Progress of Theoretical Physics, Vol. 48, No. 4, October 1972

Wave Modulations in Anharmonic Lattices

Akira TSURUI

Department of Applied Mathematics and Physics
Faculty of Engineering, Kyoto University, Kyoto

(Received April 12, 1972)

Wave modulations in one-dimensional anharmonic lattices are studied by the use of a perturbation method established by Taniuti and Yajima. A system of equations to determine the evolution of the slowly varying parts in the lowest order of an asymptotic expansion is derived. One interesting result is that the nonlinearly modulated wave must be accompanied by the other slowly varying wave which tends to stabilize the modulated one.

§ 1. Introduction

Many physical properties of real crystals are directly related to nonlinear effects produced by anharmonic forces. It is important to examine the properties of wave propagations in anharmonic lattices in connection with the thermal expansion of lattices,[1] the non-ergodic character of nonlinear lattices[2],[3] and the nonlinear propagation of heat observed by Narayanamulti and Varma.[4]

For special problems on harmonic lattices two- or three-dimensional ones have been studied but the problems on anharmonic lattices, even in the one-dimensional case, are complicated to be studied. Under certain conditions, however, real crystals can be approximated by one-dimensional lattice models.[5] Thus in this paper we will focus our attention on the wave modulations in one-dimensional anharmonic monatomic lattices.

Recently, Tappert and Varma[5] considered this problem in a continuum limit, assuming that the cubic term in the interaction potential is sufficiently small. In 1970 Lowell[1] also examined this problem according to Whitham's variational method[6] and showed that for frequencies smaller than a certain critical value the uniform wave is unstable against changes in wavenumber and amplitude. However, he did not take an essential feature acting upon the stabilization of the modulated waves into account. Namely he did not adopt correctly the interactions between an envelope wave and the other slowly varying wave accompanied by the envelope one.

In this paper, using the perturbation method established by Taniuti and Yajima,[7] the wave modulations in anharmonic lattices are investigated. We perform the perturbation with due regard to the above effect without the continuum approximation for carrier waves, and obtain the following results: The modulated wave must be accompanied by the other slowly varying wave with the same order as the modulated one, and the both are simultaneously determined with a coupled system of equations. Attention may be paid to the fact that this slowly varying wave tends to stabilize the modulated one. In addition we can show that for the existence of the unstable region the potential must be subject to a certain restriction. Lastly we discuss the lattice expansions by the calculation of the Grüneisen ratio.[8]

§ 2. Equations of motion

We consider an infinite one-dimensional monatomic lattice with nearest neighbour interactions. When the interaction potential is given by $V(r)$, where r is the relative separation, the Hamiltonian of this system is

$$H=\tfrac{1}{2}M\sum_{n}\dot{x}_n^2+\sum_{n}V(h+x_{n+1}-x_n), \tag{2·1}$$

where M stands for mass of a particle, h the static equilibrium separation, x_n the displacement of the n-th particle from the equilibrium position, and $\dot{x}_n$ the velocity of the n-th particle.

The potential $V(r)$ is assumed to be expanded in power series about the equilibrium separation:

$$V(r)=-V_0+\frac{f}{2}(r-h)^2-\frac{f}{3}p\frac{(r-h)^3}{h}+\frac{f}{4}q\frac{(r-h)^4}{h^2}+\cdots, \tag{2·2}$$

where f is the harmonic force constant and p and q are non-dimensional parameters related to the strength of the anharmonicity. So long as the motions with small amplitude are dealt with, in Eq. (2·2) we may neglect the terms higher than fourth degree.

