ON THE DISSIPATION OF ENERGY IN A CHAIN OF
COUPLED HARMONIC OSCILLATORS

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The article deals with processes which occur in coupled oscillator chains following an initial impulse imparted to any one of the atoms. In considering one-dimensional chains of coupled harmonic oscillators, their obvious deficiencies are analyzed and taken into account. The effects which energy dissipation losses and transverse vibrations have on propagation of collision waves through a one-dimensional atom chain are evaluated. It stands to reason, of course, to consider only small transverse displacements of atoms in a chain, since otherwise the simplest models become obviously inadequate.

In a theoretical study of interactions between atoms and crystal surfaces one can take two approaches. The first approach is to try to investigate computable networks which approximate most closely a certain actual physical situation (a realistic formulation of interaction potentials, three-dimensionality, a concrete example of lattice symmetry, etc., e.g., [1]). The second approach is to conduct studies based on using simulations and applicable analytic engineering techniques [2-4]. Pioneering work in the latter direction was done by Frenkel [5]. At the present time, collision between an atom and a surface is most often simulated by an interaction between the atom and a linear chain of oscillators, each of them coupled to its neighbors through harmonic forces.

Let us assume that at some instant of time any one atom (to be called here atom number zero) of a two-dimensional medium, after having previously been at rest, is displaced by an initial amount from its equilibrium position. Bearing in mind that small displacements are considered here and that the displacement amplitudes decrease as the distance from atom number zero increases, we will analyze the processes occurring in two infinite rows of atoms which pass through the equilibrium position of atom number zero at right angles to each other. Atom number zero is, therefore, the only one which belongs to both chains. For an infinite medium we have the following system of equations:

$$M x_n^{\cdot\cdot}(t) = K\left(x_{n-1} - 2x_n + x_{n+1}\right) - K\left(\delta_{1n}\frac{y_0^2}{l} - \delta_{-1n}\frac{y_0^2}{l} + 2\frac{x_0^3}{l^2}\delta_{0n}\right) \quad (-\infty < n < \infty) \tag{1}$$

$$M y_k^{\cdot\cdot}(t) = K\left(y_{k-1} - 2y_k + y_{k+1}\right) - K\left(\delta_{1k}\frac{x_0^2}{l} - \delta_{-1k}\frac{x_0^2}{l} + 2\frac{y_0^3}{l^2}\delta_{0k}\right) \quad (-\infty < k < \infty) \tag{2}$$

Here M is the atom mass; n, k are the order numbers of atoms in the "horizontal" and in the "vertical" direction, respectively; x, y are the atom displacements; K is a force constant of interaction between atoms; δ is the Kronecker delta; l is the interatomic distance considered, for simplicity, the same in both directions.

For the generating function

$$G_x(s, \tau) = \sum_{n=-\infty}^{\infty} x_n(\tau) s^{2n}, \qquad \tau = 2(K/M)^{1/2} t$$

the analog of system (1) is the equation

$$\frac{d^2 G_x}{d\tau^2} = \frac{1}{4}\left(s - \frac{1}{s}\right)^2 G_x - \frac{1}{4l}\left(s^2 - \frac{1}{s^2}\right)y_0^2 - \frac{x_0^3}{2l^2} \tag{3}$$

There is a similar correspondence with Eqs. (2). From (3) we have

$$x_n(\tau) = x_0(0)J_{2n}^{''}(\tau) - \frac{1}{2l}\int_0^\tau y_0^2(u)[J_{2n-1} - J_{2n+1}](\tau - u)\,du \;\; -\frac{1}{l^2}\int_0^\tau \sum_{m=0}^\infty J_{2n+2m+1}(\tau - u)\,x_0^3(u)\,du \tag{4}$$

where J_i is i-th order Bessel function. Equation (4) describes the displacement of all atoms in the horizontal row. For the x component of the movement of atom number zero, Eq. (4) yields a nonlinear integral Volterra equation

$$x_0(\tau) = x_0(0)J_0(\tau) - \frac{1}{l^2}\int_0^\tau \sum_{m=0}^\infty J_{2m+1}(\tau - u)\,x_0^3(u)\,du \tag{5}$$

This means that, with an accuracy down to third-order terms in $y_0 l^{-1}$, the x movement of atom number zero does not depend on how large the projections of the displacements on the vertical axis are. The effect of transverse couplings is accounted for by the second term on the right-hand side of (5).

