J. Phys. Soc. Jpn.
Downloaded from journals.jps.jp by 73.229.135.170 on 02/01/18

Check for updates

JOURNAL OF THE PHYSICAL SOCIETY OF JAPAN, Vol. 22, No. 2, FEBRUARY, 1967

Vibration of a Chain with Nonlinear Interaction

Morikazu TODA
Department of Physics, Faculty of Science, Tokyo University of Education, Tokyo

(Received September 27, 1966)

Vibration of a chain of particles interacting by nonlinear force is investigated. Using a transformation exact solutions to the equation of motion are aimed at. For a special type of interaction potential of the form

$$\phi(r)=\frac{a}{b}e^{-br}+ar+\text{const.},\ (a,\ b>0)$$

exact solutions are actually obtained in terms of the Jacobian elliptic functions. It is shown that the system has N "normal modes". Expansion due to vibration or "thermal expansion" of the chain is also discussed.

§ 1. Introduction

Our aim here is to study a simple mechanical model, a chain of particles. We assume that interaction is limited to the nearest neighbors, and that the interaction force is nonlinear. Recent studies on nonlinear oscillator systems using perturbation methods[1] and computers[2] indicate that they have many properties in common with linear systems. Thus J. Ford and J. Waters[2] found by computer analysis that nonlinear system have "normal modes where a normal mode is defined as motion in which each oscillator moves at essentially constant amplitude (energy) and at a given frequency". It is therefore anticipated that nonlinear systems will admit analytic solutions. Here we shall show that we have actually analytic solutions. These solutions reduce to the normal modes in linear limit or in the limit of

J. Phys. Soc. Jpn.
Downloaded from journals.jps.jp by 73.229.135.170 on 02/01/18

small amplitude, and cover all the modes of the linear chain.

Though the system treated in this paper is a particular chain, it seems that a wide scope of nonlinear systems is susceptible to analysis and solutions to the equation of motion may not necessarily be incredibly complex. Existence of normal modes implies nonergodic character of the system and the nonergodicity of nonlinear systems might have a wide range of validity.

The complete solution to a nonlinear system is not just a sum of normal mode solutions. To answer the problems of an approach to equilibrium, of the capacity of a system as a heat bath, of heat conduction and of other interesting problems which have connection with the ergodicity, the behavior of the complete solution must be investigated. The complete solution which satisfies an arbitrary initial condition is not given at present.

In § 2 the method of dual transformation[3,4] is described. This method also serves in classifying the type of nonlinear interactions.

In § 3 a system with a special type of interaction is treated. The normal modes are given explicitly. This system exhibit "thermal" expansion, which is shown to be in agreement with the result of conventional method in the limit of small anharmonicity.

§ 2. Dual Transformation

We are interested in the vibration of a uniform chain of particles with nonlinear interaction. The equation of motion for the n-th particle in the chain is

$$m\ddot{u}_n=-\phi'(u_n-u_{n-1})+\phi'(u_{n+1}-u_n)\ , \quad (2.1)$$

where m stands for the mass of the particles, $\phi(r)$ the interaction energy between adjacent particles as a function of r, the mutual displacement, and $\phi'(r)$ its derivative with respect to r. We consider displacement of particles along the chain, that is, londitudinal displacement. The mutual displacement r_n is defined by

$$r_n=u_n-u_{n-1}\ . \quad (2.2)$$

We consider the chain to be of finite length and label the particles from 0 to N ($n=0,\cdot\cdot,N$). The kinetic energy of the system is then given by

$$K=\frac{m}{2}\sum_{n=0}^{N}\dot{u}_n^2 \quad (2.3)$$

where for convenience we have not taken aside the part responsible for the motion of the 0-th particle, which we assume to be subject to a given condition. Though the equation of motion (1) does not include the boundary conditions explicitly, it does implicitly. We impose the boundary condition that the displacement of the 0-th particle is a given function of time, *i.e.*,

$$u_0\equiv r_0(t)\ \text{(given)} \quad (2.4)$$

and assume the force $f(t)$ applied to the N-th particle. The potential energy U of the system can be written as

$$U=\sum_{n=1}^{N}\phi(r_n)+\sum_{n=0}^{N}r_nf(t) \quad (2.5)$$

and the kinetic energy as

$$K=\frac{m}{2}\sum_{n=0}^{N}\left(\sum_{j=0}^{n}\dot{r}_j\right)^2 . \quad (2.6)$$