For simplicity we choose a time unit so that the harmonic force constant f equals the mass M. Since we consider the motion with a small but finite amplitude, we introduce the dimensionless displacement

$$\varepsilon u_n=\frac{x_n}{h}, \tag{2·3}$$

where ε is a small parameter related to the smallness of the amplitude and u_n ($n=0, \pm1, \pm2, \cdots$) are variables of order unity. Then from Eqs. (2·1) and (2·2) the equations of motion have the following form:

$$\frac{d^2u_n}{dt^2}=u_{n+1}-2u_n+u_{n-1}$$
$$-p\varepsilon\{(u_{n+1}-u_n)^2-(u_n-u_{n-1})^2\}+q\varepsilon^2\{(u_{n+1}-u_n)^3-(u_n-u_{n-1})^3\}. \tag{2·4}$$

§ 3. Equations for wave modulation

Following the method developed by Taniuti and Yajima,[7] we perform an asymptotic expansion and derive the equations to describe the development of the modulation of the amplitude in the lowest order of the expansion. Namely we investigate how the narrow-band wave packets evolve by nonlinear effects.

Thus we look for a solution expanded in terms of a small parameter ε.

$$u_n=\sum_{\nu=0}^{\infty}\varepsilon^{\nu}u_n^{(\nu)}. \tag{3·1}$$

And each $u_n^{(\nu)}$ is also expanded in terms of harmonics $\exp(il\theta)$, where $\theta=knh-\omega t$:

$$u_n^{(\nu)}=\sum_{l=-\infty}^{\infty}u_l^{(\nu)}(\tau,\xi)e^{il\theta}. \tag{3·2}$$

Here τ and ξ are slowly varying variables defined by

$$\left.\begin{aligned}\tau&=\varepsilon^2 t,\\ \xi&=\varepsilon(nh-\lambda t),\end{aligned}\right\} \tag{3·3}$$

where λ denotes the group velocity

$$\lambda=\frac{\partial\omega}{\partial k}. \tag{3·4}$$

In addition, the wavenumber k and the frequency ω are assumed to satisfy the dispersion relation

$$\omega^2=4\sin^2\frac{kh}{2}. \tag{3·5}$$

It is also noted that the reality conditions

$$u_l^{(\nu)}=u_{-l}^{(\nu)*} \tag{3·6}$$

hold for all ν and l.

Substituting Eqs. (3·1) and (3·2) into Eq. (2·4) and equating the coefficients of various powers of ε to zero, we get

$$\sum_l\left\{-l^2\omega^2+4\sin^2\frac{lkh}{2}\right\}u_l^{(0)}e^{il\theta}=0, \tag{3·7}$$

$$\sum_l\left\{2i(l\omega\lambda-h\sin lkh)\frac{\partial u_l^{(0)}}{\partial\xi}+\left(-l^2\omega^2+4\sin^2\frac{lkh}{2}\right)u_l^{(1)}e^{il\theta}\right.$$

$$=p\sum_l\sum_{l'}8i\sin^2\frac{lkh}{2}\sin l'khu_l^{(0)}u_{l'}^{(0)}e^{i(l+l')\theta}, \tag{3·8}$$

$$\sum_l\left\{(\lambda^2-h^2\cos lkh)\frac{\partial^2u_l^{(0)}}{\partial\xi^2}-2il\omega\frac{\partial u_l^{(0)}}{\partial\tau}\right.$$

$$\left.+2i(l\omega\lambda-h\sin lkh)\frac{\partial u_l^{(1)}}{\partial\xi}+\left(-l^2\omega^2+4\sin^2\frac{lkh}{2}\right)u_l^{(2)}\right\}e^{il\theta}$$

$$=p\sum_{l}\sum_{l'}\left\{8i\sin^2\frac{lkh}{2}\sin l'kh(u_l^{(1)}u_{l'}^{(0)}+u_l^{(0)}u_{l'}^{(1)})\right.$$

$$\left.+8h\sin^2\frac{lkh}{2}\cos l'khu_l^{(0)}\frac{\partial u_{l'}^{(0)}}{\partial\xi}+4h\sin lkh\sin l'kh\frac{\partial u_l^{(0)}}{\partial\xi}u_{l'}^{(0)}\right\}e^{i(l+l')\theta}$$

