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A model calculation for vibrational propagation in a chain of nonlinear oscillators II: Effects of optical dispersion and of initial conditions

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We extend our previous analysis of vibrational propagation in a chain of nonlinear oscillators to obtain explicit expressions for oscillator displacements and mean-square-displacements of the vibrational excitation for optical dispersion and study the effects of the interplay of initial conditions with nonlinearity.

1. Introduction and the model

In a previous paper [1] (hereafter referred to as I) we analyzed vibrational propagation in a chain of nonlinear oscillators. The motivation was, in part, the desire to understand thermal conduction [2–5] in unusual materials such as boron carbides. Encouraged by the quantitative success of a preliminary analysis [6] we carried out in explaining a part of the thermal observations on boron carbides, viz. the flat temperature-independent behaviour of the thermal conductivity of B_9C, we undertook in I an investigation of the nonlinear dynamics of a system involving interactions between two kinds of oscillators ("optical" and "acoustic") whose characteristic times differ significantly. The analysis in I was carried out with the help of several simplifying assumptions. We relax some of those assumptions in this paper and thereby extend that analysis to more physical systems. As in I, our results here represent some simple aspects of the transfer of vibrational excitation in a specific nonlinear model rather than being directly applicable to the thermal conductivity problem which motivated the investigation.

As in I, the model considered is a chain of alternating masses m_1 and m_2 connected by identical linear springs, or one of identical masses connected by alternating springs k_1 and k_2, which is enriched by additional interactions between the optical and acoustic vibrations. The system has the Hamiltonian

$$\begin{aligned}H=&\sum\omega_q(x_q x_{-q}+p_q{}^x p_{-q}{}^x)\\&+\sum\Omega_q(u_q u_{-q}+p_q{}^u p_{-q}{}^u)\\&+\sum A_q(u_q+u_{-q})\,|x_q|^2\end{aligned}\tag{1.1}$$

where all summations are over the modes q, the frequencies and the mode coordinates of the optical phonons are ω and x respectively, the frequencies and the mode coordinates of the acoustic phonons are Ω and u respectively, p^x and p^u are the respective momenta (or conjugate variables) of the two branches, and ω_q, Ω_q, and A_q are all even in the wavevector q. The last term in (1.1) denotes the nonlinear interaction between the optical and the acoustic oscillators. It increases the optical mode frequency by a term proportional to the amplitude of the acoustic mode and changes the equilibrium position of the acoustic mode by an amount proportional to the square of the amplitude of the optical mode. The time evolution of the mode amplitudes x_q and u_q is given by

$$(\mathrm{d}^2/\mathrm{d}t^2)\,x_q+\omega_q^2\,x_q=-A_q\,\omega_q(u_q+u_{-q})\,x_q,\tag{1.2}$$

$$(\mathrm{d}^2/\mathrm{d}t^2)\,u_q+\Omega_q^2\,u_q=-A_q\,\Omega_q|x_q|^2\tag{1.3}$$

which, under the assumption that the frequencies ω and Ω are disparate in magnitude, reduces to the single closed equation for the x modes:

$$(\mathrm{d}^2/\mathrm{d}t^2)\,x_q+\omega_q^2\,x_q-B_q\,x_q|x_q|^2=0\tag{1.4}$$

where $B_q = 2A_q^2\,\omega_q/\Omega_q$. As in I we continue to analyze only "even initial conditions", i.e. those in which $x_q = x_{-q}$ so that $|x_q|^2$ may be replaced by x_q^2, assume $(dx_q/dt)_{t=0} = 0$, and denote $(x_q)_{t=0}$ by x_q^0. The result (see I) is the explicit solution

$$x_q = x_q^0\, sn(\lambda_q t + K_q | k_q), \tag{1.5}$$

$$K_q = \int_0^{\pi/2} d\theta (1 - k_q^2 \sin^2\theta)^{-\frac{1}{2}}, \tag{1.6}$$

$$k_q = (1/\lambda_q)\,[\tfrac{1}{2} B_q (x_q^0)^2]^{\frac{1}{2}}, \tag{1.7}$$

$$\lambda_q = [\omega_q^2 - \tfrac{1}{2} B_q (x_q^0)^2]^{\frac{1}{2}}, \tag{1.8}$$

where sn is the Jacobian elliptic sine function and K_q is the complete elliptic integral of the first kind. The argument of K_q or the modulus of sn function is given by (1.7).

