

Dynamics of energy characteristics in one-dimensional crystal

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Abstract

Dynamics of one-dimensional crystal — a chain, containing equal particles connected by linear strings, is considered. The energy characteristics that are quadratic forms of displacements and velocities of the particles are introduced. They can represent dispersions and correlations of displacements and velocities. For the energy characteristics the closed system of equations is obtained. In a particular case these equations are equal to the equations of the chain dynamics with double frequency. It is shown that specific energies of the chain can be expressed in the terms of the energy characteristics.

1 Introduction

Rational derivation of macroscopic thermoelasticity equations for perfect crystals still remains a serious problem for the modern science. In one-dimensional case these equations can be derived in adiabatic approximation [1, 2]. However if thermal conductivity is taken into account then obtaining a closed system of equations became a serious challenge [3, 4, 5]. The recent molecular dynamics experiments show that the heat transfer in perfect crystals disagrees with the classical theory of thermal conductivity [6].

From the general reasons it follows that the thermal conductivity should be connected with the energy transfer in the crystal. From molecular dynamics experiments it is known that for most of initial conditions the specific kinetic and potential energies perform high frequency oscillations with decreasing amplitude [7]. It seems that this behavior of energies can be key for the description of the thermal processes in the crystals. The main aim of this paper is to obtain a closed system of dynamics equations for energy characteristics. Then solution of these equation gives the specific energies as functions of time and space coordinates.

2 Definitions

Let us consider one-dimensional crystal — a chain, containing particles of mass m , connected by linear strings with stiffness C . The equations of the chain dynamics

have the form

$$\ddot{u}_n = \omega_0^2(u_{n-1} - 2u_n + u_{n+1}); \quad \omega_0 \stackrel{\text{def}}{=} \sqrt{C/m}; \quad (1)$$

where u_n is displacement of the particle number n .

Let us consider variables f_n and g_n . Let us define position vectors

$$\mathbf{f} = \mathbf{f}_{pq} \stackrel{\text{def}}{=} [f_p, f_q], \quad \mathbf{g} = \mathbf{g}_{pq} \stackrel{\text{def}}{=} [g_p, g_q], \quad (2)$$

containing values of variables f_n and g_n for indexes p and q . For the position vectors we define the following productions

$$\mathbf{f} \cdot \mathbf{g} \stackrel{\text{def}}{=} \frac{1}{2} \langle f_p g_q + f_q g_p \rangle, \quad \mathbf{f} \times \mathbf{g} \stackrel{\text{def}}{=} \frac{1}{2} \langle f_p g_q - f_q g_p \rangle. \quad (3)$$

These productions depend on the indexes p, q , but for shortness the indexes are not shown. The brackets $\langle \dots \rangle$ in (3) stand for the averaging operator over some space interval:

$$\langle Z_{pq} \rangle \stackrel{\text{def}}{=} \frac{1}{\Lambda} \sum_{l=-\Lambda/2}^{\Lambda/2} Z_{p+l, q+l}, \quad (4)$$

where Z_{pq} is any two-index variable, Λ is an averaging interval. If $\Lambda = 1$ then $\langle Z_{pq} \rangle = Z_{pq}$. If $\Lambda = N$ (the total number of particles in chain) then the averaging is performed over the whole crystal and $\langle Z_{pq} \rangle$ depends on the difference $p - q$ only. If $1 \ll \Lambda \ll N$ then $\langle Z_{pq} \rangle$ can be considered as a variable, which is changing slowly along the chain, and for this variable a long-wave approximation can be used.

There is an analogy between productions (3) and scalar (vector) productions of 2D vectors, however the exact definition is different. In case $p = q = n$ we have

$$\mathbf{f} \cdot \mathbf{g} = f_n g_n, \quad \mathbf{f} \times \mathbf{g} = 0. \quad (5)$$

3 Dynamics equations for energy characteristics

Let us introduce \mathbf{u} and \mathbf{v} — position vectors for particle displacements and velocities, then

$$\begin{aligned} \dot{\mathbf{u}} &= \mathbf{v}, & \ddot{\mathbf{u}} &= \omega_0^2 \mathcal{D}^2 \mathbf{u}; \\ \mathbf{u} &\stackrel{\text{def}}{=} [u_p, u_q], & \mathbf{v} &\stackrel{\text{def}}{=} [v_p, v_q]; \end{aligned} \quad (6)$$

$$\mathcal{D}^2 \mathbf{u} \stackrel{\text{def}}{=} [u_{p+1} - 2u_p + u_{p-1}, u_{q+1} - 2u_q + u_{q-1}].$$