$$-q\sum_{l}\sum_{l'}\sum_{l''}4\sin^2\frac{lkh}{2}\{(e^{il'kh}-1)(e^{il''kh}-1)+(e^{il'kh}-1)(1-e^{-il''kh})$$

$$+(1-e^{-il'kh})(1-e^{-il''kh})\}u_l^{(0)}u_{l'}^{(0)}u_{l''}^{(0)}e^{i(l+l'+l'')\theta}, \tag{3·9}$$

and the equations corresponding to higher order of ε. To derive these equations, we have expanded the terms $u_l^{(\nu)}(\tau,\xi\pm\varepsilon h)$ in Taylor series of εh, since $u_l^{(\nu)}$'s are assumed to be slowly varying functions of its arguments.

In Eq. (3·7) the coefficients of the m-th harmonics are taken to be zero for all m, then because of Eq. (3·5), the following relations are easily shown:

$$u_m^{(0)}=0 \quad \text{for } |m|\geq 2\,. \tag{3·10}$$

To the lowest order, it should be noted that the non-zero terms are at most $u_0^{(0)}$ and $u_{\pm1}^{(0)}$. Next in Eq. (3·8) the same process is performed for $m=0$, ±1 and ±2. In view of Eqs. (3·4) and (3·5), we see that the relations for $m=0$ and ±1 identically hold. Making use of Eqs. (3·4), (3·5) and (3·10), however, we obtain the equation for $m=\pm2$ as follows:

$$u_{\pm2}^{(1)}=\mp pi\cot\frac{kh}{2}u_{\pm1}^{(0)2}. \tag{3·11}$$

By the same calculation as above, we have from Eq. (3·9) the following two relations for $m=0$ and ±1:

$$\frac{\partial^2u_0^{(0)}}{\partial\xi^2}=\frac{8p}{h}\frac{\partial}{\partial\xi}|u_{\pm1}^{(0)}|^2 \tag{3·12}$$

and

$$h^2\sin^2\frac{kh}{2}\frac{\partial^2u_{\pm1}^{(0)}}{\partial\xi^2}\mp 2i\omega\frac{\partial u_{\pm1}^{(0)}}{\partial\tau}$$

$$\pm 8pi\left(\sin^3kh-\sin^2\frac{kh}{2}\sin 2kh\right)u_{\mp1}^{(0)}u_{\pm2}^{(1)}-8ph\sin^2\frac{kh}{2}u_{\pm1}^{(0)}\frac{\partial u_0^{(0)}}{\partial\xi}$$

$$+24q\sin^2\frac{kh}{2}(1-\cos kh)u_{\pm1}^{(0)2}u_{\mp1}^{(0)}=0\,, \tag{3·13}$$

respectively. Equations (3·4), (3·5) and (3·10) are in use in the derivation of these expressions.

If Eq. (3·11) is substituted into this equation, together with Eq. (3·12), a system of differential equations describing the nonlinear wave modulation in the lowest order of the asymptotic expansion is obtained. Expressing the coefficients of these equations in terms of frequency, we find the coupled system of equations

$$\frac{\partial^2 u_0^{(0)}}{\partial\xi^2}=\frac{8p}{h}\frac{\partial}{\partial\xi}|u_{\pm1}^{(0)}|^2,$$

$$\pm i\frac{\partial u_{\pm1}^{(0)}}{\partial\tau}=\frac{h^2}{8}\omega\frac{\partial^2 u_{\pm1}^{(0)}}{\partial\xi^2}+\omega\left\{\frac{3}{2}q\omega^2+p^2(4-\omega^2)\right\}|u_{\pm1}^{(0)}|^2u_{\pm1}^{(0)} \qquad (3\cdot14)$$

$$-ph\omega\frac{\partial u_0^{(0)}}{\partial\xi}u_{\pm1}^{(0)}.$$

It is interesting that if $p\neq0$, $u_0^{(0)}$ and $u_{\pm1}^{(0)}$ must be determined simultaneously, that is, the modulated wave must be accompanied by the other slowly varying wave of the same order as that. The properties of the modulated wave much differ from Lowell's ones[1] due to the appearance of the wave $u_0^{(0)}$.

