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Thermal echo in a finite one-dimensional harmonic crystal

A S Murachev¹ , A M Krivtsov^{1,2} and D V Tsvetkov¹

¹ Peter the Great Saint Petersburg Polytechnic University, Saint Petersburg, Russia

² Institute for Problems in Mechanical Engineering RAS, Saint Petersburg, Russia

E-mail: andrey.murachev@gmail.com, akrivtsov@bk.ru and dvtsvetkov@ya.ru

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Abstract

An instant homogeneous thermal perturbation in the finite harmonic one-dimensional crystal is studied. Previously it was shown that for the same problem in the infinite crystal the kinetic temperature oscillates with decreasing amplitude described by the Bessel function of the first kind. In the present paper it is shown that in the finite crystal this behavior is observed only until a certain period of time when a sharp increase of the oscillation amplitude is realized. This phenomenon, further referred to as the thermal echo, occurs periodically, with the period proportional to the crystal length. The amplitude for each subsequent echo is lower than for the previous one. It is obtained analytically that the time-dependence of the kinetic temperature can be described by an infinite sum of the Bessel functions with multiple indices. It is also shown that the thermal echo in the thermodynamic limit is described by the Airy function.

Keywords: thermal processes, temperature, finite crystals, harmonic crystals

(Some figures may appear in colour only in the online journal)

1. Introduction

Analytical and experimental results demonstrate an anomalous nature of thermal processes in ultrapure materials [1–9]. These processes can be caused by shock waves [10–13] or by ultrashort laser pulses [14–20]. One-dimensional crystal lattices are subject of an extensive research since they admit analytical solutions and allow verification of fundamental phenomena inherent also for higher dimensional systems [21–25]. An analytical description of the thermal processes in non-equilibrium harmonic crystals can be obtained on the basis of the covariance analysis [1, 3, 4, 26]. The corresponding description of the anomalous heat propagation is presented in papers [3, 27, 28] for one dimension and in works [4, 29–31] for two and three dimensions.

One of the specific phenomena of the nonequilibrium thermal processes in discrete molecular systems is the high-frequency oscillations of the kinetic temperature, which have long been known from the results of numerical simulation [32]. Covariance analysis admit analytical description of this phenomenon, for example in the case of the instantaneous thermal perturbation of the simplest model of one-dimensional

harmonic crystal these oscillations are described by the Bessel function of the first kind and the zero order [26], similar result was obtained earlier by direct analytical solution of the equations of the atoms motion by Ilya Prigogine [33]. For the case of the one-dimensional crystal on an elastic substrate the same problem is solved in [24], for higher dimensions in papers [4, 30].

Unlike previous papers [3, 24, 26, 27], where the main attention is focused on infinite crystals, the present paper investigates thermal processes in *finite* crystals [34]. The systems with a finite number of particles are of practical importance, especially because nanotechnologies are actively developing [35–39]. In the current paper it is demonstrated that for the finite crystals the temperature oscillation amplitude is decreasing only until a certain moment in time when a sharp increase of the amplitude of the kinetic temperature oscillations is realized. This phenomenon can be interpreted as a thermal echo, which will be analyzed in detail in the present paper. Exact and asymptotic formulas describing the oscillations of the kinetic temperature are obtained. These results, in particular, are important for description of the anomalous heat propagation in ultrapure materials [3, 5, 40].

2. Dynamics of the crystal

2.1. The mathematical model

We consider a one-dimensional harmonic crystal containing N identical particles connected by harmonic springs. The equation of motion for the particles is

$$\ddot{u}_k = \mathcal{L}u_k, \quad \mathcal{L}u_k \stackrel{\text{def}}{=} \omega_e^2(u_{k+1} - 2u_k + u_{k-1}), \quad (1)$$

where u_k is the displacement of the k th particle ($k = 0..N - 1$), \mathcal{L} is the linear difference operator, $\omega_e = \sqrt{C/m}$ is the elementary frequency, C is the stiffness of the interparticle spring, m is the particle mass. Periodic boundary conditions are used:

$$u_0 \stackrel{\text{def}}{=} u_N, \quad u_{N+1} \stackrel{\text{def}}{=} u_1. \quad (2)$$

The initial conditions are

$$u_k = 0, \quad v_k \stackrel{\text{def}}{=} \dot{u}_k = \sigma \rho_k, \quad (3)$$

where ρ_k are independent random numbers with zero mathematical expectation and unit variance, σ is the initial velocity variance. These initial conditions correspond to an instantaneous temperature perturbation, such as perturbations caused by an ultrashort laser pulse [14, 15, 17]. The crystal temperature before the perturbation is zero.

The initial problem (1)–(3) describes stochastic dynamics of the particles in the crystal. Further the deterministic equations for the statistical characteristics of motion (covariances) are analyzed to describe the thermal processes in the crystal.