Let us use the following differential inequalities valid for any position vector \mathbf{u}

$$\begin{aligned} (\mathbf{u} \cdot \mathbf{u})'' &= 2\dot{\mathbf{u}} \cdot \dot{\mathbf{u}} + 2\mathbf{u} \cdot \ddot{\mathbf{u}}, \\ (\dot{\mathbf{u}} \cdot \dot{\mathbf{u}})' &= 2\dot{\mathbf{u}} \cdot \ddot{\mathbf{u}}, \\ (\mathbf{u} \times \dot{\mathbf{u}})' &= \mathbf{u} \times \ddot{\mathbf{u}}. \end{aligned} \quad (7)$$

Then, substitution of (6) to (7) gives

$$\begin{aligned} (\mathbf{u} \cdot \mathbf{u})'' &= 2\mathbf{v} \cdot \mathbf{v} + 2\omega_0^2 \mathbf{u} \cdot \mathcal{D}^2 \mathbf{u}, \\ (\mathbf{v} \cdot \mathbf{v})' &= 2\omega_0^2 \mathbf{v} \cdot \mathcal{D}^2 \mathbf{u}, \\ (\mathbf{u} \times \mathbf{v})' &= \omega_0^2 \mathbf{u} \times \mathcal{D}^2 \mathbf{u}. \end{aligned} \quad (8)$$

Let us introduce the following finite difference operators for any two-index variable $Z_{p,q}$

$$\begin{aligned}\Delta Z_{p,q} &\stackrel{\text{def}}{=} (\mathcal{D}_p^2 + \mathcal{D}_q^2)Z_{p,q}, & \Delta_{\times} Z_{p,q} &\stackrel{\text{def}}{=} (\mathcal{D}_p^2 - \mathcal{D}_q^2)Z_{p,q}; \\ \mathcal{D}_p^2 Z_{p,q} &\stackrel{\text{def}}{=} Z_{p+1,q} - 2Z_{p,q} + Z_{p-1,q}, & \mathcal{D}_q^2 Z_{p,q} &\stackrel{\text{def}}{=} Z_{p,q+1} - 2Z_{p,q} + Z_{p,q-1}.\end{aligned}\tag{9}$$

Then equations (8) can be written in the form

$$\begin{aligned}(\mathbf{u}\cdot\mathbf{u})'' &= 2(\mathbf{v}\cdot\mathbf{v}) + \omega_0^2 \Delta(\mathbf{u}\cdot\mathbf{u}), \\ (\mathbf{v}\cdot\mathbf{v})' &= \frac{1}{2}\omega_0^2 \Delta(\mathbf{u}\cdot\mathbf{u}) + \omega_0^2 \Delta_{\times}(\mathbf{u}\times\mathbf{v}), \\ (\mathbf{u}\times\mathbf{v})' &= -\frac{1}{2}\omega_0^2 \Delta_{\times}(\mathbf{u}\cdot\mathbf{u}).\end{aligned}\tag{10}$$

Thus we obtained the closed system of equations for variables $\mathbf{u}\cdot\mathbf{u}$, $\mathbf{v}\cdot\mathbf{v}$, $\mathbf{u}\times\mathbf{v}$. Elimination of $\mathbf{u}\times\mathbf{v}$ from the above system gives the closed system of equations for variables $\mathbf{u}\cdot\mathbf{u}$, $\mathbf{v}\cdot\mathbf{v}$

$$\begin{aligned}(\mathbf{u}\cdot\mathbf{u})'' &= 2(\mathbf{v}\cdot\mathbf{v}) + \omega_0^2 \Delta(\mathbf{u}\cdot\mathbf{u}), \\ (\mathbf{v}\cdot\mathbf{v})'' &= \frac{1}{2}\omega_0^2 \Delta(\mathbf{u}\cdot\mathbf{u})'' - \frac{1}{2}\omega_0^4 \Delta_{\times}^2(\mathbf{u}\cdot\mathbf{u}).\end{aligned}\tag{11}$$

Quantities $\mathbf{u}\cdot\mathbf{u}$ and $\mathbf{v}\cdot\mathbf{v}$ we will name as energy characteristics, since, as it will be shown below, the specific energies of the crystal can be expressed in the terms of these quantities. Elimination of $\mathbf{v}\cdot\mathbf{v}$ from system (11) gives for $\xi \stackrel{\text{def}}{=} \mathbf{u}\cdot\mathbf{u} = \langle u_p u_q \rangle$ the following equation

$$\xi''' - 2\omega_0^2 \Delta \xi'' + \omega_0^4 \Delta_{\times}^2 \xi = 0.\tag{12}$$

