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# Transition to thermal equilibrium in a crystal subjected to instantaneous deformation

A M Krivtsov<sup>1,2,\*</sup>  and A S Murachev<sup>1,2,\*</sup> 

<sup>1</sup> Peter the Great St. Petersburg Polytechnic University, Saint Petersburg, Russia

<sup>2</sup> Institute for Problems in Mechanical Engineering of the Russian Academy of Sciences, Saint Petersburg, Russia

E-mail: [akrivtsov@bk.ru](mailto:akrivtsov@bk.ru) and [andrey.murachev@spbstu.ru](mailto:andrey.murachev@spbstu.ru)

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## Abstract

An adiabatic transition between two equilibrium states corresponding to different stiffnesses in an infinite chain of particles is studied. Initially, the particles have random displacements and random velocities corresponding to uniform initial temperature distributions. An instantaneous change in the parameters of the chain initiates a transitional process. Analytical expressions for the chain temperature as a function of time are obtained from statistical analysis of the dynamic equations. It is shown that the transition process is oscillatory and that the temperature converges non-monotonically to a new equilibrium state, in accordance with what is usually unexpected for thermal processes. The analytical results are supplemented by numerical simulations.

Keywords: energy oscillations, thermal equilibration, FPU crystal, temperature, covariance analysis

## 1. Introduction

Nonequilibrium processes in solids at the nano- and microscale are currently a subject of intensive research, partly driven by the development of nanotechnologies [1–9]. At the microscale, the transition to an equilibrium state in harmonic crystals is a gradual equalization of the kinetic and potential energies of atomic motion according to the virial theorem [10–14]. However, this theorem does not describe the processes that occur during the transition. A macroscopic description of such a transition is also challenging since it requires the application of special constitutive equations for ultrafast atomic processes. Therefore, we have developed a simple model that analytically describes both the microscopic and macroscopic transitional processes.

Crystals with simple lattices are convenient models for the study of nonequilibrium processes in solids [15–18]. Numerical simulations [19] have shown that the process of energy equalization in molecular systems is accompanied by high-

frequency oscillations. In the pioneering paper by Klein and Prigogine [20], the equations of atomic motion for a one-dimensional harmonic crystal were solved directly and it was shown that the energy oscillations following an instantaneous thermal perturbation were described by the Bessel function of the first kind. In later work [21], this problem was solved by analysing the dynamics equations of the velocity covariances, which allowed generalization of these results to more complex systems, including multidimensional crystals [22–28].

In the above mentioned works, the nanoscale thermal processes were studied separately from the mechanical processes. The advances in modern technologies have produced ultrafast mechanical processes where the speed of the mechanical load is comparable or even faster than the rate of the local thermal equilibration in the system being considered. This condition is fulfilled if the material is rapidly loaded by forces uniformly distributed along the length of the sample. Such loads occur in the nanoscale electronic components of experimental equipment requiring fast magnetic field switches which are, for example, necessary in condensed matter physics, plasma physics, or inertial confinement synthesis [29]. Electric pulses

\* Authors to whom any correspondence should be addressed.

can create distributed electromagnetic loads on circular samples for times up to several tens of nanoseconds [30, 31]. In [32], the idea of an ultrafast photodetector capable of converting femtosecond light pulses into electric pulses of the same length was proposed. Paper [29] demonstrates an all-optical method for generating magnetic field impulses on the order of several tesla for a duration of tens of femtoseconds. In the near future it is expected that experimental electromagnetic impulses will reach a duration of less than a femtosecond; femtosecond lasers already exist [33] and attoseconds lasers are under development [34–36]. Therefore, an analytical study of the impact of ultrafast mechanical loads on thermal equilibration is needed to provide a theoretical basis for the upcoming experimental studies.