2.2. The dynamics of covariances

One of the key statistical characteristics of the crystal is the kinetic temperature T , which can be determined by the mathematical expectation $\langle \dots \rangle$ of the square of the centered velocity. The corresponding formula for a one-dimensional case is

$$T = \frac{m}{k_B} \langle \tilde{v}_k^2 \rangle, \quad (4)$$

where

$$\tilde{v}_k \stackrel{\text{def}}{=} v_k - \bar{v}, \quad \bar{v} \stackrel{\text{def}}{=} \frac{1}{N} \sum_{k=0}^{N-1} v_k. \quad (5)$$

Here \bar{v} is the center of mass velocity and k_B is the Boltzmann constant. In order to obtain a closed system of equations for statistical characteristics it is imperative that we consider the covariances of the particle velocities [3, 26, 30]:

$$\kappa_n = \langle \tilde{v}_k \tilde{v}_{k+n} \rangle, \quad (6)$$

which are the quantities characterizing motion of the particle pairs. The following initial problem for the velocity covariances can be obtained by differentiating the covariances using relations (1)–(3) (see appendix A):

$$\begin{aligned} \dot{\kappa}_n - 4\mathcal{L}\kappa_n &= -2\mathcal{L}\kappa_n^0, \\ t = 0: \quad \kappa_n &= \kappa_n^0 \stackrel{\text{def}}{=} \sigma^2 \delta_n^N - \frac{\sigma^2}{N}, \quad \dot{\kappa}_n = 0, \end{aligned} \quad (7)$$

where δ_n^N is the periodical Kronecker symbol: $\delta_n^N = 1$ for n divisible by N (including $n = 0$), otherwise $\delta_n^N = 0$. Additionally the covariances satisfy the periodicity conditions: $\kappa_{n+N} = \kappa_n$. After solving the initial problem (7), the kinetic temperature of the crystal can be found using formula (4), which can be written as

$$T = \frac{m}{k_B} \kappa_n \Big|_{n=0}. \quad (8)$$

2.3. Representation via Bessel functions

Solution of the initial problem (7) yields the following expression for the temperature of the crystal (see appendix B):

$$T = T_E + \frac{\delta T}{2N} \sum_{k=0}^{N-1} \cos\left(4\omega_e t \sin \frac{\pi k}{N}\right) \quad (9)$$

where

$$T_E \stackrel{\text{def}}{=} \frac{\Delta T}{2} \left(1 - \frac{1}{N-1}\right) \quad (10)$$

is an equilibrium temperature³,

$$\Delta T \stackrel{\text{def}}{=} \frac{m}{k_B} \kappa_n^0 \Big|_{n=0} = \sigma^2 \left(1 - \frac{1}{N}\right) \quad (11)$$

is the temperature jump initially caused by the thermal perturbation and

$$\delta T \stackrel{\text{def}}{=} \Delta T \left(1 + \frac{1}{N-1}\right). \quad (12)$$

Expression (9) accurately describes the time dependence of the kinetic temperature of the harmonic crystal after an instant heat perturbation. Formula (9) can be effectively used for computations, however it is less appropriate for an analytical analysis. Therefore an alternative representation for the crystal temperature in terms of the Bessel functions is obtained below.

Let us consider identity [41]

$$\cos(z \sin \vartheta) = \sum_{p=-\infty}^{\infty} J_{2p}(z) \cos(2p \vartheta), \quad (13)$$

where $J_{2p}(t)$ is the Bessel function of the first kind of order $2p$. Substitution $\vartheta = \pi k/N$ and summation over k yields

$$\frac{1}{N} \sum_{k=0}^{N-1} \cos\left(z \sin \frac{\pi k}{N}\right) = \sum_{p=-\infty}^{\infty} J_{2p}(z) \delta_p^N, \quad (14)$$

where

$$\delta_p^N = \frac{1}{N} \sum_{k=0}^{N-1} \cos\left(p \frac{2\pi k}{N}\right). \quad (15)$$

³ For an infinite crystal the kinetic temperature is tending to T_E ; for a finite crystal the temperature is oscillating in the vicinity of T_E .

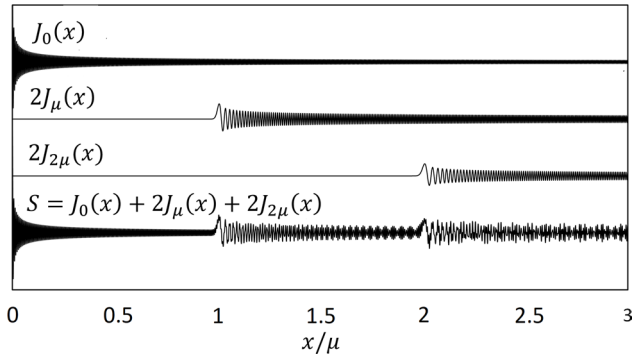


Figure 1. Bessel functions multiple orders, $\mu = 10^3$ (the top three graphs); sum of the Bessel functions (the lower lines).

