\alpha a^2 N/3)^{1/2}, \tag{16}$$

$$\Delta = \{2(1 - 3A/4)/\alpha N\}^{1/2}. \tag{17}$$

This solution is possible for arbitrary value of the mass ratio m/M.

§3 Coupled waves

In this section we study the coupled waves described by Eqs.(11a) and (11b). The equations are still rather complex to study analytically. Here we assume a slow modulation of the optical waves. Let ψ be defined by

$$r = \frac{1}{2}(\psi e^{-i\Omega t} + \psi^* e^{i\Omega t}), \tag{18}$$

where asterisk denotes complex conjugate. The amplitude ψ varies slowly with respect to x and t. We then obtain

$$r_{tt} + \Omega^2 r \simeq -i\Omega\psi_t e^{-i\Omega t} + i\Omega\psi_t^* e^{i\Omega t}. \tag{19}$$

Furthermore, we suppose the slowness of spatial variation and the smallness of amplitude of acoustic wave are in the same order, i.e., $a\partial_x \sim O(\varepsilon)$ and $\alpha R \sim O(\varepsilon)$. As for the amplitude of modulated wave, we consider the following two cases; $\alpha|\psi| \sim O(\varepsilon)$ (Case I) and $\alpha|\psi| \sim O(\varepsilon^2)$ (Case II). We substitute Eqs.(14) and (19) into Eqs.(11a) and (11b), keep the leading terms of nonlinear couplings and neglect the higher order terms in ε. Then we find the equations for n and ψ by averaging the fast oscillating parts; for Case I,

$$n_{tt} - \frac{1}{4}\Omega^2 A a^2 n_{xx} = \frac{1}{8}\alpha\Omega^2 A(|\psi|^2)_{xx}, \tag{20a}$$

$$-i\Omega\psi_t + \frac{1}{8}\Omega^2\Lambda a^2\psi_{xx} = -\alpha\Omega^2 a^2 n\psi, \tag{20b}$$

and for Case II,

$$n_{tt} - \frac{1}{4}\Omega^2\Lambda a^2[n + \frac{1}{3}(1 - \frac{3}{4}\Lambda)a^2 n_{xx} + \alpha a^2 n^2]_{xx}$$

$$= \frac{1}{8}\alpha\Omega^2\Lambda(|\psi|^2)_{xx}, \tag{21a}$$

$$-i\Omega\psi_t + \frac{1}{8}\Omega^2\Lambda a^2\psi_{xx} = -\alpha\Omega^2 a^2 n\psi. \tag{21b}$$

If the propagation speed of coupled waves is nearly equal to the sound speed (= $\sqrt{\Omega^2\Lambda a^2/4}$), the dispersive and nonlinear terms neglected in obtaining Eq.(20a) become important and, therefore, Eq.(21a) should apply.

Both of the coupled equations have arised in the study of nonlinear wave propagation in a plasma,[13),14)] where ψ denotes the amplitude of Langmuir waves and n the density fluctuation of ions. Equations (20) and (21) are known to have coupled wave solutions which describe an optical soliton accompanied with an acoustic wave. The forms of such soliton solutions depend on whether the effect of nonlinearity and dispersion of acoustic waves is included or not.

Here we show the coupled wave solutions for both cases. We look for a solution of Eqs.(20a) and (20b) in the following form,

$$\psi = \phi(\eta)\exp\{i(\kappa x - \nu t)\}, \tag{22a}$$

$$n = n(\eta), \tag{22b}$$

$$\eta = x - \lambda t. \tag{23}$$

Case I Substituting Eqs.(22) and (23) into Eqs.(20a) and (20b) yields

$$(\lambda^2 - \frac{1}{4}\,\Omega^2\Lambda a^2)n = \frac{1}{8}\alpha\Omega^2\Lambda\phi^2, \tag{24a}$$

$$\frac{1}{8}\,\Lambda a^2\phi_\eta^2 = (\frac{\nu}{\Omega} + \frac{2\lambda^2}{\Omega^2\Lambda a^2})\phi^2 - \frac{1}{16}\,\frac{\alpha^2\Omega^2\Lambda a^2}{(\lambda^2-\Omega^2\Lambda a^2/4)}\,\phi^4, \tag{24b}$$

$$\lambda = -\Omega\Lambda a^2\kappa/4. \tag{25}$$

From these equations we obtain

$$n = N\ \mathrm{sech}^2\{(x-\lambda t)/\Delta\}, \tag{26a}$$

$$\psi = \phi\ \exp[-i\{(2\mu\sqrt{\Lambda})x/a - (\mu^2 - \alpha a^2 N)\Omega t/2\}], \tag{26b}$$

$$\phi = [2(\mu^2-1)a^2N/\alpha]^{1/2}\ \mathrm{sech}\{(x - \lambda t)/\Delta\}, \tag{26c}$$

where

$$\Delta = [\Lambda/(4\alpha N)]^{1/2}, \tag{27}$$

$$\mu = \lambda/[\sqrt{\Lambda}\Omega a/2], \tag{28}$$

and N is arbitrary. This solution is possible only for $\lambda^2 > \Omega^2\Lambda a^2/4$, i.e., the propatation speed > the sound speed, $(\mu^2 > 1)$.