In the present paper, we study an adiabatic non-equilibrium process analogous to those considered previously [22–27]. This process is, however, initiated by instantaneous loading instead of instantaneous heating. The material is deformed by forces uniformly distributed along the length of the sample [30, 31], hence in this case the orders of the velocities of the mechanical and thermal processes are the same. We note that in this paper we neglect the effects of inertia during crystal loading. The interaction between mechanical and thermal processes requires an accounting for non-linearity, therefore an  $\alpha$ -FPU one-dimensional crystal [37–39] is considered. The non-linearity is assumed to be strong enough to cause adiabatic heating in the crystal, but also sufficiently weak to analyse the resulting energy oscillations in the framework of the harmonic approximation.

The paper is organized as follows: in section 2 the mathematical formulation of the problem is presented. Two problems are then solved, where the first is the problem of the equilibrium value of the kinetic temperature after loading at large times  $t \rightarrow \infty$  (section 3). The second problem that this paper addresses is an analytical description of the transition to a new state of equilibrium (section 4). It is shown that the crystal temperature oscillates during the transition process via the Bessel function, and the analytical solution is compared with a numerical one. In section 5 an estimation of the temperature jump for the real crystal is represented.

## 2. Formulation of the problem

We consider a model of an infinite one-dimensional crystal—a chain of point masses connected by massless springs. It is assumed that the chain particles interact only with their nearest neighbours. At thermodynamic equilibrium, particle velocities  $v_n$  and bond deformations  $\varepsilon_n$  are independent stochastic quantities, and all the statistical characteristics of the crystal are constant over time. To describe the statistical behaviour of the system, we introduce the following quantities:

$$K \stackrel{\text{def}}{=} \frac{1}{2} m \langle v_n^2 \rangle, \quad T \stackrel{\text{def}}{=} \frac{2K}{k_B}, \quad (1)$$

where  $K$  is the mathematical expectation of the kinetic energy,  $T$  is the kinetic temperature,  $n = 1, 2, 3, \dots$  is the index of the particle,  $\langle \cdot \cdot \cdot \rangle$  is the operator for the mathematical expectation,  $v_n$  is the particle velocity,  $k_B$  is the Boltzmann constant, and  $m$

is the particle mass. The statistical characteristics of this system depend on such crystal parameters as the particle mass and bond stiffness. Variation of these parameters transfers the crystal to a non-equilibrium state and begins the transition process, which eventually brings the crystal to a new equilibrium state.

One of the natural ways to change the bond stiffness of the crystal is by a homogeneous crystal deformation by external loading. For example, such a loading can be realized by applying distributed electromagnetic forces to a circular sample [30, 31]. Based on the approach described in [21], we investigate the evolution of the kinetic temperature of the crystal during this transition process.

In addition to the mathematical expectation of kinetic energy  $K$ , this paper uses the mathematical expectation of the potential energy  $U$ :

$$U(\varepsilon + \varepsilon_n) \stackrel{\text{def}}{=} \langle \Pi(\varepsilon + \varepsilon_n) \rangle, \quad \varepsilon_n \stackrel{\text{def}}{=} u_n - u_{n-1}, \quad \Pi(\varepsilon) \stackrel{\text{def}}{=} \frac{C}{2} \varepsilon^2 + \frac{\alpha}{3} \varepsilon^3, \quad (2)$$

where  $\Pi$  is the interparticle potential,  $C$  and  $\alpha$  are the stiffnesses of the interparticle bonds of the first and the second order,  $u_n$  is the displacement of a particle from its equilibrium position, and deformation is the sum of the homogeneous deformation  $\varepsilon$  and stochastic deformation  $\varepsilon_n$ . The homogeneous deformation  $\varepsilon(t)$  is applied instantaneously:

$$\varepsilon(t) = \begin{cases} 0, & t < 0 \\ \varepsilon, & t \geq 0, \end{cases} \quad (3)$$

where  $\varepsilon$  is a constant. The force  $F_n$  imposed on particle  $n - 1$  by particle  $n$  is

$$F_n \stackrel{\text{def}}{=} -F(\varepsilon + \varepsilon_n), \quad F(\varepsilon) = -\Pi'(\varepsilon) = -C\varepsilon - \alpha\varepsilon^2, \quad (4)$$

where prime stands for differentiation. The equation of particle dynamics for the crystal is

$$m\dot{v}_n = F_{n+1} - F_n. \quad (5)$$

We consider weak non-linearity, therefore the second terms in the formulae for  $\Pi(\varepsilon)$  (2) and  $F(\varepsilon)$  (4) are small compared to the first. Since the non-linear term is weak, a harmonic (linear) approximation is used to describe the thermal processes. At relatively small times, the harmonic approximation is quite accurate in describing thermal processes in a crystal with weak non-linearity [23, 28, 39]. However, a non-zero stiffness of the second order allows us to take the influence of the homogeneous deformation  $\varepsilon$  on inter-particle potential into account.