As mentioned before, $\delta_p^N = 1$ if p is divisible by N , otherwise $\delta_p^N = 0$. Identity (15) is derived in appendix C. Using properties of δ_p^N formula (14) can be reduced to

$$\frac{1}{N} \sum_{k=0}^{N-1} \cos\left(z \sin \frac{\pi k}{N}\right) = \sum_{p=-\infty}^{\infty} J_{2pN}(z). \quad (16)$$

Substitution of the obtained formula to expression (9) gives

$$T = T_E + \frac{\delta T}{2} \sum_{p=-\infty}^{\infty} J_{2pN}(4\omega_e t). \quad (17)$$

Using identity $J_{-2pN} \equiv J_{2pN}$ formula (17) can be rewritten as

$$T = T_E + \frac{\delta T}{2} J_0(4\omega_e t) + \delta T \sum_{p=1}^{\infty} J_{2pN}(4\omega_e t), \quad (18)$$

where T_E and δT is defined in (10) and (12). Thus, the kinetic temperature can be represented as the equilibrium temperature plus the sum of terms proportional to the Bessel functions of multiple orders.

Both expressions (9) and (18) are exact, but expression (18) is more suitable for the analytical analysis. Indeed, for a positive integer index μ the Bessel function $J_\mu(x)$ is almost zero for all positive x up to a vicinity of the point $x = \mu$. Therefore, for a finite moment in time only a finite number of terms gives noticeable contribution to representation (18). For illustration consider series

$$S(x) = J_0(x) + 2J_\mu(x) + 2J_{2\mu}(x) + \dots + 2J_{p\mu}(x) + \dots \quad (19)$$

Graphs for $S(x)$ and the first three terms of its representation (19) are shown in figure 1. The figure shows that for almost⁴ the entire interval $[0, \mu)$ the sum $S(x)$ is determined only by the first term in the expression (19). Similarly, for almost the entire interval $[\mu, 2\mu)$ the sum $S(x)$ is determined by the first two terms, and so on.

If the crystal has a nonzero initial temperature T_0 before the heat perturbation then the equilibrium temperature (10) contains additional term T_0 :

$$T_E \stackrel{\text{def}}{=} T_0 + \frac{\Delta T}{2} \left(1 - \frac{1}{N-1}\right), \quad (20)$$

⁴Except a small vicinity of the right boundary $x = \mu$, where the width of this vicinity can be determined by expression (34).

while expressions (17) and (18) remain unchanged. This is a direct consequence of the superposition principle, which is valid for harmonic systems

$$\begin{aligned} \tilde{T} &= T - T_E \\ &= \frac{\delta T}{2} \left(J_0(4\omega_e t) + 2 \sum_{p=1}^{\infty} J_{2pN}(4\omega_e t) \right), \end{aligned} \quad (21)$$

where $\delta T = \Delta T \left(1 + \frac{1}{N-1}\right)$ (12), ΔT is the temperature jump⁵ caused by temperature perturbation. As follows from expression (21) the equilibrium temperature T_E is the temperature reached when $N \rightarrow \infty$, $t \rightarrow \infty$ (equilibrium state of an infinite crystal).

3. Oscillations of the kinetic temperature

3.1. Thermal echo

According to the virial theorem [42, 43] in harmonic systems a time average for both kinetic and potential energies tends to the same value. Earlier studies [26, 33] have shown that in the one-dimensional infinite harmonic crystal this equilibration process is accompanied by the energy (and, consequently, the temperature) oscillations described by the Bessel function of the zero order. According to formula (17) or (18) the same process in the finite harmonic crystal is described by an infinite series of the Bessel functions with multiple orders.

This phenomenon referred to as thermal echo can be explained as follows. The solution of the initial problem (1)–(3) due to the linearity of the system can be represented as a superposition of N problems for each individual particle, where only this certain particle was randomly disturbed. For each particle elastic waves propagate to the right and left from its position in the crystal and superposition of these waves for all particles describes the thermal process in the crystal. Since the crystal is periodic (circular), the elastic waves meet each other after they have passed half-length of the crystal. All particles were disturbed instantly, therefore the waves initiated from each particle meet simultaneously, causing a sharp short-term increase of the system’s kinetic temperature—the first thermal echo. Then the waves travel further and meet again—the second thermal echo is realized, and so on. Each thermal echo (18) is expressed in terms of the Bessel functions of order $2pN$, where $p = 1, 2, 3, \dots$ is the echo number.

The crystal is discrete system that possesses dispersion—the wave speed depends on the wave length. The fastest are the long waves that travel with the speed of sound $c_s = a\omega_e$ [44, 45], where ω_e is an elementary frequency (1), a is the lattice step. These waves meet after they pass half-length of the crystal, therefore the thermal echo period is

⁵The temperature jump is the difference between the temperature of the crystal at the point in time immediately after the temperature perturbation, and the temperature at the point in time immediately preceding the temperature perturbation.

