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# Solitons in a One-Dimensional Lennard-Jones Lattice

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Nonlinear waves in a one-dimensional lattice with $(2n, n)$ Lennard-Jones potential are studied in small-amplitude and long-wavelength approximations. Equations derived are classified into three types according to the value of the force-range parameter $n$. For $n=2$ and $\geqq 4$, we get the Benjamin-Ono equation and the Korteweg-de Vries equation, respectively.

## § 1. Introduction

Since the discovery of solitons by Zabusky and Kruskal,[1] many studies have been made on the nonlinear wave propagation in one-dimensional anharmonic lattices.[2] Important equations in this problem are the Zabusky equation (or the Boussinesq equation), the Korteweg-de Vries (K-dV) equation, the modified K-dV equation, the nonlinear Schrödinger equation, the Sine-Gordon equation, the Toda lattice equation and so on.[2),3] They all were investigated in detail both numerically and analytically and are known to have $N$-soliton solutions.[3] In these lattices, solitons play an important role for the physical properties such as heat conduction.[4]

The equations mentioned above are derived for a lattice with the nearest-neighbor interaction. In some lattices such as metals,[5] however, interatomic forces may extend further than the nearest neighbors. A lattice with the long-range interaction has, as is well known, the dispersion relation different from that of a lattice with the nearest-neighbor interaction, and may have soliton solutions not observed before.

In this paper, we investigate this problem. As a model of the nonlinear lattice, we take a one-dimensional lattice with $(2n, n)$ Lennard-Jones (L-J) potential expressed as

$$U(r)=4U_0\left[\left(\frac{\sigma}{r}\right)^{2n}-\left(\frac{\sigma}{r}\right)^{n}\right], \tag{1·1}$$

where $U_0$ is the potential depth, $2\sigma$ the diameter of constituent particle and $n$ is a positive integer. The smaller the value of parameter $n$ is, the longer the range of force is. Under the nearest-neighbor approximation, formerly Visscher et al.[6] studied the (12, 6) L-J lattice in connection with thermal conductivity in the nonlinear lattice and recently Yoshida and Sakuma[7] presented the Boussinesq-like equation for the (2, 1) L-J lattice. We shall investigate the general $(2n, n)$ L-J lattice with effects of the long-range interactions fully taken into account.

The plan of this paper is as follows. In § 2, we present the general equations of motion for small vibration. In § 3, introducing the continuum approximation, we derive three types of nonlinear wave equations according to the value of the parameter $n$. Solitary wave solutions of them are also examined. Concluding remarks are given in § 4.

## § 2. Equations of motion for small vibration

We consider a lattice consisting of an infinite number of equally spaced identical particles of mass $M$, lying along a straight line. Let the equilibrium spacing between the particles be $a$ and the longitudinal displacement of the $p$th particle from its equilibrium position be $u_p$. Then the total potential energy of the lattice, $V$, is given by

$$V=\sum_p \sum_{m>0} U(x_{p+m}-x_p), \tag{2·1}$$

where $x_p$ is the position of the $p$th particle and given by

$$x_p=pa+u_p\,. \tag{2·2}$$

We assume that the particle displacement is very small compared with the interparticle distance. Expanding $U(x_{p+m}-x_p)$ in the displacement $u_p$ and neglecting terms higher than $O(u_p{}^3)$, we obtain from Eqs. (2·1) and (2·2)

$$V=V_0+\frac{1}{2}\sum_p \sum_{m>0} U''(ma)(u_{p+m}-u_p)^2+\frac{1}{6}\sum_p \sum_{m>0} U'''(ma)(u_{p+m}-u_p)^3\,, \tag{2·3}$$

where $V_0$ is the potential energy of the lattice corresponding to the equilibrium configuration,

$$V_0=\sum_p \sum_{m>0} U(ma). \tag{2·4}$$

We have also used the fact that the terms linear in $u_p$ vanish because the lattice is in equilibrium when $u_p=0$ for all $p$. Requiring that $V_0$ be a minimum with respect to variations in the lattice spacing $a$,[5] we have from Eqs. (1·1) and (2·4)

$$a=\left[\frac{2\zeta(2n)}{\zeta(n)}\right]^{1/n}\sigma\,, \tag{2·5}$$

where $\zeta(n)$ is the Riemann zeta function. We observe that for $n=1$ the lattice spacing is zero. From now on we will assume $n\geqq 2$.