The purpose of present paper is to relax two simplifying assumptions of I and thereby explore further the transport properties of the vibrational excitation in chains of nonlinear oscillators. In the next section we investigate the effect of *optical* dispersion on the time evolution of the vibrational excitation propagation. In Sect. 3 initial condition effects are studied through the calculation of the mean-square-displacements for the optical dispersion relation. Concluding remarks are presented in Sect. 4.

The first of the two assumptions we will modify here is

$$B_q = 2f^2\,\omega_q^2 (x_q^0)^{-2} \tag{1.9}$$

for the interaction term appearing in (1.4), (1.7) and (1.8). The second is the dispersion relation

$$\omega_q = \omega^0 |\sin \tfrac{1}{2} q|. \tag{1.10}$$

where ω^0 is a constant. The purpose of making these assumptions in I was to arrive, in the most economical manner possible, at some essential consequences of nonlinearity. However, the first of these assumptions, which had been pointed out in I as being rather drastic, suffers from the fact that knowledge of the initial condition is preassumed in the interaction expression (1.9) – alternatively, the system is changed (through the prescription (1.9) for B_q) every time the initial condition is changed. In the present paper we remove this shortcoming from the analysis. We take the interaction A_q in the Hamiltonian (1.1) to be given, independently of the initial condition, by

$$A_q^2 = A^2\,\Omega_q\,\omega_q \tag{1.11}$$

where A is a constant. The resulting expression for B_q is

$$B_q = 2\omega_q^2 A^2. \tag{1.12}$$

We will see that this generalization makes it impossible to get the extreme simplifications obtained in I and modifies the results considerably for general initial conditions. However, for the limits of *(i)* the initially localized condition, wherein all masses in the chain, except the one at site 0, are at rest and in their equilibrium positions initially, with $x_m(0) = \delta_{m,0}$, and *(ii)* the grating initial condition wherein the vibrational excitation is initially sinusoidal in space, with $x_m = x_0 \cos(\eta m)$, nothing is changed with respect to the previous analysis. The changes introduced for intermediate initial conditions will be discussed in Sect. 3.

2. Effects of optical dispersion

The other assumption made in I, viz. (1.10), is not representative of the dispersion of optical vibrations which x denotes. The acoustic dispersion of (1.10) was assumed in I only for simplicity. As is well-known [7], the exact dispersion for a system of identical masses and alternating springs is

$$\omega_q^+ = \{(G+V) + [1 - (2GV/(G+V)^2) \cdot \sin^2(q/2)]^{1/2}\}^{1/2}, \tag{2.1}$$

$$\omega_q^- = \{(G+V) - [1 - (2GV/(G+V)^2) \cdot \sin^2(q/2)]^{1/2}\}^{1/2} \tag{2.2}$$

where the force constants for the alternating springs are G and V, respectively. From (2.2) one can derive, for the higher (optical) branch, the approximate dispersion

$$\omega_q = \omega_0 + \omega_1 \cos q \tag{2.3}$$

under the condition

$$\omega_0 \gg \omega_1 \tag{2.4}$$

where ω_0 and ω_1 are given by

$$\omega_0 = [2(G+V)]^{1/2} \tag{2.5}$$

$$\omega_1 = GV/[2(G+V)]^{3/2}. \tag{2.6}$$

Throughout this paper we will assume the dispersion relation (2.3) characteristic of optical vibrations rather than (1.10) which describes acoustic modes.