We use the mutual displacements r_n as the generalized coordinates, whose canonically conjugate momenta are given by

$$s_n=\partial K/\partial\dot{r}_n \quad (n=0,\cdots,N)\ . \quad (2.7)$$

In terms of s_n the kinetic energy is[3]

$$K=\frac{1}{2m}\sum_{n=0}^{N}(s_n-s_{n+1})^2 \quad (2.8)$$

where we have put

$$s_{N+1}=0\ . \quad (2.9)$$

The Hamilton's function is $H(r_n, s_n)=K+U$, which yields the canonical equations of motion of the form

$$\dot{r}_n=\frac{\partial H}{\partial s_n}=\frac{1}{m}(2s_n-s_{n-1}-s_{n+1})\ , \quad (2.10)$$

$$\dot{s}_n=-\frac{\partial H}{\partial r_n}=-\left\{\frac{\partial\phi(r_n)}{\partial r_n}+f(t)\right\} . \quad (2.11)$$

The set (s_n, $-r_n$) can be regarded as that of general coordinate and momentum, which furnishes the dual transformation described in a preceding paper.[4]

Consider next the case where eq. (2.11) affords single valued solution, which we shall write as

$$r_n=-\frac{1}{m}\chi(\dot{s}_n) \quad (2.12)$$

In general χ is also a function of $f(t)$. Equation (2.10) then gives the equation of motion for the dual chain of the form

$$\frac{d}{dt}\chi(\dot{s}_n)=-2s_n+s_{n-1}+s_{n+1}\ . \quad (2.13)$$

Thus the equation of motion takes the form quite similar to the linear case. Alternately we may write eq. (2.13) as

$$\chi(\ddot{S}_n)=-2S_n+S_{n-1}+S_{n+1} \quad (2.14)$$

J. Phys. Soc. Jpn.
Downloaded from journals.jps.jp by 73.229.135.170 on 02/01/18

with

$$S_n=\int^t s_n dt\ . \tag{2.15}$$

If the applied force f is constant or if no external force is applied, we have

$$\chi'(\dot{s}_n)\ddot{s}_n=-2s_n+s_{n-1}+s_{n+1}\ . \tag{2.16}$$

We see that the characteristics of the nonlinear interaction is now reflected in the functional form of $\chi(\dot{s}_n)$. Therefore we may classify the type of nonlinear interaction by the form of the function χ.

Though the above treatment assumes finite length of the chain, we may treat travelling wave solution. Physically this is accomplished by choosing appropriate input and output, or $r_0(t)$ and $f(t)$ at the both ends of the chain.

§ 3. Nonlinear Chain

As an example of nonlinear interaction we shall treat the anharmonic potential of the form

$$\phi(r)=\frac{a}{b}e^{-br}+ar+\text{const.}\quad (a,\ b>0) \tag{3.1}$$

The two terms imply repulsive and attractive forces respectively. The parameters are so chosen as the minimum of the potential is just at $r=0$, or

$$\phi'(0)=0\ . \tag{3.2}$$

We assume the case of no external force, and then eq. (2.11) is

$$\dot{s}_n=-\frac{\partial\phi(r_n)}{\partial r_n}=-a\{1-\exp(-br)\}\ , \tag{3.3}$$

which yields

$$r_n=-\frac{1}{b}\log\frac{a+\dot{s}_n}{a}=-\chi(\dot{s}_n)\ . \tag{3.4}$$

Therefore the equation of motion is (mass $m=1$)

$$\frac{\ddot{s}_n}{a+\dot{s}_n}=-b(2s_n-s_{n-1}-s_{n+1})\ . \tag{3.5}$$

It is shown in Appendix I. that the travelling wave solution for eq. (3.5) is of the form

$$s_n=\frac{2K\nu}{b}Z\left\{2K\left(\nu t\pm\frac{n}{\lambda}\right)\right\} \tag{3.6}$$

where

$$2K\nu=\sqrt{ab\Big/\left\{\frac{1}{sn^2(2K/\lambda)}-1+\frac{E}{K}\right\}}\ , \tag{3.7}$$

$$Z(u)=\int_0^u dn^2u du-\frac{E}{K}u\ . \tag{3.8}$$

In the above formula sn and dn represent the Jacobian elliptic functions[5]; K and E are the complete elliptic integrals of the first and the second kind. These are all of the same modulus which we shall write k. The complete elliptic integrals are

$$K=K(k)=\int_0^{\pi/2}\frac{d\theta}{\sqrt{1-k^2\sin^2\theta}}\ , \tag{3.9}$$

$$E=E(k)=\int_0^{\pi/2}\sqrt{1-k^2\sin^2\theta}\,d\theta\ . \tag{3.10}$$

The Z-function has the periodicity of $2K$,

$$Z(u+2K)=Z(u)\ , \tag{3.11}$$

and ν and λ represent the frequency and the wave length respectively. The modulus k is responsible for the amplitude of the wave as will be shown below. Given the wave length λ and the modulus k, eq. (3.7) gives the frequency ν. From eq. (3.4), (3.6) and (3.8) we have

$$r_n=-\frac{1}{b}\log\left(1+\frac{4(K\nu)^2}{ab}\left[dn^2\left\{2K\left(\nu t\pm\frac{n}{\lambda}\right)\right\}-\frac{E}{K}\right]\right)\ . \tag{3.12}$$