Let $F_p$ denote the total force acting on the $p$th particle. Then it is given by $-\partial V/\partial u_p$, so that the equation of motion of the $p$th particle is

$$M\frac{d^2}{dt^2}u_p=F_p \tag{2·6}$$

with

$$F_p=\sum_{m>0}U''(ma)(u_{p+m}+u_{p-m}-2u_p)$$
$$+\frac{1}{2}\sum_{m>0}U'''(ma)[(u_{p+m}-u_p)^2-(u_{p-m}-u_p)^2]. \tag{2·7}$$

If the interactions only among nearest neighbors are taken into account, then Eq. (2·6) with Eq. (2·7) reduces to

$$M\frac{d^2}{dt^2}u_p=U''(a)(u_{p+1}+u_{p-1}-2u_p)$$
$$+\frac{1}{2}U'''(a)[(u_{p+1}-u_p)^2-(u_{p-1}-u_p)^2]. \tag{2·8}$$

As is well known, a continuum limit of this equation yields the Boussinesq equation or the K-dV equation which has sech$^2$-type soliton solution.[2)]

## § 3. Nonlinear waves with long-wavelengths

In this section we study the nonlinear waves described by Eq. (2·6) with Eq. (2·7) which includes long-range force components. For the $(2n, n)$ L-J potential, Eq. (2·6) with Eq. (2·7) is rather complicated to study analytically. Here we consider smooth waves with wavelengths which are long compared with the lattice spacing, so that we adopt a continuum approximation.

For this purpose, it is convenient to introduce the Fourier expansion for $u_p$,

$$u_p=\sum_k Q_k e^{ikx} \tag{3·1}$$

with

$$|k|<\frac{\pi}{a}, \tag{3·2}$$

where $x$ is the equilibrium position of the $p$th particle, $x=pa$. Because $u_p$ is real, we have $Q_{-k}=Q_k^*$. With use of Eq. (3·1), the expression for $F_p$ is written as

$$F_p=\sum_k[-2I(k)]Q_k e^{ikx}+\sum_k\sum_{k'}[iJ(k+k')-2iJ(k)]Q_kQ_{k'}e^{i(k+k')x}, \tag{3·3}$$

where

$$I(k)=\sum_{m=1}^{\infty}U''(ma)[1-\cos(mka)] \tag{3·4}$$

and

$$J(k)=\sum_{m=1}^{\infty}U'''(ma)\sin(mka). \tag{3·5}$$

For the $(2n, n)$ L-J potential (1·1), $I(k)$ and $J(k)$ are given by

$$I(k)=\frac{2n\zeta(n)U_0}{\zeta(2n)a^2}\left[\frac{(2n+1)\zeta(n)}{\zeta(2n)}A_{2n+2}(ka)-(n+1)A_{n+2}(ka)\right], \tag{3·6}$$

$$J(k)=\frac{2n(n+1)\zeta(n)U_0}{\zeta(2n)a^3}\left[-\frac{(4n+2)\zeta(n)}{\zeta(2n)}B_{2n+3}(ka)+(n+2)B_{n+3}(ka)\right], \tag{3·7}$$

where $A_n(ka)$ and $B_n(ka)$ are defined by Eqs. (A·1) and (A·2) in the Appendix. We note here that the exact dispersion relation of the linear wave is expressed from the linearized version of Eq. (3·3) as

$$\omega_k{}^2=\frac{2}{M}I(k), \tag{3·8}$$

where $\omega_k$ is the frequency of the wave with wavevector $k$.