In I we have derived the method to obtain the time evolution of the displacement of the nonlinear oscillators $x_m(t)$. The method carries through essentially unchanged for optical dispersion. We first consider the localized initial condition, i.e. $x_m(0)=x_0\,\delta_{m,0}$ where x_0 denotes the amplitude of the localized excitation at time $t=0$. As in I, the displacement of the nonlinear oscillators in real space can be constructed through a superposition of an infinite number of the solutions of the corresponding *linear* equation with the replacement of the characteristic frequencies ω by the nonlinearly reduced frequencies ω^f. The coefficients in the superposition have the same form for every term and depend only on the nonlinearity:

$$x_m(t)/x_0=\sum_r R_r\cos(\omega_0^f t)(-1)^{m/2}J_m((2r+1)\,\omega_1^f t) \tag{2.7}$$

for m even and

$$x_m(t)/x_0=\sum_r R_r\sin(\omega_0^f t)(-1)^{(m+1)/2}J_m((2r+1)\,\omega_1^f t) \tag{2.8}$$

for m odd. Here, the reduction factor R_r is given by

$$R_r=(\pi/kK)(-1)^r\operatorname{cosech}((2r+1)(\pi/2)K'/K) \tag{2.9}$$

K, K' have their usual meanings in the context of elliptic integrals, J_m is the ordinary Bessel function of order m, and ω_1^f and ω_0^f are the two frequencies ω_0 and ω_1 reduced by the identical factor $(\pi/2K)(1-f^2)^{1/2}$ as a result of nonlinearity:

$$\omega_1^f=\omega_1(\pi/2K)(1-f^2)^{1/2} \tag{2.10}$$

$$\omega_0^f=\omega_0(\pi/2K)(1-f^2)^{1/2} \tag{2.11}$$

$$f\ =Ax_0 \tag{2.12}$$

and, in the present case, the modulus k has the form

$$k=f(1-f^2)^{1/2} \tag{2.13}$$

We notice that the *linear* equation of motion in momentum space for the "approximate" optical phonon branch treated above, which corresponds to the nonlinear equation (1.4), is

$$(\mathrm{d}^2/\mathrm{d}t^2)\,x_q+(\omega_0+\omega_1\cos q)^2\,x_q=0 \tag{2.14}$$

and is the Fourier transform of the equation of motion in real space given by

$$(\mathrm{d}^2/\mathrm{d}t^2)\,x_m+g_1\,x_m-g_2(2x_m-x_{m-1}-x_{m+1})=0 \tag{2.15}$$

where g_1 and g_2 are constants related to the spring force constants in the linear vibrational chain. For the initial condition $x_m(0)=x_0\,\delta_{m,0}$ this linear chain

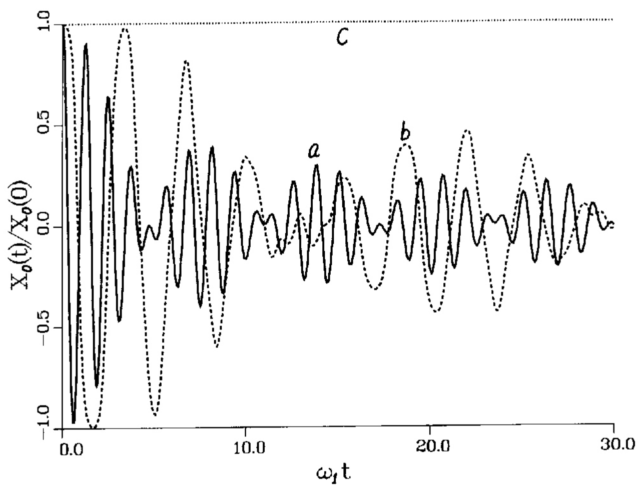

Fig. 1. Effects of optical dispersion and nonlinearity on the propagation of an localized vibrational excitation shown through a plot of the time dependence of the displacement from equilibrium of the initial excited site in Fig. 1. The respective displacement $x_0(t)$ normalized to the initial value of $x(0)$ is plotted along y-axis and time is plotted in units of $1/\omega_1$ along X-axis. Curve a shows the extreme linear limit ($f=0$), curve c shows the extreme nonlinear limit ($f=2^{-1/2}$), and curves b represents the intermediate value of nonlinearity ($f=0.7$). The frequency ω_1 is chosen equal to 0.5 and ω_0 equal to 5.0