If the modulus k is very small, we have

$$sn\,u\cong\sin u\ ,\qquad \frac{E}{K}\cong 1-\frac{k^2}{2}\ ,\qquad Z(u)\cong\frac{k^2}{4}\sin 2u\ ,\qquad K\cong\frac{\pi}{2}\ . \tag{2.13}$$

Therefore if $k\ll 1$, we have, for the dual chain.

$$s_n\cong\frac{\omega k^2}{8b}\sin\left(\omega t\pm\frac{2\pi n}{\lambda}\right)\ , \tag{3.14}$$

$$\omega\cong 2\sqrt{\gamma}\,\sin\frac{\pi}{\lambda}\ ,\qquad \gamma=ab\ . \tag{3.15}$$

Thus if the amplitude of the wave is small, our solution (3.6) reduces to that of the linear case with the force constant γ. For sufficiently small k or small amplitude of the wave, we have the wave, for the original chain,

J. Phys. Soc. Jpn.
Downloaded from journals.jps.jp by 73.229.135.170 on 02/01/18

$$r_n \cong -\frac{\omega^2 k^2}{8ab^2}\cos\left(\omega t \pm \frac{2\pi n}{\lambda}\right). \tag{3.16}$$

By adjusting appropriately the end conditions r_0 for the 0-th and $f(t)$ for the N-th particles, cyclic boundary condition can be realized to yield the N "normal modes" in the sense that they reduce to the N normal modes in the limit of small amplitude.

We consider the ensemble of the chains. If each normal mode is excited in each chain, it will exhibit expansion because of the anharmonicity. If the amplitude is small we may expand the right-hand side of eq. (3.4) as

$$r_n \cong -\frac{1}{b}\left\{\frac{\dot{s}_n}{a} - \frac{1}{2}\left(\frac{\dot{s}_n}{a}\right)^2 + \cdots\right\}. \tag{3.17}$$

Since the time average of $\dot{s}_n$ vanishes, the time average of r_n is, to the first approximation,

$$\overline{r_n} = \frac{1}{2a^2 b}\overline{\dot{s}_n{}^2}, \tag{3.18}$$

in which we may use the zero-th approximation for $\dot{s}_n$. In the zero-th approximation in turn we have $r_n \cong -\dot{s}_n/ab$ and the chain reduces to a linear chain with force constant $\gamma = ab$. Therefore in this approximation the equipartition of energy gives (k_B=Boltzmann const.)

$$\frac{\gamma}{2}\overline{r_n{}^2} = \frac{\gamma}{2(ab)^2}\overline{\dot{s}_n{}^2} = \frac{k_B T}{2}. \tag{3.19}$$

Thus it is shown that

$$\overline{r_n} = \frac{b}{2\gamma}k_B T. \tag{3.20}$$

On the other hand if we expand $\phi'(r)$ for small r we have

$$-\phi'(r) = -\gamma r + \alpha r^2 + \cdots, \qquad \gamma = ab, \qquad \alpha = \frac{1}{2}ab^2. \tag{3.21}$$

Therefore eq. (3.20) can be written as

$$\overline{r_n} = \frac{\alpha}{\gamma^2}k_B T. \tag{3.22}$$

This is in accordance with the result which is given by the conventional method of statistical mechanics.

Appendix I.

The following relation can be verified easily:

$$sn^2(u+v) - sn^2(u-v) = 2\frac{d}{dv}\frac{sn\,u\,cn\,u\,dn\,u\,sn^2\,v}{1-k^2\,sn^2\,u\,sn^2\,v}, \tag{AI·1}$$

where k denotes the modulus of these Jacobian elliptic functions. Since

$$dn^2\,u = 1 - k^2\,sn^2\,u, \tag{AI·2}$$

if we define the function

$$\varepsilon(u) = \int_0^u dn^2 u\,du \tag{AI·3}$$

and use its derivatives

$$\varepsilon'(u) = dn^2 u, \qquad \varepsilon''(u) = -2k^2\,sn\,u\,cn\,u\,dn\,u, \tag{AI·4}$$