Let us take a continuum limit of Eqs. (3·3), (3·6) and (3·7). Assuming that $|ka|\ll 1$, keeping the leading terms of $A_n(ka)$ and $B_n(ka)$ and neglecting the higher order terms in $ka$, we find that $F_p$ has three types of expressions for $n=2, 3, 4, \cdots$ (see the Appendix):

$$F_p=M\sum_k(-\omega_k{}^2)Q_ke^{ikx}-3(n+1)Mc^2\sum_k\sum_{k'}(ik)(ik')^2Q_kQ_{k'}e^{i(k+k')x}, \tag{3·9}$$

where $c$ is the sound speed given by

$$c^2=\frac{2n^2[\zeta(n)]^2U_0}{\zeta(2n)M}, \tag{3·10}$$

and $\omega_k{}^2$ is written as

$$\left.\begin{aligned}\omega_k{}^2&=c^2(k^2+\delta|k|^3),\\ \delta&=\frac{\pi a}{4\zeta(2)},\end{aligned}\right\}\quad\text{for } n=2, \tag{3·11}$$

$$\left.\begin{aligned}\omega_k{}^2&=c^2(k^2-\delta k^4\log|ka|),\\ \delta&=\frac{a^2}{9\zeta(3)},\end{aligned}\right\}\quad\text{for } n=3 \tag{3·12}$$

and

$$\left.\begin{aligned}&\omega_k{}^2=c^2(k^2-\delta k^4),\\&\delta=\frac{a^2}{12n}\left[(2n+1)\frac{\zeta(2n-2)}{\zeta(2n)}-(n+1)\frac{\zeta(n-2)}{\zeta(n)}\right],\end{aligned}\right\}\quad \text{for } n\geqq 4\,. \tag{3·13}$$

These equations show that the value of the force-range parameter $n$ mainly contributes to the form of the dispersion relation.

We will derive from these expressions the equations governing $u_p=u(x,t)$ and study solitary wave solutions of them.

*Case $n=2$.* Substituting Eq. (3·1) into Eqs. (3·9) and (3·11), we have from Eq. (2·6)

$$u_{tt}=c^2[u_{xx}-\delta H(u_{xxx})-9u_x u_{xx}], \tag{3·14}$$

where $H$ is the Hilbert transform operator defined by

$$H[f(x)]=\frac{1}{\pi}P\int_{-\infty}^{\infty}\frac{f(x)}{x'-x}dx'\,. \tag{3·15}$$

We have also used the identity

$$H(e^{ikx})=i(\operatorname{sgn}k)e^{ikx}\,. \tag{3·16}$$

A solitary wave solution of Eq. (3·14) is written as

$$u=\frac{4}{9}\delta\tan^{-1}[(x-\lambda t)/\Delta], \tag{3·17a}$$

$$\lambda^2=c^2[1-(\delta/\Delta)], \tag{3·17b}$$

$$\Delta>\delta\,, \tag{3·17c}$$

where we have used the identity

$$H\left(\frac{1}{x^2+\Delta^2}\right)=\frac{-x}{\Delta(x^2+\Delta^2)}\,. \tag{3·18}$$

It is well known that a solitary wave solution of the Zabusky equation which is derived as a continuum limit of Eq. (2·8) is compressive and supersonic. However, in the above solution, the propagation speed is smaller than the sound speed and the lattice is expanded around a solitary wave. Equation (3·14) can be reduced to the equation which describes the waves moving in one direction in the rest frame, by using the reductive perturbation method.[8] Let us introduce the stretched coordinates

$$\xi=\varepsilon(x-ct), \tag{3·19a}$$

$$\tau=\varepsilon^2 t\,, \tag{3·19b}$$

and expand $u_x$ as

$$u_x = \varepsilon v + \varepsilon^2 w + \cdots . \tag{3·20}$$

Substituting Eqs. (3·19) and (3·20) into Eq. (3·14) and collecting terms of order $\varepsilon^3$, we obtain

$$v_\tau - \frac{\delta c}{2} H(v_{\xi\xi}) - \frac{9c}{2} v v_\xi = 0 . \tag{3·21}$$