This is the desired dynamics equation for the energy characteristics. The variable ξ in (12) depends on the indexes p, q : $\xi = \xi_{p,q}$, but for shortness the indexes are not shown. In more detailed form the equation can be written as

$$\xi''' - 2\omega_0^2(\mathcal{D}_p^2 + \mathcal{D}_q^2)\xi'' + \omega_0^4(\mathcal{D}_p^2 - \mathcal{D}_q^2)^2 \xi = 0.\tag{13}$$

This equation can be also written in the factorized operator form

$$\left(\frac{\partial^2}{\partial t^2} - \omega_0^2(\mathcal{D}_p + \mathcal{D}_q)^2\right) \left(\frac{\partial^2}{\partial t^2} - \omega_0^2(\mathcal{D}_p - \mathcal{D}_q)^2\right) \xi = 0.\tag{14}$$

The initial conditions can be found using formulae

$$\begin{aligned}\xi &= \mathbf{u}\cdot\mathbf{u}, & \dot{\xi} &= 2\mathbf{u}\cdot\mathbf{v}, & \ddot{\xi} &= 2(\mathbf{v}\cdot\mathbf{v}) + \omega_0^2 \Delta(\mathbf{u}\cdot\mathbf{u}), \\ \xi'' &= 4\omega_0^2 \Delta(\mathbf{u}\cdot\mathbf{v}) + 2\omega_0^2 \Delta_{\times}(\mathbf{u}\times\mathbf{v}).\end{aligned}\tag{15}$$

If the values of u_n, v_n for $t = 0$ are known then formulae (15) allow to obtain the necessary initial conditions for ξ . As for boundary conditions, any possible variant can be considered, however the simplest and usually the most convenient variant is periodic boundary conditions.

4 Specific energies

Let us define the specific kinetic energy K and specific potential energy U of the crystal as

$$K \stackrel{\text{def}}{=} \frac{1}{2} m \langle v_n^2 \rangle, \quad U \stackrel{\text{def}}{=} \frac{1}{4} C \langle (u_{n+1} - u_n)^2 + (u_n - u_{n-1})^2 \rangle. \quad (16)$$

These energies can be expressed in the terms of the energy characteristics like

$$K = \frac{1}{2} m (\mathbf{v} \cdot \mathbf{v}) \big|_{p=q}, \quad U = \frac{1}{4} C (\mathcal{D}^2 - \Delta) (\mathbf{u} \cdot \mathbf{u}) \big|_{p=q}, \quad (17)$$

where operator \mathcal{D}^2 for a two-index variable $Z_{p,q}$ is defined as

$$\mathcal{D}^2 Z_{p,q} \stackrel{\text{def}}{=} Z_{p+1,q+1} - 2Z_{p,q} + Z_{p-1,q-1}. \quad (18)$$

Since from (11) quantity $\mathbf{v} \cdot \mathbf{v}$ can be expressed in the terms of $\xi = \mathbf{u} \cdot \mathbf{u}$ as

$$\mathbf{v} \cdot \mathbf{v} = \frac{1}{2} \left(\frac{\partial^2}{\partial t^2} - \omega_0^2 \Delta \right) \xi, \quad (19)$$

then specific energies can be also expressed in the terms of $\xi = (\mathbf{u} \cdot \mathbf{u}) = \langle u_p u_q \rangle$

$$\begin{aligned} K &= \frac{m}{4} \left(\frac{\partial^2}{\partial t^2} - \omega_0^2 \Delta \right) \xi \big|_{p=q}, & U &= \frac{m}{4} \omega_0^2 (\mathcal{D}^2 - \Delta) \xi \big|_{p=q}; \\ E &= \frac{m}{4} \left(\frac{\partial^2}{\partial t^2} + \omega_0^2 \mathcal{D}^2 - 2\omega_0^2 \Delta \right) \xi \big|_{p=q}, & L &= \frac{m}{4} \left(\frac{\partial^2}{\partial t^2} - \omega_0^2 \mathcal{D}^2 \right) \xi \big|_{p=q}; \end{aligned} \quad (20)$$

where E and L are the specific total energy and Lagrange function:

$$E \stackrel{\text{def}}{=} K + U, \quad L \stackrel{\text{def}}{=} K - U. \quad (21)$$

Thus, after the equation (6) is solved, all specific energies can be determined from equations (20).