problem with optical dispersion relation has the solution

$$x_m^{\text{lin}}(t)/x_0=\cos(\omega_0 t)(-1)^{m/2}J_m(\omega_1 t) \tag{2.16}$$

for m even and

$$x_m^{\text{lin}}(t)=x_0\sin(\omega_0 t)(-1)^{(m+1)/2}J_m(\omega_1 t) \tag{2.17}$$

for m odd. Comparison with (2.7), (2.8) and (2.16), (2.17) shows that nonlinearity has two effects as in I: the reduction of the frequencies, here ω_0, ω_1, by the factor $(\pi/2K)(1-f^2)^{1/2}$ and the appearance of the summation over r.

The solutions (2.7) and (2.8) of our nonlinear vibrational excitation problem are exact and plotted in Fig. 1 where the displacements of the mass at site 0 are shown as functions of time t. The three curves represent different nonlinearity. As in I, the effect of the nonlinearity is to slow down the propagation of the vibrational excitation. The new feature in the present optical branch case is the appearance of *two* characteristic frequencies: one describes "intercell" motion whereas the other describes "intracell" motion, the "cell" being a pair of masses.

For the "grating" initial condition, i.e. $x_m(0)=x_0\cos(m\eta)$ in real space where η is a constant, and $x_q(0)=x_0(\delta_{\eta,q}+\delta_{\eta,-q})/2$ in momentum space, the time evolution of the displacement of the nonlinear oscillators are found to be

$$x_m(t)=(x_0/\pi)\cos(m\eta)\, sn(\omega^f\, t\,|\,k) \tag{2.18}$$

$$\omega^f \;=\pi/(2K)(1-f^2)^{1/2}(\omega_0+\omega_1\cos\eta) \tag{2.19}$$

where the nonlinearity parameter is again given by $f=Ax_0$. However, the symbol x_0 represents the *grating amplitude* here. The frequency reduction in (2.10) is represented through the factor $(1-f^2)^{1/2}$ and the separation of the spatial evolution and the temporal variation is shown here clearly. The linear counterpart is

$$x_m(t)=(x_0/\pi)\cos(m\eta)\sin[(\omega_0+\omega_1\cos\eta)\,t] \tag{2.20}$$

and is obtained as the limit of (2.18), (2.20) as $k\to 0$.

3. Initial condition effects

In our nonlinear model, the vibrational amplitude of the qth mode has been found in (1.5)–(1.8) in Sect. 1. We will now use the more physical expression (1.12) for B_q rather than (1.9). Then, (1.8) reduces to

$$\lambda_q=\omega_q[1-A^2(x_q^0)^2]^{1/2} \tag{3.1}$$

rather than to

$$\lambda_q=\omega_q(1-f^2)^{1/2} \tag{3.2}$$

which was the consequence of (1.9), i.e. of the analysis in I. Equation (3.1) contains the effect of initial conditions on λ_q. The elliptic parameter k_q in (1.7) now has the form

$$k_q=Ax_q^0[1-A^2(x_q^0)^2]^{-1/2} \tag{3.3}$$

which is sensitive to initial conditions unlike the result in I, viz.,

$$k_q=f(1-f^2)^{-1/2} \tag{3.4}$$

which is not. We notice that the quantity Ax_q^0 now takes the place of the constant f. It is very clear that, as state in Sect. 1, initial conditions have little interplay with nonlinearity when they are of the extreme kind: localized as in (2.7) and (2.8) or grating as in (2.18) and (2.19). We will therefore study an intermediate initial condition, viz. a Gaussian:

$$x_q^0=x_0\exp(-q^2/\sigma^2) \tag{3.5}$$

where σ is the width of the Gaussian, and x_0 is a constant.