This equation is equivalent to the Benjamin-Ono (B-O) equation which describes internal waves in stratified fluids of great depth.[9] A soliton solution of Eq. (3·21)[9),10] is

$$v = A[1 + (\xi - \lambda\tau)^2/\Delta^2]^{-1} , \tag{3·22a}$$

$$A = -\frac{4\delta}{9|\Delta|} , \tag{3·22b}$$

$$\lambda = -\frac{c\delta}{2|\Delta|} , \tag{3·22c}$$

which has the Lorentzian profile vanishing algebraically as $|x| \to \infty$. The B-O equation has a solution describing a multiple collision of $N$ solitons.[10] The B-O solitons have no phase shift after the collisions of them unlike those which take place between K-dV solitons.

*Case $n=3$.* Substituting Eq. (3·1) into Eqs. (3·9) and (3·12), we have from Eq. (2·6)

$$u_{tt} = c^2[u_{xx} - \delta T(u_{xxxxx}) - 12 u_x u_{xx}], \tag{3·23}$$

where $T$ is the integral transform operator defined by

$$T[f(x)] = \frac{1}{\pi}\int_{-\infty}^{\infty} \mathrm{sgn}(x'-x)[\log|(x'-x)/a| + \gamma] f(x') dx' , \tag{3·24}$$

and $\gamma$ is Euler's constant. We have also used the identity

$$T(e^{ikx}) = \frac{\log|ak|}{ik} e^{ikx} . \tag{3·25}$$

At present, analytic solutions of Eq. (3·23) have not been found.

*Case $n \geqq 4$.* Substituting Eq. (3·1) into Eqs. (3·9) and (3·13), we get from Eq. (2·6)

$$u_{tt} = c^2[u_{xx} + \delta u_{xxxx} - 3(n+1) u_x u_{xx}], \tag{3·26}$$

which is essentially the same as a long-wave equation of nearest-neighbor system (2·8), namely the Zabusky equation. A solitary wave solution is expressed as

$$u=-\frac{4}{n+1}\left(\frac{\delta}{\Delta}\right)\tanh[(x-\lambda t)/\Delta], \tag{3·27a}$$

$$\lambda^2=c^2(1+4\delta/\Delta^2), \tag{3·27b}$$

where $\Delta$ is an arbitrary constant. Unlike the case $n=2$, this solution describes a compressed wave with supersonic speed. If instead of Eqs. (3·19) we introduce the stretched coordinates

$$\xi=\varepsilon^{1/2}(x-ct), \tag{3·28a}$$

$$\tau=\varepsilon^{3/2}t, \tag{3·28b}$$

then we can reduce Eq. (3·26) to the K-dV equation. It follows that

$$v_\tau+\frac{c\delta}{2}v_{\xi\xi\xi}-\frac{3(n+1)c}{2}vv_\xi=0. \tag{3·29}$$

A soliton solution of Eq. (3·29) is

$$v=A\ \mathrm{sech}^2[(\xi-\lambda\tau)/\Delta], \tag{3·30a}$$

$$A=-\frac{4\delta}{n+1}\frac{1}{\Delta^2}, \tag{3·30b}$$

$$\lambda=2\delta c\frac{1}{\Delta^2}, \tag{3·30c}$$

where $\Delta$ is an arbitrary constant.

We note here that the total compression by a K-dV soliton takes various values depending on the amplitude of the soliton but the total expansion by a B-O soliton is determined only by $\delta$ which depends on the lattice constant $a$ and the potential parameter $n$.