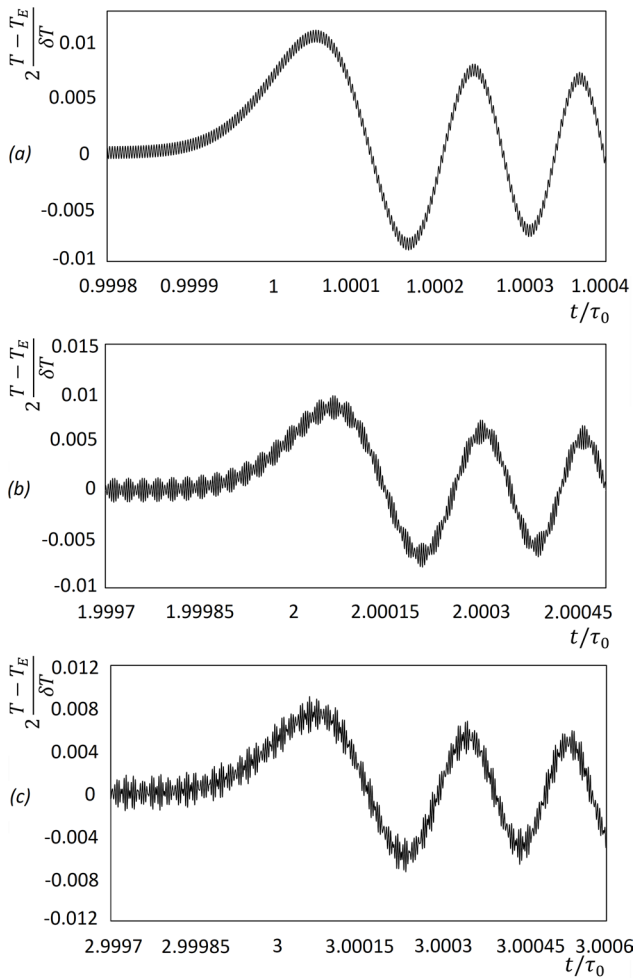


Figure 2. Beats of temperature imposed on three successive thermal echoes. The number of particles $N = 10^6$, T_E is the equilibrium temperature, $\delta T = \Delta T \left(1 + \frac{1}{N-1}\right)$, ΔT is the temperature jump of the crystal caused by the thermal perturbation, t is time, τ_0 is the period of realization of the thermal echo.

$$\tau_0 = \frac{L}{2c_s} = \frac{N}{2\omega_e}, \quad (22)$$

where $L = Na$ is the crystal length. The number of thermal echoes in the system up to the time t can be obtained using ratio t/τ_0 . Shorter waves are slower and meet later—therefore the thermal echo has a finite width, and consequently each next thermal echo is less prominent.

The time $t = p\tau_0$ we will call the reference time for the thermal echo number p . At that time the long waves from the initial disturbances have the meeting number p , that causes the temperature oscillations of corresponding the thermal echo.

3.2. Thermal echo implementations

Using formula (18) the kinetic temperature can be represented in the form:

$$T = T_E + T_B + T_1 + T_2 + \dots + T_p + \dots; \\ T_B = \frac{\delta T}{2} J_0(4\omega_e t), \quad T_p = \delta T J_{2pN}(4\omega_e t); \quad (23)$$

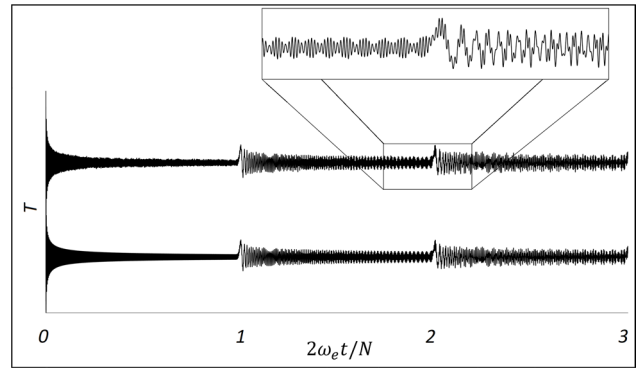


Figure 3. Oscillations of kinetic temperature T in the finite crystal. Numerical (top) and analytical (bottom) solutions. The averaging is performed using 100 numerical experiments. The number of particles $N = 10^3$, t is time and ω_e is the elementary frequency.

where T_E is the equilibrium temperature (18), T_B is the basic thermal mode, and the subsequent terms T_p are the thermal modes with the number $p = 1, 2, 3, \dots$

The temperature oscillations in a crystal containing 10^6 particles are shown in figure 2. The plots show the time vicinity of the first, second and third thermal echo. The first thermal echo is initiated for $t \approx \tau_0$. The corresponding temperature oscillations (23) are described by the first thermal mode T_1 .

Each thermal mode is represented by the corresponding Bessel function. Bessel functions are not periodic, however it is convenient to consider a quasiperiod—the interval between two consequent maximums of the Bessel function. This quasiperiod is not a constant, its value decreases for each next maximum.