The first iteration of Eq. (5) yields

$$x_0(\tau) = x_0(0)J_0(\tau) - \frac{x_0^3(0)}{l^2}\left\{[1 + 2J_0(\tau) - J_0^2(\tau)]\sin^2\frac{\tau}{2} - [1 - J_0(\tau)]\tau J_1(\tau) - \tau\sin\tau\right\} \tag{6}$$

The first term inside the large brackets of (6) is bounded, the second term here grows as $\sim \tau^{\frac{1}{2}}$, and the third term here grows as τ. Using the asymptotic formula for function J_0, it is easy to establish that for large values of τ the last term of Eq. (6) decelerates the decay of the vibrations of atom number zero.

Substitution of the expressions for $x_0(\tau)$ and $y_0(\tau)$ into Eq. (4) will yield the x displacements of atoms $|n| > 0$ as functions of time. The transverse movement of atom number zero is more significant here than in its own x vibrations. Since for $n \neq 0$ the last term of Eq. (4) has the same structure as that of Eq. (5), and since the third term of (4) is of a higher order of smallness with respect to the magnitude of the initial displacement than the second term, we will consider only the significance of the second term of (4) describing the effect which the transverse vibrations of atom number zero have on the longitudinal displacements of atoms in the horizontal row. We have

$$x_n(\tau) = x_0(0)J_{2n}(\tau) - \frac{y_0^2(0)}{l}\left\{[1 - J_0(\tau)]J_{2n}(\tau) - 2\sum_{m=0}^\infty (-1)^m J_{2n+2m+2}(\tau)\right\} \tag{7}$$

It becomes evident that the initial displacement of atom number zero produces significant changes in the longitudinal vibrations only at large values of τ. The initial vibration of the n-th atom at $\tau \approx 2n$ is practically independent of the transverse vibrations [if, of course, $x_0(0) > y_0(0)$]. We also note that the transverse vibrations of atom number zero, beginning at some value of τ, impart to atoms $|n| > 0$ a certain background noise represented by vibrations whose amplitude is of the order of $y_0^2 l^{-1}$. For n = 1, for example, Eq. (7) corresponds to the equation

$$x_1(\tau) = x_0(0)J_2(\tau) + \frac{y_0^2(0)}{l}\{\cos - J_0 + J_2 + J_0 J_2\}(\tau) \tag{8}$$

Obviously, formulas for the displacements of atoms in the vertical row, including also $y_0(\tau)$, can be derived by interchanging x_i and y_i in formulas (4)-(8).

It was assumed earlier that the atom rows are infinite in both directions. The effect of boundaries has been studied in several works (e.g., [4-6]). We will, therefore, mention only that, if atom number zero (i.e., the one initially displaced) lies on a surface, then the gist of the analysis is to consider the interaction between the longitudinal wave traveling from the surface depthwise into the medium and the wave which travels within the surface layer of the solid.

Using the same symbols as before, the analyzed system of equations for a chain with friction will be written down as follows:

$$x_n^{\cdot\cdot}(\tau) = \tfrac{1}{4}(x_{n-1} - 2x_n + x_{n+1})(\tau) - \tfrac{1}{2}\gamma x_n^{\cdot}(\tau) \quad (-\infty < n < \infty) \tag{9}$$

where γ characterizes the magnitude of friction forces. Substituting

$$x_n(\tau) = U_n(\tau)\, e^{-\frac{1}{4}\gamma\tau} \tag{10}$$

into (9) and performing a Laplace transformation of (9) will then yield the following system of algebraic equations:

$$\varphi_{n-1}(p) - (4p^2 + 2 - \tfrac{1}{4}\gamma^2)\varphi_n(p) + \varphi_{n+1}(p) + 4px_0(0)\delta_{n0} = 0 \tag{11}$$

where $\varphi_n(p)$ is the transform of function $U_n(\tau)$, the latter determined according to (10). It is assumed, for simplicity, that the initial velocities of all atoms are zero and that only atom number zero is initially displaced.

System (11) gives

$$G(p, s) = \sum_{n=-\infty}^{\infty} \varphi_n(p)\, s^n = -\frac{4px_0(0)}{s - (4p^2 + 2 - \tfrac{1}{4}\gamma^2) + s^{-1}} \tag{12}$$

Resolving (12) into positive-power and negative-power terms in s, we find after a subsequent inverse Laplace transformation:

$$U_n(\tau) = x_0(0) \sum_{m=0}^{\infty} \left(\frac{\tau}{2}\right)^{2n+2m} \frac{1}{(2n+2m)!} \sum_{i=0}^{m} \frac{(n+m)!\, a^{m-i}}{(m-i)!\,(\tfrac{1}{2}i + n)!\,\tfrac{1}{2}i!} \tag{13}$$

$$a = \tfrac{1}{4}\gamma^2 - 2, \quad n \geqslant 0$$

The internal summation in Eq. (13) involves only even i terms.