5 Averaging over whole crystal

Let us consider the case $\Lambda = N$. In this case the averaging operator $\langle \dots \rangle$ gives an average over all particles in the crystal, and the corresponding specific energies are average energies over the whole crystal. Then all quantities depend only on $k = q - p$ and we can define

$$\xi_{q-p} \stackrel{\text{def}}{=} \xi_{p,q} = \langle u_p u_q \rangle. \quad (22)$$

This definition can be written as

$$\xi_k \stackrel{\text{def}}{=} \frac{1}{N} \sum_{n=1}^N u_n u_{n+k}. \quad (23)$$

Then we obtain for $k = q - p$

$$\mathcal{D}_k^2 \xi_k \stackrel{\text{def}}{=} \mathcal{D}_p^2 \xi_k = \mathcal{D}_q^2 \xi_k = \xi_{k+1} - 2\xi_k + \xi_{k-1}; \quad (24)$$

$$\Delta\xi_k = 2\mathcal{D}_k^2 \xi_k, \quad \Delta_\times \xi_k = 0, \quad \mathcal{D}^2 \xi_k = 0. \quad (25)$$

The dynamics equation for the energy characteristics (12) takes the form

$$\overset{\cdot\cdot\cdot}{\xi}_k - 4\omega_0^2 \mathcal{D}_k^2 \overset{\cdot\cdot}{\xi}_k = 0. \quad (26)$$

This equation can be rewritten as

$$\overset{\cdot\cdot}{\zeta}_k - 4\omega_0^2 \mathcal{D}_k^2 \zeta_k = 0, \quad \zeta_k \stackrel{\text{def}}{=} \frac{1}{2} \overset{\cdot\cdot}{\xi}_k. \quad (27)$$

Thus we obtain for ζ_k the equation, which is almost identical to the equation of the chain dynamics (1) with the only difference that the partial frequency in this case is $2\omega_0$ instead of ω_0 :

$$\overset{\cdot\cdot}{\zeta}_k = 4\omega_0^2 (\zeta_{k+1} - 2\zeta_k + \zeta_{k-1}). \quad (28)$$

The initial conditions for ζ_k can be found using formulae (15):

$$\zeta_k = (\mathbf{v} \cdot \mathbf{v})_k + \omega_0^2 \mathcal{D}_k^2 (\mathbf{u} \cdot \mathbf{u})_k, \quad \dot{\zeta}_k = 4\omega_0^2 \mathcal{D}_k^2 (\mathbf{u} \cdot \mathbf{v})_k; \quad (29)$$

where

$$(\mathbf{u} \cdot \mathbf{u})_k = \frac{1}{N} \sum_{n=1}^N u_n u_{n+k}, \quad (\mathbf{u} \cdot \mathbf{v})_k = \frac{1}{N} \sum_{n=1}^N u_n v_{n+k}, \quad (\mathbf{v} \cdot \mathbf{v})_k = \frac{1}{N} \sum_{n=1}^N v_n v_{n+k}. \quad (30)$$

If values of u_n, v_n for $t = 0$ are known then formulae (29)–(30) allows obtaining the necessary initial conditions for ζ_k .

From (20) we can see that variable ζ_k for $k = 0$ defines the Lagrange function — the difference between kinetic and potential energies of the chain:

$$L = K - U = \frac{m}{2} \zeta_0. \quad (31)$$

Since E is constant in the considered case (it is $1/N$ of the total energy of the crystal), then kinetic and potential energies can be found as

$$K(t) = \frac{1}{2}E + \frac{m}{4} \zeta_0(t), \quad U(t) = \frac{1}{2}E - \frac{m}{4} \zeta_0(t). \quad (32)$$

Thus solution of equation (28) allows to obtain the kinetic and potential energies of the crystal as functions of time for any initial distribution of displacements and velocities.

6 Conclusions

In the current paper the closed system of equations with initial conditions for energy characteristics is obtained. If this system is solved then the specific energies can be found as functions of time and space coordinates. The energy characteristics that are quadratic forms of displacements and velocities of the particles are introduced. These characteristics can represent dispersions and correlations of displacements and velocities. The obtained equations in addition to the time and space coordinates

have also correlational coordinate, which describes correlation of dynamics in different points of the crystal. From the obtained equations it follows that correlations between displacements and velocities of different particles are essential for describing the energy transfer processes, which probably can not be explained without taking into account redistribution of oscillations along the correlational coordinate.

In the case when the energy characteristics are obtained as average over all particles in the crystal it was shown that they can be described by the same equation as the dynamics of the particles in the chain, but with double partial frequency. This allows to examine analytically the phenomenon of high-frequency energy oscillations, which is known from molecular dynamics computer experiments.

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