As can be seen from figure 2(a), for $t \approx \tau_0$ the oscillations are superposition (18) of the basic mode T_B (small short oscillations on the graph) and the first mode T_1 (global oscillations on the graph). For $t \approx \tau_0$ the quasiperiod of the basic mode is much smaller than the quasiperiod of the first mode. The larger is the crystal, the more significant is the discrepancy. For times $t \approx 2\tau_0$, the oscillation parameters of the basic and the first thermal modes become close, which leads to a beat phenomena. For $t \approx 2\tau_0$, the second thermal echo is realized, superimposed by the mentioned beatings—see figure 2(b). For $t \approx 3\tau_0$, the third thermal echo is realized (see figure 2(c)). Numerical experiments show that for large times plural realizations of the thermal echo result in an increasingly complex form of beats. The realizations of the thermal echo with large ordinal numbers is less pronounced against the background of residual oscillations from previous implementations of the thermal echo. As a result, at large times the temperature fluctuations acquire a quasi-stochastic character resembling thermal noise.

Figure 3 shows comparison of the analytical solution (bottom) and the computer simulation of the crystal dynamics (top). The crystal under consideration contains 10^3 particles. The analytical solution is described by formula (9) or (18). The computer simulation uses the method of central differences to solve numerically the system of 10^3 differential equations of the chain dynamics (1) with the integration step $0.02/\omega_e$. The results are regarded over 100

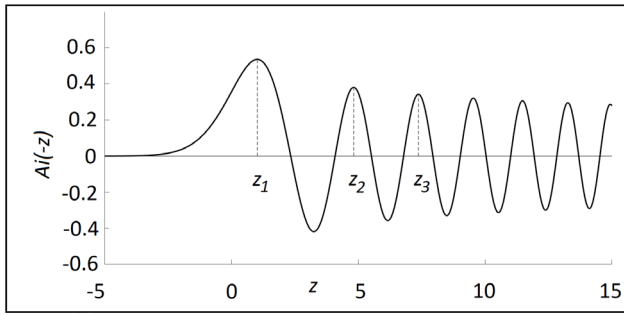


Figure 4. The Airy function. Such a form takes any thermal echo for a sufficiently large number of particles N .

realizations of such chain with an independent random initiation. As it can be seen from figure 3 the graphs of the computer simulation and the analytical solution are almost identical.

3.3. Asymptotics

Expression (18), which describes the temperature oscillations in the crystal, includes Bessel functions of multiple orders. In the time-vicinity of the thermal echo appearance the following asymptotic representation of the Bessel functions [41] can be used:

$$J_\mu(x) = \left(\frac{2}{\mu}\right)^{1/3} \text{Ai}\left(\left(\frac{2}{\mu}\right)^{1/3}(\mu - x)\right) + O(\mu^{-1}), \quad (24)$$

where Ai is the Airy function⁶ [41]. This representation is valid⁷ for $x \approx \mu \gg 1$. More general asymptotics, which is valid for any x is given in appendix D. The important advantage of these asymptotic representations is that they express special function $J_\mu(x)$ of two variables x, μ in terms of a special Airy function of a single variable. Therefore each thermal mode (23) except the basic mode can be obtained from the Airy function by a linear transformation. Substitution $\mu = 2pN$ and $x = 4\omega_e t$ to (24) allows to obtain asymptotics the thermal echo. The Airy function graph in a form of $\text{Ai}(-z)$ is plotted in figure 4. This graph demonstrates the shape of the thermal echo in the thermodynamic limit ($N \rightarrow \infty$), where the value $z = 0$ corresponds to the reference time $t = p\tau_0$ of the thermal echo number p . It is a bit unexpected that the significant temperature increase starts before the reference time, that is before the long waves from the initial disturbance formally meet each other. Probably this is due to the nature of discrete systems, where some energy can be transferred faster than the speed of sound of the corresponding continuum system.

Then the temperature (18) can be represented as

⁶The Airy function can be defined as: $\text{Ai}(x) = \frac{1}{\pi} \int_0^\infty \cos\left(\frac{t^3}{3} + xt\right) dt$.

⁷The representation (24) is given by the formula 9.3.23 [41]. It is valid for $|\mu - x|/\sqrt[3]{\mu} \leq A$, where A is an arbitrary positive constant.

$$T \approx T_E + \frac{\delta T}{2} J_0(4\omega_e t) + \delta T \sum_{p=1}^{\infty} \frac{1}{\sqrt[3]{pN}} \text{Ai}\left(\frac{2pN - 4\omega_e t}{\sqrt[3]{pN}}\right). \quad (25)$$

For large values of arguments $x \gg \mu + 1$ the following asymptotics for the Bessel functions fulfils [41]:

$$J_\mu(x) = \sqrt{\frac{2}{\pi x}} \cos\left(x - \frac{\pi\mu}{2} - \frac{\pi}{4}\right) + O(x^{-3/2}). \quad (26)$$

Asymptotic representations (24) and (26) for the Bessel functions allows to obtain the basic characteristics of the temperature oscillations for large N .

3.4. Characteristics of thermal echo

Let us consider the thermal mode number p :

$$T_p = \nu_p \delta T J_{2pN}(4\omega_e t) \quad (27)$$

for large values of N , where $\nu_p = \frac{1}{2}$ for $p = 0$ (the basic thermal mode) and $\nu_p = 1$ otherwise.