Case II Substituting Eqs.(22) and (23) into Eqs.(21a) and (21b), we obtain

$$(\lambda^2 - \frac{1}{4}\,\Omega^2\Lambda a^2)n - \frac{1}{12}\,\Omega^2\Lambda(1 - \frac{3}{4}\Lambda)a^4 n_{\eta\eta} - \frac{1}{4}\,\alpha\Omega^2\Lambda a^3 n^2 = \frac{1}{8}\,\alpha\Omega^2\Lambda\phi^2, \tag{29a}$$

$$\frac{1}{8}\,\Omega\Lambda a^2\phi_{\eta\eta} = (\nu + \frac{2\lambda^2}{\Omega\Lambda a^2})\phi - \alpha\Omega a^2 n\phi, \tag{29b}$$

$$\lambda = -\Omega\Lambda a^2\kappa/4. \tag{25}$$

We suppose that n is expressed as, with arbitrary N,

$$n = N\,\mathrm{sech}^2(\eta/\Lambda). \tag{30}$$

If we consider $n = N\,\mathrm{sech}^m(\eta/\Lambda)$ for $m = 1,2,\cdots$, we see that only the case $m = 2$ satisfies Eqs.(29a) and (29b). The solution ϕ is determined by substituting Eq.(30) into Eqs.(29a) and (29b). There are three possible types of soliton solutions for $\alpha a^2 N > 0$.

(Case II-1)

$$\phi = 0, \tag{31a}$$

$$\Lambda = \{2(1 - 3A/4)/\alpha N\}^{1/2}, \tag{31b}$$

$$\lambda = (\sqrt{A}\Omega a/2)(1 + 2\alpha a^2 N/3)^{1/2}. \tag{31c}$$

This solution is equivalent to the acoustic soliton solution, Eqs.(15)-(17), and always possible for arbitrary value of the mass ratio m/M when $\lambda > \sqrt{A}\Omega a/2$.

(Case II-2)

$$\psi = \phi\, \exp[-i\{(2\mu/\sqrt{A})x/a - \{1 - 8(1-2/3A)\alpha a^2 N/3\}\Omega t/2\}], \tag{32a}$$

$$\phi = (16/3A - 6)^{1/2}\, a^2 N\, \mathrm{sech}^2(\eta/\Lambda), \tag{32b}$$

$$\Lambda = (3A/4\alpha N)^{1/2}, \tag{32c}$$

$$\lambda = (\sqrt{A}\Omega a/2)[1 + (4/3)\{4/(3A) - 1\}\alpha a^2 N]^{1/2}. \tag{32d}$$

This solution is realized for $A < 8/9$. The condition is expressed in terms of the mass ratio as $m/M > 2$ or $m/M < 1/2$.

(Case II-3)

$$\psi = \phi\, \exp[-i\{(2\mu/\sqrt{A})x/a - \{1 + 4(1-2/3A)\alpha a^2 N/3\}\Omega t/2\}], \tag{33a}$$

$$\phi = (6 - 16/3A)^{1/2} a^2 N \operatorname{sech}(\eta/\Delta)\tanh(\eta/\Delta), \tag{33b}$$

$$\Delta = (3A/4\alpha N)^{1/2}, \tag{33c}$$

$$\lambda = (\sqrt{A}\Omega a/2)[1 + (5/3)\{1 - (8/15A)\}\alpha a^2 N]^{1/2}, \tag{33d}$$

This solution is realized for $A > 8/9$, i.e., $1/2 < m/M < 2$.

We note here that the form of optical soliton depends on the mass ratio of two adjacent particles of the diatomic lattice.

§4 Concluding remarks

We have investigated the continuum limit of the nonlinear diatomic lattice. The long wave equations written by the normal mode coordinates express a nonlinear interaction between acoustic and optical modes. In an approximation of slow variations of the system, the equations are reduced to the coupled wave equations which are known to describe an interaction of Langmuir waves with ion acoustic waves in a plasma. The existence of the coupled solitn solutions is an essential feature of these equations.

In Case I, the optical soliton couples with the compressive acoustic soliton for positive α and with the rarefactive acoustic soliton for negative α. In any case the propagation speed of solitons is greater than the sound speed, while for the case of plasmas the soliton speed does not exceed the ionic sound speed.[13] In Case II, one of the interesting results is that the wave form of the optical soliton depends on the mass ratio of adjacent particles in the diatomic lattice. If the mass ratio is greater than 2, the optical field trapped by the acoustic soliton has no nodal point. On the other hand, if the mass ratio is less than 2, the optical field has one node. It should be noted that an acoustic soliton trapping the optical waves does not exsist when the mass ratio is just equal to 2.

A numerical investigation of the coupled wave equations (20a) and (20b) has shown that the breaking-up or fusion of solitons occurs in their collisions.[15] The similar situation is expected for lattice waves even if the long wavelength approximation is not assumed. It is worth while studying numerically the diatomic lattice system, Eqs.(1a) and (1b), in order to see the existence of a steady coupled lattice soliton and the behavior of interaction among the coupled solitons.

Finally, we remark that the discussions made here hold in the case of m=M. For this case, though an optical mode does not exist, the mode, r, corresponds to the oscillation in which the adjacent particles move in the opposite phase each other. Therefore, the coupled soliton is considered to be due to the interaction between the long acoustic-wave and the modulation of the oscillation of the highest frequency.

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