As in I, we define a "mean-square-displacement" by

$$\langle m^2\rangle=\sum_m m^2[x_m(t)/x_0] \tag{3.6}$$

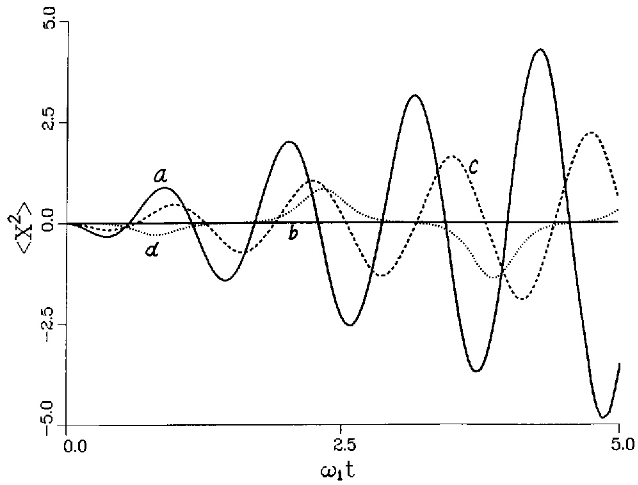

Fig. 2. Time evolution of the mean-square-displacement $\langle x^2(t)\rangle$ for the vibrational excitation for an initial Gaussian distribution. The four curves indicate different nonlinearities: extreme linear limit $f=0$ for a, extreme nonlinear limit $f=2^{-1/2}$ for b, and two intermediate cases $f=0.4$ and $f=0.7$ for c and d. The width $\sigma=10$. The values of ω_1 and ω_0 are the same as in Fig. 1

We find that from (1.5)–(1.8), (1.12) and (2.3) the Gaussian initial condition gives

$$\langle m^2\rangle=(((1-f^2)^{1/2}\,\omega_1-(2/\sigma^2)f^2(\omega_0+\omega_1))\,t-(2/\sigma^2)\,k^2 \cdot(1-f^2)^{-1/2}F(u|k))\,cn(u|k)\,dn(u|k) +(2/\sigma^2)\,sn(u|k) \tag{3.7}$$

where the nonlinearity parameter f is given by $f=x_0\,A$, and the functions $sn(u|k)$, $cn(u|k)$ and $dn(u|k)$ are Jacobian elliptic functions with modulus

$$k=f/(1-f^2)^{1/2} \tag{3.8}$$

and argument u given by

$$u=(\omega_0+\omega_1)(1-f^2)^{1/2}\,t+K_0 \tag{3.9}$$

where K_0 is the complete elliptic integral given in (1.6) with modulus k_q replaced by k given by (3.8). The function $F(u|k)$ is defined as [8]

$$F(u|k)=\int_{\pi/2}^{\phi} dx\{\sin^2 x/[(1-k\sin^2 x)]^{3/2} \tag{3.10}$$

where ϕ is given by

$$\sin\phi=sn(u|k). \tag{3.11}$$

By solving (2.14) directly, the mean-square-displacement for the linear chain (2.15) may be written as

$$\langle m^2\rangle=-\omega_1\,t\sin[(\omega_0+\omega_1)\,t]+(2/\sigma^2) \cdot\cos[(\omega_0+\omega_1)\,t] \tag{3.12}$$

Equation (3.12) is seen to be recovered from (3.7) by putting $f=0$.