In the vicinity of the reference time $t = p\tau_0$ the thermal mode T_p with the use of asymptotics (24) can be represented as

$$T_p \approx \frac{\nu_p \delta T}{\sqrt[3]{pN}} \text{Ai}\left(\frac{2pN - 4\omega_e t}{\sqrt[3]{pN}}\right). \quad (28)$$

The Airy function $\text{Ai}(-z)$ is depicted in figure 4. Let z_k be the successive points of the local maximums of this function, where $k = 1, 2, 3, \dots$ is the point number; $A_k \stackrel{\text{def}}{=} \text{Ai}(-z_k)$ are the corresponding maximums of the function. The first three values of these constants are [46]:

$$\begin{aligned} z_1 \approx 1.0 : \quad A_1 \approx 0.53, \\ z_2 \approx 4.8 : \quad A_2 \approx 0.38, \\ z_3 \approx 7.4 : \quad A_3 \approx 0.34. \end{aligned} \quad (29)$$

Then the corresponding points of the first local maximums t_p and the maximum values M_p for the thermal mode (28) are

$$t_p \approx \frac{1}{4\omega_e} \left(2pN + \sqrt[3]{pN}\right), \quad M_p \approx \frac{\nu_p \delta T}{\sqrt[3]{pN}} A_1. \quad (30)$$

The formula for t_p can be rewritten in the form

$$t_p \approx p\tau_0 \left(1 + \frac{1}{2(pN)^{2/3}}\right). \quad (31)$$

Hence the relative difference between the reference time and the time of the temperature maximum t_p decreases with increase of N , which proves that these times coincide in the continuum limit.

In the vicinity of the reference time $t = p\tau_0$ the previous thermal mode T_{p-1} (27) with the use of asymptotics (26) can be represented as

$$T_{p-1} \approx (-1)^N \nu_{p-1} \frac{\delta T}{\sqrt{\pi N p}} \cos\left(4\omega_e t - \pi N p - \frac{\pi}{4}\right). \quad (32)$$

Let us define the relative height of the thermal echo h_p as a ratio of the maximum value of the thermal mode number p (30) to the amplitude of the residual oscillations from the previous thermal mode (32), which gives⁸

$$h_p \simeq \frac{\sqrt{\pi} A_1 \sqrt[6]{pN}}{\nu_{p-1}}. \quad (33)$$

Thus the relative height of the thermal echo h_p increases with increasing N . Therefore for very large N the residual oscillations can be considered as negligible. However this increase is very slow—proportional to $N^{1/6}$, hence even for $N = 10^6$ the residual oscillations are quite noticeable.

To analyze the thermal echo properties let us introduce its relative width w_k as the ratio of the quasiperiod of the corresponding Bessel function to the asymptotic period of Bessel functions at infinity. From formulas (24)–(26) it follows that the relative width is proportional to $N^{1/3}$ (see appendix E):

$$w_k \simeq \frac{z_{k+1} - z_k}{2\pi} \sqrt[3]{pN}. \quad (34)$$

From relations (33) and (34) it follows that for large N the residual oscillations from the previous thermal echo are small and frequent in comparison with the current thermal echo wave—see figure 2.

3.5. Example

As an example consider a chain of $N = 10^3$ carbon atoms with the periodic boundary conditions and initial temperature $T_0 = 0$ °C. The heat perturbation instantaneously increases the temperature up to the value

$$T_0 + \Delta T = 100 \text{ °C}. \quad (35)$$

The chosen value of ΔT is sufficiently small in comparison with the melting temperature of carbon (3500 °C), so as not to take into account the nonlinearity of the interatomic interaction. As a result of this perturbation the temperature oscillations near the equilibrium value of $T_E \approx 50$ °C are realized in the crystal. The graph of the temperature oscillations for the crystal calculated using numerical and analytical solution is shown in figure 3. Formula (30) gives for the maximum value of the first thermal mode

$$M_1 \approx 5.3 \text{ °C} \quad \implies \quad T_E + M_1 \approx 55.3 \text{ °C}. \quad (36)$$

Thus the thermal echo brings approximately 10% change of the temperature comparing to the final temperature raise $T_E - T_0 \approx 50$ °C.

These results are slightly perturbed by the residual oscillations from the previous (the basic) thermal mode. Formulas (33) and (34) yield

$$h_1 \approx 5.9, \quad w_1 \approx 11.3, \quad (37)$$

hence the residual oscillations are approximately six times weaker and have an 11 times shorter period than the oscillations caused by the first thermal echo. The residual oscillations according to formula (32) have the amplitude of approximately 0.9 °C, which is about 17% of M_1 . If the residual oscillations

⁸ For $p = 1$ the previous mode is T_B with twice less amplitude—see (23).

are taken into account the maximum temperature achieved by the first thermal echo is approximately 56.2 °C.