The analytical expression for the kinetic temperature at large times after the homogeneous deformation can be obtained using the virial theorem, and is given in the following section.

## 3. Crystal in the thermodynamic equilibrium

In this section, we first derive expressions for the kinetic temperature of the crystal before loading and show how it relates to potential energy. We then present a solution to the problem of finding the asymptotic value of the kinetic temperature at

long times after loading. The following section compares the obtained asymptotic solution with the exact solution for the kinetic temperature.

### 3.1. Prior to loading

At  $t < 0$ , according to (3), the energies are

$$K = \frac{1}{2}m\langle v_n^2 \rangle, \quad U = \frac{C}{2}\langle \varepsilon_n^2 \rangle + \frac{\alpha}{3}\langle \varepsilon_n^3 \rangle \quad (6)$$

and the crystal is assumed to be at thermodynamic equilibrium. Since only the mathematical expectations of the energies are considered, henceforth the term ‘mathematical expectation’ is omitted. Following [11], the kinetic energy (1) of the system can be represented by (see appendix A):

$$K = \frac{1}{2}\langle \varepsilon_n F_n \rangle. \quad (7)$$

Formula (7) allows us to obtain expressions for the equilibrium kinetic temperature of the crystal before and after the instantaneous deformation, as follows:

$$m\langle v_n^2 \rangle = \langle \varepsilon_n F_n \rangle = C\langle \varepsilon_n^2 \rangle + \alpha\langle \varepsilon_n^3 \rangle, \quad (8)$$

By neglecting the small term  $\alpha\langle \varepsilon_n^3 \rangle$  in equation (8) we can obtain expressions for the kinetic temperature of the crystal prior to loading

$$k_B T_0 = m\langle v_n^2 \rangle = C\langle \varepsilon_n^2 \rangle. \quad (9)$$

From expression (9) it can be seen that the initial kinetic temperature is proportional to the crystal potential energy (6).

In the next subsection, we consider the kinetic temperature after loading.

### 3.2. After loading

At  $t \geq 0$ , the kinetic and potential energies of the crystal are

$$K = \frac{1}{2}m\langle v_n^2 \rangle, \quad U = \Pi(\varepsilon) + U_T, \quad (10)$$

$$U_T = \frac{1}{2}(C + 2\alpha\varepsilon)\langle \varepsilon_n^2 \rangle + \frac{1}{3}\alpha\langle \varepsilon_n^3 \rangle,$$

where  $U_T$  is the thermal part of the potential energy. We note that in formula (10) the term  $\alpha\varepsilon\langle \varepsilon_n^2 \rangle$  corresponds in order of magnitude to the term  $C\langle \varepsilon_n^2 \rangle$ . However, to remain within the framework of the harmonic theory, we neglect the term  $\alpha\langle \varepsilon_n^3 \rangle$  below. The term  $\alpha\varepsilon\langle \varepsilon_n^2 \rangle$  allows us to describe the thermoelastic effects. In the state of thermodynamic equilibrium the kinetic energy  $K$  and the thermal part of the potential energy  $U_T$  are equal, therefore the expression for kinetic temperature (1) is

$$k_B T|_{t \rightarrow \infty} = 2K = U_T + K. \quad (11)$$

We note that  $U_T + K$  is constant for  $t \geq 0$  in the transition process by virtue of the energy conservation law. An expression for this sum can be obtained by substitution into (11) of the initial values of the corresponding quantities:

$$k_B T = \frac{1}{2}m\langle v_n^2 \rangle \Big|_{t=0} + \frac{1}{2}(C + 2\alpha\varepsilon)\langle \varepsilon_n^2 \rangle \Big|_{t=0}, \quad (12)$$

where the term  $\alpha\langle \varepsilon_n^3 \rangle/3$  is omitted. Substitution of expressions (9) into (12) yields:

$$T|_{t \rightarrow \infty} = T_0 \left( 1 + \frac{\alpha\varepsilon}{C} \right). \quad (13)$$

From expression (13) it follows that the change in kinetic temperature  $T$ , in the first approximation, is proportional to the deformation  $\varepsilon$ .