J. Phys. Soc. Jpn.
Downloaded from journals.jps.jp by 73.229.135.170 on 02/01/18

we have

$$\varepsilon(u+v)+\varepsilon(u-v)-2\varepsilon(u)=\frac{\varepsilon''(u)}{\dfrac{1}{sn^2v}-1+\varepsilon'(u)}\,. \tag{AI·5}$$

By simple transformations we easily arrive at eq. (3.6) in the text. The same conclusion can be drawn by using the relation to the ϑ-function ($\vartheta_4\equiv\vartheta_0$)

$$Z(u)=\varepsilon(u)-\frac{E}{K}u=\frac{\partial}{\partial u}\log\vartheta_4\left(\frac{u}{2K}\right) \tag{AI·6}$$

and the relations

$$\frac{\partial^2}{\partial v^2}\log\vartheta_4(v)=\frac{\vartheta_4''(0)}{\vartheta_4(0)}-\left[\frac{\vartheta_1'(0)}{\vartheta_4(0)}\right]^2\left[\frac{\vartheta_1(v)}{\vartheta_4(v)}\right]^2, \tag{AI·7}$$

$$\vartheta_4(v+w)\vartheta_4(v-w)[\vartheta_4(0)]^2=[\vartheta_4(v)\vartheta_4(w)]^2-[\vartheta_1(v)\vartheta_1(w)]^2\,. \tag{AI·8}$$

Appendix II.

We shall here treat the wave with the shortest wave length. This wave exhibits the character of stationary wave as well. Consider the mode

$$r_{2n}=\varDelta+2x\,,\qquad r_{2n+1}=\varDelta-2x\,, \tag{AII·1}$$

in an infinite chain. Here $\varDelta$ denotes the average value of r_n, and $\pm x$ represents the displacement of each particle from their average positions. The equation of motion for a particle is seen to be of the form (mass $m=1$)

$$\ddot{x}=a\{e^{-b(\varDelta+2x)}-e^{-b(\varDelta-2x)}\}\,, \tag{AII·2}$$

or

$$\ddot{x}=-a'\sinh 2bx\,, \tag{AII·3}$$

with

$$a'=ae^{-b\varDelta}\,. \tag{AII·4}$$

The solution of the above equation is

$$e^{\pm 2bx}=c\,dn^2(\sqrt{a'bc}t,\,k) \tag{AII·5}$$

where k is the modulus, and

$$c=\frac{1}{\sqrt{1-k^2}}\,. \tag{AII·6}$$

If there is no external force, $\varDelta$ represents the natural expansion of the chain as it vibrates. In this case $\varDelta$ is given by the condition that the average value of $\dot{s}_n$ is zero, or

$$\overline{\frac{\partial\phi}{\partial r}}=a-a'\overline{e^{-2bx}}=0\,, \tag{AII·7}$$

However

$$\overline{e^{-2bx}}=c\int_0^{2K/\sqrt{a(bc}}dn^2(\sqrt{a'bc}\,t)dt\Big/\frac{2K}{\sqrt{a'bc}}=c\frac{E}{K} \tag{AII·8}$$

where K and E are the complete elliptic integrals of the first and the second kind of modulus k. We have therefore

$$a-a'c\frac{E}{K}=0\,. \tag{AII·9}$$

J. Phys. Soc. Jpn.
Downloaded from journals.jps.jp by 73.229.135.170 on 02/01/18

The coefficient of t in (AII·5) is therefore

$$\sqrt{a'bc}=\sqrt{ab}\sqrt{\frac{K}{E}}\ . \tag{AII·10}$$

This wave has the wave length $\lambda=2$. On the other hand eq. (3.7) gives, for $\lambda=2$, the coefficient of t in eq. (3.12)

$$2K\nu=\sqrt{ab}\Big/\sqrt{\frac{E}{K}}\ . \tag{AII·11}$$

Further, since we have the relation[5)]

$$\frac{1}{\sqrt{1-k^2}}dn^2(2K\nu t+K)=\sqrt{1-k^2}/dn^2(2K\nu t)\ , \tag{AII·12}$$

we see that the wave treated here is in agreement with the special case $\lambda=2$ of the wave given by eq. (3.12).

References

1) J. Ford: J. math. Phys. **2** (1961) 387.
2) J. Ford and J. Waters: J. math. Phys. **4** (1963) 1293.
3) M. Toda: J. Phys. Soc. Japan **20** (1955) 2095.
4) M. Toda: Progr. theor. Phys. Suppl. **36** (1966) 113.
5) H.B.S. Jeffereys: *Mathematical Physics* (Cambridge University Press, 1956), 3rd. ed., Chapter. 25. E. T. Whittaker and G. N. Watson: *Modern Analysis* (Cambridge University Press, 1927), 4 th ed., Chapter 20–22.