## § 4. Concluding remarks

In this paper we have investigated nonlinear wave propagations in the one-dimensional lattice with the $(2n, n)$ L-J potential. Introducing the approximations of small amplitude and long-wavelength, we have obtained Eq. (3·14) or the B-O equation for $n=2$, Eq. (3·23) for $n=3$ and the Zabusky equation or the K-dV equation for $n\geqq 4$. The results show that the value of the force-range parameter $n$ contributes not to the nonlinear terms but to the dispersion terms of the equations. It is well known that both the B-O and K-dV equations have soliton solutions formed by balancing of the nonlinearity and dispersion effects of the systems. The reason why the B-O soliton is algebraic is that the B-O equation is more dispersive than the K-dV equation. It is interesting to study whether Eq. (3·23) having an intermediate dispersion term between the B-O and

K-dV equations gives soliton solutions or not, though the problem is still open.

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## Appendix

*—— Formulas of Fourier Series ——*

Here we give some formulas of the Fourier series which are used in the text. We define the functions $A_n(ka)$ and $B_n(ka)$ as

$$A_n(ka)=\sum_{l=1}^{\infty}\frac{1}{l^n}[1-\cos(lka)], \tag{A·1}$$

$$B_n(ka)=\sum_{l=1}^{\infty}\frac{1}{l^n}\sin(lka), \tag{A·2}$$

where $n\geqq 2$. Then, for $|ka|\leqq\pi$, we have the recurrence formulas for them:

$$A_2(ka)=\frac{\pi}{2}|ka|-\frac{1}{4}(ka)^2, \tag{A·3}$$

$$A_3(ka)=-\frac{1}{2}\log 2\cdot(ka)^2+\int_0^{|ka|}(t_1-|ka|)\log(\sin t_1/2)dt_1$$

$$=-\frac{1}{2}(ka)^2\log|ka|+\frac{3}{4}(ka)^2+\frac{1}{288}(ka)^4+\cdots, \tag{A·4}$$

$$A_{n+2}(ka)=\frac{1}{2}\zeta(n)(ka)^2-\int_0^{ka}\int_0^{t_2}A_n(t_1)dt_1dt_2, \tag{A·5}$$

$$B_n(ka)=A_{n+1}(ka). \tag{A·6}$$

From these equations we find that if $|ka|\ll 1$ we obtain

$$A_4(ka)=\frac{1}{2}\zeta(2)(ka)^2-\frac{\pi}{12}|ka|^3+O[(ka)^4], \tag{A·7}$$

$$A_5(ka)=\frac{1}{2}\zeta(3)(ka)^2+\frac{1}{24}(ka)^4\log|ka|+O[(ka)^4], \tag{A·8}$$

$$A_6(ka)=\frac{1}{2}\zeta(4)(ka)^2-\frac{1}{24}\zeta(2)(ka)^4+O[(ka)^5], \tag{A·9}$$

$$A_7(ka)=\frac{1}{2}\zeta(5)(ka)^2-\frac{1}{24}\zeta(3)(ka)^4+O[(ka)^6\log|ka|], \tag{A·10}$$

$$B_5(ka)=\zeta(4)(ka)-\frac{1}{6}\zeta(2)(ka)^3+O[(ka)^4], \tag{A·11}$$

$$B_6(ka)=\zeta(5)(ka)-\frac{1}{6}\zeta(3)(ka)^3+O[(ka)^5\log|ka|], \tag{A·12}$$

and for $n\geqq 8$

$$A_n(ka)=\frac{1}{2}\zeta(n-2)(ka)^2-\frac{1}{24}\zeta(n-4)(ka)^4+O[(ka)^6], \tag{A·13}$$

$$B_n(ka)=\zeta(n-2)(ka)-\frac{1}{6}\zeta(n-4)(ka)^3+O[(ka)^5]. \tag{A·14}$$

Substitution of these equations into Eqs. (3·3), (3·6) and (3·7) gives Eqs. (3·9) ~(3·13).

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