## 4. Dynamics of the transition process

In the previous section, the problem of finding the asymptotic value of the temperature at large times was solved. This section is focussed on the second problem of this paper, which is to derive an expression for the temperature as a function of time. By substituting expression (4) into (5) we obtain the following equation of motion:

$$m\dot{v}_n = C\Delta\varepsilon_n + 2\alpha\varepsilon\Delta\varepsilon_n + \alpha\Delta\varepsilon_n^2, \quad \dot{\varepsilon}_n = \Delta v_n. \quad (14)$$

The term  $\alpha\Delta\varepsilon_n^2$  can be neglected in the case of small deformations. Thus, equation (14) become linear:

$$\dot{v}_n = \omega^2(\varepsilon_n - \varepsilon_{n-1}), \quad \dot{\varepsilon}_n = v_n - v_{n-1} \quad (15)$$

where  $\omega \stackrel{\text{def}}{=} \sqrt{\frac{C+2\alpha\varepsilon}{m}}$ . Note that the sum  $C + 2\alpha\varepsilon$  plays the role of first order stiffness after external loading. The initial conditions for the system (15) are determined from equation (9):

$$v_n|_{t=0} = \sqrt{\frac{k_B T_0}{m}}\rho_n, \quad \varepsilon_n|_{t=0} = \sqrt{\frac{k_B T_0}{C}}\varrho_n, \quad (16)$$

where  $\rho_n$  and  $\varrho_n$  are independent random numbers with zero mathematical expectation and unit variance:

$$\langle \rho_n \rho_{n+k} \rangle = \delta_k, \quad \langle \varrho_n \varrho_{n+k} \rangle = \delta_k. \quad (17)$$

Here,  $\delta_k = 1$  for  $k = 0$  and  $\delta_k = 0$  otherwise. Equation (16) operates under the assumption that particle velocities and bond deformations are independent at thermodynamic equilibrium. The initial value problem (15) and (16) describes the stochastic dynamics of the particles. The kinetic temperature of the crystal as a function of time can then be found using the covariance analysis approach [21, 25], by introducing the generalized energies

$$\mathcal{K}_k \stackrel{\text{def}}{=} \frac{1}{2}m\langle v_n v_{n+k} \rangle, \quad \mathcal{U}_k \stackrel{\text{def}}{=} \frac{1}{2}m\omega^2\langle \varepsilon_n \varepsilon_{n+k} \rangle, \quad (18)$$

$$\mathcal{L}_k \stackrel{\text{def}}{=} \mathcal{K}_k - \mathcal{U}_k,$$

where  $\mathcal{K}_k$  and  $\mathcal{U}_k$  are generalized kinetic and potential energies, and  $\mathcal{L}_k$  is the generalized Lagrangian. Differentiation of (18) and the equations of motion (14) leads to the following initial problem value for the generalized Lagrangian:

$$\ddot{\mathcal{L}}_k = 4\omega^2(\mathcal{L}_{k-1} - 2\mathcal{L}_k + \mathcal{L}_{k+1}),$$

$$t = 0: \quad \mathcal{L}_k = -\frac{T_0 k_B \alpha \varepsilon}{C} \delta_k, \quad \dot{\mathcal{L}}_k = 0. \quad (19)$$

The initial conditions for (19) are obtained from (9) and (16). A solution for a similar initial problem is obtained in [21]. According to that solution, the generalized Lagrangian oscillates with a decreasing amplitude:

$$\mathcal{L}_k = -\frac{T_0 k_B \epsilon \alpha}{C} J_{2k}(4\omega t), \quad (20)$$

where  $J_k(x)$  is the Bessel function of the  $k$ th order [40].