§ 4. Stabilities of plane waves

By the use of Eq. (3·14), we are able to investigate the dynamical stability of the plane waves. The first equation of (3·14) is easily integrated once and written as

$$\frac{\partial u_0^{(0)}}{\partial\xi}=\frac{8p}{h}\{|u_{\pm1}^{(0)}|^2-C\}, \qquad (4\cdot1)$$

where $-(8p/h)C$ is the integration constant. Therefore from Eq. (3·14) we make up the single equation to determine $u_{\pm1}^{(0)}$.

$$\pm i\frac{\partial u_{\pm1}^{(0)}}{\partial\tau}=\frac{h^2}{8}\omega\frac{\partial^2 u_{\pm1}^{(0)}}{\partial\xi^2}+\omega\left\{\frac{3}{2}q\omega^2-p^2(4+\omega^2)\right\}|u_{\pm1}^{(0)}|^2u_{\pm1}^{(0)}$$

$$+8p^2\omega Cu_{\pm1}^{(0)}. \qquad (4\cdot2)$$

Putting

$$\left.\begin{aligned}\varphi_{\pm1}&=\exp\left(\pm i8p^2\omega\int Cd\tau\right)u_{\pm1}^{(0)},\\ \varphi_0&=u_0^{(0)},\\ s&=\omega\tau,\\ \eta&=\frac{2}{h}\xi\end{aligned}\right\} \qquad (4\cdot3)$$

and

$$\kappa=\frac{3}{2}q\omega^2-p^2(4+\omega^2), \qquad (4\cdot4)$$

we get the so-called nonlinear Schrödinger equation[7),9),10)]

$$\pm i\frac{\partial\varphi_{\pm1}}{\partial s}=\frac{1}{2}\frac{\partial^2\varphi_{\pm1}}{\partial\eta^2}+\kappa|\varphi_{\pm1}|^2\varphi_{\pm1} \tag{4·5}$$

and

$$\frac{\partial\varphi_0}{\partial\eta}=4p\{|\varphi_{\pm1}|^2-C\}. \tag{4·6}$$

The asymptotic behavior of the amplitude of nonlinearly modulated wave is described by these equations.

Recently the properties of the nonlinear Schrödinger equation (4·5) are investigated by many workers.[9),10)] And it is well known that in the region of $\kappa>0$, the plane wave is unstable, namely modulational instability occurs, otherwise it does not occur.

In our case, it is shown from Eq. (4·4) that if the condition

$$0<\frac{8p^2}{3q-2p^2}<\omega^2\leq 4 \tag{4·7}$$

is satisfied, the instability occurs. This unstable region is shown in Fig. 1. Thus we know that if $\frac{3}{4}<p^2/q$, then the plane wave is stable for any wavenumber but if $0<p^2/q<\frac{3}{4}$, then it becomes unstable above the critical frequency ω_c, where

$$\omega_c^2=\frac{4(p^2/q)}{3/2-p^2/q}. \tag{4·8}$$

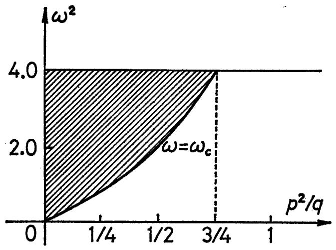

Fig. 1. Critical frequency ω_c vs. p^2/q. In the shaded region plane waves are modulationally unstable.

As we can easily see from Eq. (3·14), the interaction of the waves between $u_0^{(0)}$ and $u_{\pm1}^{(0)}$ plays an essential role for the stabilization. Due to this effect the stable region is extremely different from that of Lowell.[1)]

When $\kappa>0$, Eq. (4·5) has the solitary wave solution[9)]

$$\varphi_{\pm1}=A\exp\{\pm i(\kappa A^2/2)s\}\ \mathrm{sech}\{A\kappa\eta\}. \tag{4·9}$$

Substituting this expression into Eq. (4·6), we have

$$\varphi_0=4p\frac{A}{\sqrt{\kappa}}\tanh\{A\sqrt{\kappa}\,\eta\}-4pC\eta+D, \tag{4·10}$$

where D is the integration constant. This form of φ_0 is similar to a solitary wave solution in *K-d V* limit,[2),3)] but the wave φ_0 propagates with the group velocity λ.