The time evolution (3.7) of the mean-square-displacement is shown in Fig. 2 where the 4 curves refer,

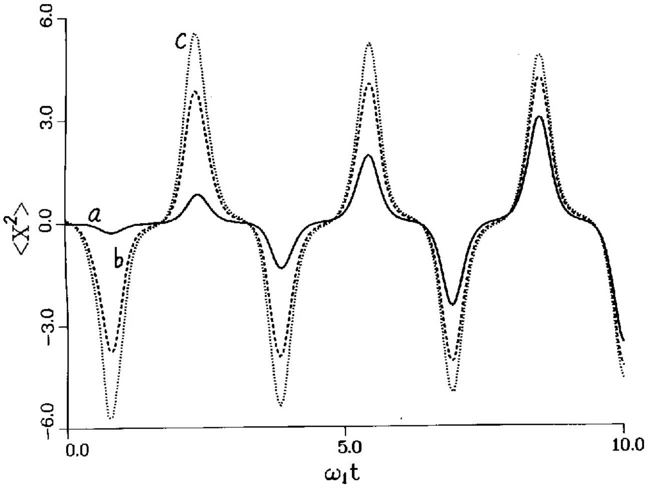

Fig. 3. Effects of varying the width of the initial Gaussian on the propagation of vibrational excitation. Curves a, b and c represent $\sigma=100$, $\sigma=5$ and $\sigma=4$, respectively. The nonlinear parameter f is equal to 0.7 for all three curves. Other parameters are the same as in Fig. 2

respectively, to the nonlinear parameter f being equal to 0 (linear limit), 0.35, 0.7 and $2^{-1/2}$ (this is the extreme nonlinear limit since $k=1$). The propagation of the vibrational excitation in the nonlinear chain is seen to have retained the features of the linear chain (optical branch) that the mean-square-displacement increases linearly and that it oscillates as time increases. The shape of the curve for large nonlinearity deviates dramatically from the sinusoidal function characteristic of the linear case and represents the shape of the elliptic function. The phenomenon that the nonlinearity causes slowing down in the propagation of the vibrational excitation, which we have seen in I, is seen in Fig. 2. If one examines the small-time portion of the curve, however, the peak value of the first peak (or the second or the third, etc.) is seen to *decrease* as the nonlinearity increases.

The effects of the Gaussian width σ on the propagation of the excitation are shown in Fig. 3 where the nonlinear parameter f is taken to be 0.7 for all three curves. The curves a, b and c, referring to $\sigma=100$, 5 and 4, respectively, describe the time evolution of the mean-square-displacement. It is well known that the Gaussian distribution will become a δ-function when the real space width $1/\sigma$ tends to zero. The curve a shows this large σ case. We find that the straightforward effect of σ is the same as that of the nonlinearity f: Larger σ's (more localized initial conditions) reduce the short-time amplitude of the mean-square-displacement, i.e., the mobility of the quasiparticle.

4. Concluding remarks

In the present paper we have extended the work done in the paper I in two ways. First, the restriction on the nonlinearity parameter B_q made in (2.5) in I has been relaxed to make it more general and not dependent on the initial condition: see (1.11) and (1.12). Second, the optical dispersion relation (2.3) is used for the x-oscillators instead of the acoustic dispersion relation (1.10) which was used in I. This replacement is important in the light of the original motivation for the investigation: at high temperature, heat carriers are optical phonons. With those improvements, and by means of the general methods described in I we have obtained here explicit expressions for the real-space displacement evolving in time for both localized and "grating" initial conditions. We have also given results for the mean-square-displacement for a Gaussian initial condition and studied the effect of initial conditions by varying the width of the Gaussian. The results are given by (2.8) and (3.7).

The mobility reduction effect and the frequency reduction effect caused by the nonlinearity which was explored earlier in I are also seen in the present optical branch case. The new feature arising from the optical dispersion relation is the appearance of *two* characteristic frequencies, one of which describes the intercell motion and the other the intracell motion.

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