The kinetic energy  $K$  and thermal part of the potential energy  $U_T$  are equal to the generalized kinetic and potential energies with zero indexes, therefore the kinetic temperature  $T$  can be expressed as follows:

$$k_B T = \mathcal{L}_0 + K + U_T. \quad (21)$$

The kinetic temperature of the crystal as a function of time can then be found using formulae (13), (20) and (21):

$$T = T_0 + \frac{T_0 \alpha \epsilon}{C} (1 - J_0(4\omega t)). \quad (22)$$

We note that, according to the asymptotic representation for the Bessel function [40],

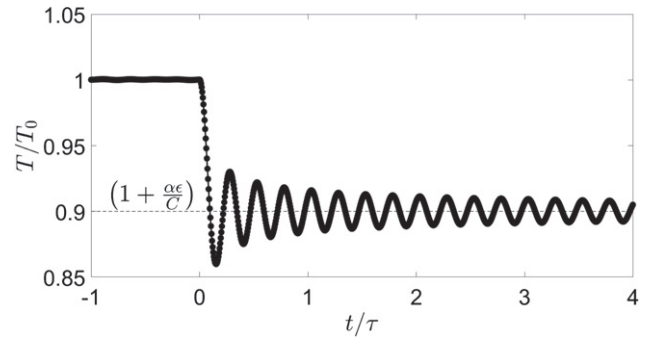
$$x \gg \mu + 1: \quad (23)$$

$$J_\mu(x) = \sqrt{\frac{2}{\pi x}} \cos\left(x - \frac{\pi\mu}{2} - \frac{\pi}{4}\right) + O(x^{-3/2}),$$

wherein the amplitude of the kinetic temperature oscillations decreases in line with  $t^{-1/2}$ .

Figure 1 shows a comparison of the analytical solution (22) with the numerical solution obtained by computer simulations of the weakly anharmonic crystal consisting of  $N = 5 \times 10^4$  particles under periodic boundary conditions. In the framework of the numerical experiment, the parameters of the problem under consideration are chosen so that  $\alpha\epsilon/C = -0.1$ . The simulation uses the method of central differences, with an integration step of  $0.01/\omega_e$ . At the initial time, the particle displacements are zero, while the particle velocities are random and correspond to the crystal temperature  $2T_0$ . The process of energy equalization results in a crystal temperature that oscillates with a decreasing amplitude about an amplitude of  $T_0$ . A homogeneous deformation is applied when the temperature oscillations have a negligibly small amplitude. After loading of the crystal, the temperature then oscillates about a new equilibrium value.

In paper [23], it was shown numerically that thermal phenomena in crystals with a sufficiently weak non-linearity do not differ greatly from those in harmonic crystals. In the simulation, a time span sufficient to describe tens of temperature oscillations after the homogeneous deformation has been chosen. The time span however is chosen to be not large so that the temperature oscillations significantly deviate from the harmonic solution. To calculate the mathematical expectations for the statistical quantities the results are averaged over all particles and  $10^3$  realizations, which are solutions of the same equations with different randomly generated initial conditions. According to paper [21], the crystal temperature before the



**Figure 1.** Oscillations of kinetic temperature  $T$  in the infinite crystal after the instantaneous loading at  $t = 0$ . Numerical (dots) and analytical (solid line) solutions are presented. The averaging is performed using  $10^3$  numerical experiments. Number of particles  $N = 5 \times 10^4$ , constant  $\tau = 2\pi/\omega_e$ , coefficient  $\alpha\epsilon/C = -0.1$ .

instantaneous deformation is the Bessel function of zero order. The instantaneous deformation is applied when the amplitude of the temperature oscillation is small compared to the absolute value of  $\alpha\epsilon/C$ .

As seen from figure 1, the analytical solution (22) practically coincides with the results of the numerical integration of the chain dynamics system equations (3)–(5) for several tens of oscillation periods.