§ 5. Some remarks

In order to consider the lattice expansions of our system we calculate the

Grüneisen ratio. As a result of the passage of the wave $\exp(\pm i\theta)$, the average separation of adjacent particles varies slightly from h. The variation is easily calculated by minimizing the potential energy averaged over the phase θ with respect to new average separation R. Thus we have

$$R \simeq h + 2ph\omega^2 |\varphi_{\pm1}|^2 \varepsilon^2. \tag{5·1}$$

If $p>0$, $R-h$ must be always positive, and only this case is discussed in what follows.

According to Karpman and Krushkal,[9] nonlinear dispersion relasion is expressed as

$$\Omega = \omega \{1 + [\tfrac{3}{2}q\omega^2 - p^2(4+\omega^2)] |\varphi_{\pm1}|^2 \varepsilon^2\}. \tag{5·2}$$

Equations (5·1) and (5·2) give the Grüneisen ratio γ,[8] i.e.,

$$\gamma = -\frac{\partial \ln \Omega}{\partial \ln R} \simeq 2p \left\{\frac{1}{\omega^2} - \frac{3q}{8p^2} + \frac{1}{4}\right\}. \tag{5·3}$$

If $0<p^2/q<\frac{3}{4}$, γ changes sign from positive to negative values at the critical frequency ω_c, but otherwise it always takes positive value. On the other hand γ can be expressed in terms of thermodynamical quantities.[8]

$$\gamma = \frac{V}{C_v}\left(\frac{\partial P}{\partial T}\right)_v, \tag{5·4}$$

where V, P, T and C_v are the volume, pressure, temperature and heat capacity of the system, respectively. Since the quantity $(\partial P/\partial T)_v$ is the ratio of the thermal expansion coefficient to the compressibility, it follows that if $0<p^2/q<\frac{3}{4}$ the thermal expansion coefficient becomes negative at sufficiently high temperature, the examples of which abound in real crystals.

In 1967, Toda[2] gave the periodic wave solution explicitly for an anharmonic potential of special form. It is noted that the small amplitude waves in this system are modulationally stable, because this potential gives $p^2/q=3/2$.

The modulated waves in optical branches will be different from the above case, for in that case u_0 is always zero in the lowest order of ε. But the wave modulations in the longitudinal and transverse acoustic branches may be approximately described by this model if the parameters p and q are adequately taken.

Acknowledgement

The author wishes to express his thanks to Professor N. Yajima for stimulating discussions and comments.

References

1) S. C. Lowell, Proc. Roy. Soc. **A318** (1970), 93.
2) M. Toda, J. Phys. Soc. Japan **23** (1967), 501.

3) N. J. Zabusky and M. D. Kruskal, Phys. Rev. Letters **15** (1965), 240.
4) V. Narayanamurti and C. M. Varma, Phys. Rev. Letters **25** (1970), 1105.
5) F. D. Tappert and C. M. Varma, Phys. Rev. Letters **25** (1970), 1108.
6) G. B. Whitham, J. Fluid Mech. **22** (1965), 273.
7) T. Taniuti and N. Yajima, J. Math. Phys. **10** (1969), 1369.
8) M. Born and K. Huang, *Dynamical Theory of Crystal Lattices* (Oxford University Press, 1954).
9) V. I. Karpman and E. M. Krushkal, Soviet Phys.-JETP. **28** (1969), 277.
10) N. Yajima and A. Outi, Prog. Theor. Phys. **45** (1971), 1997.
V. E. Zakharov and A. B. Shabat, Zh. Eksp. i Teor. Fiz. **61** (1971), 118.