It is easy to prove that for $a = -2$, i.e., when there are no dissipation terms in Eq. (9),

$$x_n(\tau) = x_0(0)\, J_{2n}(\tau) \tag{14}$$

as should be.

A second indicative special case is $a = 2$, i.e., $\gamma = 4$ (heavy friction). Then

$$x_n(\tau) = x_0(0)\, e^{-\tau} I_{2n}(\tau) \tag{15}$$

where I_{2n} is the Bessel function of the 2n-th order imaginary argument.

Thus, $x_0(\tau)$ in the last case will not change its sign when equilibrium is approached in a viscous medium. Atoms $n > 0$ behave in a similar manner, the atoms above number two practically not "responding" any more to the displacement of atom number zero. It is to be noted that the amplitude of $x_0(\tau)$ for large values of τ and without friction is only twice as large as $x_0(\tau)$ for the same values of τ in the case described by Eq. (15). This can, apparently, be explained by the "slowness" of processes in a system with "heavy" friction.

Equation (13) becomes quite simple when $\gamma = \sqrt{8}$, namely:

$$x_0(\tau) = x_0(0) \sum_{m=0}^{\infty} \left(\frac{\tau}{2}\right)^{4m} \frac{2m!}{4m!(m!)^2} \exp\frac{-\sqrt{2}\,\tau}{2} \tag{16}$$

Equation (16), as well as Eq. (15), corresponds to a rather heavy friction and, therefore, x_0 varies here with time similarly as in (15).

If we assume that $\gamma \ll 1$, then the solution to system (9) can be written as

$$x_n(\tau) = x_0(0)\left\{ J_{2n}(\tau) + \tfrac{1}{8}\gamma^2\tau \sum_{k=0}^{\infty} (-1)^k J_{2n+2k+1}(\tau) \right\} \exp - \gamma\tau/4 \tag{17}$$

This solution consists of a steady term and an additional term whose significance increases with time, Eq. (17) becomes particularly descriptive for n = 0:

$$x_0(\tau) = x_0(0)\{ J_0(\tau) + \tfrac{1}{16}\gamma^2\tau \sin\tau \} e^{-\tfrac{1}{4}\gamma\tau} \tag{18}$$

Thus, instead of the first term in (17) and (18) decreasing, the additional term here increases. It can be verified that for a sufficiently small γ and sufficiently large τ the second term signifies, in the final analysis, a decelerated decrease of $x_0(\tau)$ comparable to $J_{2n}(\tau)\exp(-\tfrac{1}{4}\gamma\tau)$.

It is not difficult to estimate the range of distances from the initially excited atom within which the displacements of atoms are comparable to that of this atom number zero. Considering that this range of distances corresponds to the propagation of waves along the chain within the time interval limited to

$$\tfrac{1}{4}\gamma\tau \lesssim 2 \tag{19}$$

then obviously atoms within

$$|n| \lesssim \tfrac{1}{4}\gamma^{-1} R_{2n} \tag{20}$$

where R_{2n} determines the order of extreme J_{2n} values for τ of the order 2n, will be displaced considerably. It is noteworthy that the region where Eqs. (17) and (18) are valid is practically identical to the region bounded by conditions (19) and (20). If $\gamma \lesssim 0.1$, then the displacement amplitudes of atoms $|n|$ up to several tens in the chain become comparable to $x_0(0)$.

In summing up the results, it must be stated that small initial transverse displacements of atoms and low friction do significantly distort the transient growth of longitudinal vibrations of atoms only for large values of τ. Least sensitive to initial small transverse displacements are the longitudinal vibrations of the very atom which has been transversely displaced. As to the other atoms, their displacement amplitudes, which correspond to a swing of a given atom caused by an elastic wave reaching it, are not significantly changed by these small transverse displacements of the initially excited atom. For large values of τ, however, a certain background noise is added to the steady vibrations of these atoms which is proportional to the magnitude of the initial displacement. With low friction present, the result is that, first of all, the displacements of all atoms in the chain decrease exponentially with time, which is not the case in a dissipationless process. The exponential factor here, by the way, is the same for all atoms. When the energy loss due to friction per vibration cycle is relatively small for the initially excited atom, then all atoms n at least up to several tens are displaced by an amount comparable to the maximum displacement of the initially excited atom. When the friction is heavier, then the range of significant atom displacements becomes narrow and the displacement of the initially excited atom tends toward zero by some slow tenfold aperiodic process.

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