Formula (13) gives the limiting value for the kinetic temperature. According to expression (21), after the instantaneous deformation, the kinetic temperature oscillates around this limiting value and tends to it at large times. Thus, as  $t \rightarrow \infty$ , expression (22) coincides with formula (13), as obtained from the virial theorem. For arbitrary times this expression gives the desired description of the nonequilibrium transition process.

## 5. Example

In order to estimate the temperature jump in the transition process, we consider a one-dimensional ring of carbon atoms, which is at a state of thermodynamic equilibrium with initial temperature  $T_0 = 300^\circ$  K. We assume that following the result of the homogeneous loading the bond deformation is 1.0% of the equilibrium interparticle distance  $a = 0.154$  nm [41]. The mass of the carbon atom is  $m = 1.99 \times 10^{-26}$  kg and the first-order stiffness coefficient is taken to be equal to the stiffness of diamonds bond  $C = 472$  N m $^{-1}$  [42]. The second-order stiffness coefficient can be found from the following formula [43]:

$$\alpha = -\frac{\beta a C^2}{k_B}, \quad (24)$$

where  $\beta = 0.7 \times 10^{-6}$  K $^{-1}$  is the coefficient of the thermal expansion of diamond [44]. The substitution of the stiffness coefficients and deformation into formula (13) gives the new equilibrium temperature value of 298.3 K. The asymptotic period of the kinetic temperature oscillations in the transient process described by formula (22), is approximately 10.2 femtoseconds. Thus 1.0% deformation leads to a change in the crystal temperature by 0.6%.

## 6. Conclusions

The paper presents an analytical approach for the analysis of the transition process in one-dimensional crystals (chains) subjected to an instantaneous homogeneous deformation. Such a deformation can be interpreted as an instantaneous change in the stiffness of the interparticle bonds in a chain. An instantaneous change of stiffness abruptly changes the potential energy of the crystal, which leads to the changes in the kinetic energy and the kinetic temperature. It is found that the transition process is accompanied by high-frequency energy oscillations, which have an analytical representation in terms of the zero Bessel function of the first kind, and consequently the amplitude of the transitional oscillations is inversely proportional to the square root of time. After the decay in the oscillations the system reaches a near equilibrium state corresponding to the predictions of equilibrium thermodynamics. However, the transition process can be studied in detail by use of the presented approach, where the analytical solution is confirmed by numerical simulations. Using the technique described in [22], the presented approach can be extended to analyses of transition processes in two-dimensional and three-dimensional materials. The obtained results are important in establishing the link between the mechanical and thermal processes in solids over the femtosecond time scale.

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## Data availability statement

No new data were created or analysed in this study.

## Appendix A. The virial relation

Following [11] the kinetic energy (1) of the system can be represented by

$$K = \frac{m}{2} \langle u_n v_n \rangle - \frac{1}{2} \langle u_n (F_{n+1} - F_n) \rangle, \quad (\text{A1})$$

where expression (5) has been used. The second term in (A1) is

$$\langle u_n (F_{n+1} - F_n) \rangle = -\langle \varepsilon_n F_n \rangle + \langle F_{n+1} u_n \rangle - \langle F_n u_{n-1} \rangle. \quad (\text{A2})$$

Defining  $g \stackrel{\text{def}}{=} \langle F_n u_{n-1} \rangle$ , equation (A1) then takes the form

$$K = \frac{1}{2} \langle \varepsilon_n F_n \rangle - \frac{1}{2} g' + \frac{m}{2} \langle u_n v_n \rangle. \quad (\text{A3})$$

where prime stands for spatial differentiation. The quantities  $g$  and  $\langle u_n v_n \rangle$  are constant in the thermodynamic equilibrium

state and their derivatives are zero. Therefore the expression for the kinetic energy is

$$K = \frac{1}{2} \langle \varepsilon_n F_n \rangle. \quad (\text{A4})$$

Formula (A4) allows us to obtain expressions for the equilibrium kinetic temperature of the crystal before and after the instantaneous deformation.

## ORCID iDs

A M Krivtsov  <https://orcid.org/0000-0002-9258-065X>

A S Murachev  <https://orcid.org/0000-0002-6311-4457>

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