The above characteristics depend only on the number of particles N , while the period τ_0 of the thermal echo realization depends on the physical properties of the crystal and the type of oscillations (longitudinal or transversal). Let us consider longitudinal oscillations, the mass of the carbon atom $m = 1.99 \times 10^{-26}$ kg and the stiffness of diamond bond $C = 1824$ N m⁻¹ [47]. Then formula (22) gives $\tau_0 = 1.65 \times 10^{-12}$ s that is a $\frac{N}{4\pi} \approx 80$ times greater than the atomic oscillation period.

The obtained numerical characteristics of the thermal echo can be used to determine its occurrence in natural experiments.

4. Conclusions

The paper considers a finite one-dimensional harmonic crystal subjected to an instant spatially uniform thermal perturbation. The numerical and analytical analysis presented in the paper demonstrates the phenomenon of the thermal echo: a sharp short-term temperature rise that is periodically realized in the crystals.

Previous papers [26, 33] have shown that in the infinite one-dimensional harmonic crystal the instant thermal perturbation produces the thermal oscillations with a monotonically decreasing amplitude, these oscillations are described by the zero order Bessel function. In the present paper it is shown that in the finite harmonic crystal the sequence of realizations of the thermal echo is described by a series of the Bessel functions of multiple orders. Any thermal echo in the thermodynamic limit is described by the Airy function. A superposition of the temperature oscillations generated by the sequential thermal echoes results in a temperature beats. Each subsequent thermal echo complicates the shape of the beats.

It follows thus from the analysis that the maximum temperature increase caused by the thermal echo decreases as $\sqrt[3]{pN}$ (30), where p the thermal echo number and N is the number of particles in the crystal. The duration of the thermal echo grows by the same law (34). Between any two thermal echoes the amplitude of the temperature oscillations decreases in proportion to the square root of time (26). The larger is the crystal, the more noticeable are the temperature increases compared the residual oscillations (33).

Thus, an analytical description of the thermal echo for one-dimensional crystals is presented. Our results can be generalized to two- and three-dimensional cases using technique presented in [4, 30]. Similar effects can be found in nanotubes, where we expect to observe two thermal echoes. The first one is caused by the elastic waves propagation along the tube direction, and the second one in the transverse direction. Influence of anharmonic effects on similar thermal processes is studied numerically in [4]. The investigation shows that harmonic approximation is quite accurate in the case of small nonlinearity.

This phenomenon is an important feature of thermal processes in finite systems and should be taken into account in the development of the modern micro- and nanosize electronic devices.

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Appendix A. The initial problem for the velocities covariance

Let us consider displacements covariance and velocities covariance:

$$\xi_n = \langle u_k u_{k+n} \rangle, \quad \kappa_n = \langle v_k v_{k+n} \rangle. \quad (\text{A.1})$$

Differentiation of expression (A.1) gives us the equation

$$\dot{\kappa}_n = \mathcal{L} \dot{\xi}_n, \quad (\text{A.2})$$

where \mathcal{L} is the operator from the problem (1). The equation (A.2) leads to the conservation law:

$$\kappa_n - \mathcal{L} \xi_n = \epsilon_n^0, \quad (\text{A.3})$$

where the constant ϵ_n^0 can be obtained from the initial conditions (3):

$$\epsilon_n^0 = \kappa_n \Big|_{t=0} = \sigma^2 \langle \tilde{\rho}_k \tilde{\rho}_{k+n} \rangle \Big|_{t=0}, \quad (\text{A.4})$$

and $\tilde{\rho}_k$ is centered random numbers. Let us consider the following expression:

$$\langle \tilde{\rho}_k \tilde{\rho}_{k+n} \rangle = \langle \rho_k \rho_{k+n} \rangle - 2 \langle \rho_k \bar{\rho} \rangle + \langle \bar{\rho}^2 \rangle, \quad (\text{A.5})$$

where $\bar{\rho}$ is the mean value of ρ_k . Let us take into account that

$$t = 0: \quad \langle \rho_k \bar{\rho} \rangle = \frac{\rho_k}{N} \sum_{n=0}^{N-1} \rho_{k+n} = \frac{1}{N}, \quad \bar{\rho}^2 = \frac{1}{N}, \quad (\text{A.6})$$

then

$$\epsilon_n^0 = \sigma^2 \delta_n - \frac{\sigma^2}{N}. \quad (\text{A.7})$$

The equations below can be obtained by differentiating twice (A.1):

$$\ddot{\xi}_n = 2(\kappa_n + \mathcal{L} \xi_n), \quad \ddot{\kappa}_n = 2\mathcal{L}(\kappa_n + \mathcal{L} \xi_n). \quad (\text{A.8})$$

The using of conservation law (A.3) allow us to close equation for each covariance:

$$\ddot{\xi}_n - 4\mathcal{L} \xi_n = 2\mathcal{L} \epsilon_n^0, \quad \ddot{\kappa}_n - 4\mathcal{L} \kappa_n = -2\mathcal{L} \epsilon_n^0. \quad (\text{A.9})$$

The second equation of (A.9) and (A.4) gives us the initial problem for κ_n .

Appendix B. Equation for velocities covariances

Let us consider the initial problem (7) with the corresponding boundary conditions:

$$\begin{aligned} \ddot{\kappa}_n - 4\mathcal{L} \kappa_n &= -2\sigma^2 \mathcal{L} \delta_n, \\ t = 0: \quad \kappa_n &= \sigma^2 \delta_n - \frac{\sigma^2}{N}, \quad \dot{\kappa}_n = 0, \\ \kappa_0 &= \kappa_N, \quad \kappa_{N+1} = \kappa_1. \end{aligned} \quad (\text{B.1})$$

Then we apply the discrete Fourier transformation

$$\kappa_k^* = \sum_{n=0}^{N-1} \kappa_n e^{\frac{-2\pi i k n}{N}} \quad (\text{B.2})$$

to the initial problem (B.1):

$$\begin{aligned} \ddot{\kappa}_k + 4\mathcal{L} \kappa_k &= 0, \\ t = 0: \quad \kappa_k &= \frac{\sigma^2}{2} - \sigma^2 \delta_k, \quad \dot{\kappa}_k = 0, \end{aligned} \quad (\text{B.3})$$

where

$$\kappa_k = \kappa_k^* - \frac{\sigma^2}{2}, \quad \mathcal{L} = 4\omega_e^2 \sin^2 \frac{\pi k}{N}. \quad (\text{B.4})$$

The solution of the problem (B.3) is

$$\kappa_k = \frac{\sigma^2}{2} (1 - 2\delta_k) \cos \left(4\omega_e t \sin \frac{\pi k}{N} \right), \quad (\text{B.5})$$

hence

$$\kappa_k^* = \frac{\sigma^2}{2} (1 - 2\delta_k) \cos \left(4\omega_e t \sin \frac{\pi k}{N} \right) + \frac{\sigma^2}{2}. \quad (\text{B.6})$$

The inverse Fourier transform for κ_k^* is

$$\kappa_n = \frac{1}{N} \frac{\sigma^2}{2} \sum_{k=0}^{N-1} \left(1 + \cos \left(4\omega_e t \sin \frac{\pi k}{N} \right) \right) e^{i \frac{2\pi n k}{N}} - \frac{\sigma^2}{N}. \quad (\text{B.7})$$

The $\kappa_n|_{n=0}$ which is proportional ΔT is

$$\kappa_n|_{n=0} = \frac{\sigma^2}{2} \left(1 - \frac{2}{N} \right) + \frac{1}{N} \frac{\sigma^2}{2} \sum_{k=0}^{N-1} \cos \left(4\omega_e t \sin \frac{\pi k}{N} \right). \quad (\text{B.8})$$

The (B.8) can be represented following form

$$\begin{aligned} \kappa_n|_{n=0} &= \frac{\sigma^2}{2} \left(1 - \frac{1}{N} \right) \left(1 - \frac{1}{N-1} \right) \\ &+ \frac{1}{N} \frac{\sigma^2}{2} \left(1 - \frac{1}{N} \right) \left(1 + \frac{1}{N-1} \right) \sum_{k=0}^{N-1} \cos \left(4\omega_e t \sin \frac{\pi k}{N} \right). \end{aligned} \quad (\text{B.9})$$

Appendix C. The formula for the sum of cosines of multiple angles

Let us demonstrate that the sum of the multiple angles of the cosine can be represented by the following form:

$$\frac{1}{N} \sum_{k=0}^{N-1} \cos \left(p \frac{2\pi k}{N} \right) = \delta_p^N. \quad (\text{C.1})$$

The sum of cosines of multiple angles can be calculated as a sum of exponentials, which is calculated as the sum of the geometric progression:

$$\frac{1}{N} \sum_{k=0}^{N-1} \cos k\phi = \operatorname{Re} \sum_{k=0}^{N-1} e^{ik\phi} = \operatorname{Re} \left(\frac{e^{iN\phi} - 1}{e^{i\phi} - 1} \right). \quad (\text{C.2})$$

Substitution $k = \pi k/N$ and the calculation of the real part (C.2) gives us the following representation:

$$\frac{1}{N} \sum_{k=0}^{N-1} \cos \left(p \frac{2\pi k}{N} \right) = \frac{\sin(2\pi p)}{2N} \operatorname{ctg} \frac{\pi p}{N} + \frac{\sin^2(\pi p)}{N}. \quad (\text{C.3})$$

For all p , except p divisible by N , the expression (C.3) is equal to 1, and for p divisible by N , the value of the expression is equal to 0.

Appendix D. Asymptotics for the Bessel functions

An asymptotic for the Bessel functions of large orders μ and arbitrary argument x is represented by the series 9.3.35 from [41]. The first term of this expression can be represented as the following composition:

$$J_\mu(x) \simeq \left(\frac{4\zeta}{1-\xi^2} \right)^{1/4} \frac{\operatorname{Ai}(\mu^{2/3}\zeta)}{\mu^{1/3}}, \quad \mu \rightarrow \infty, \quad (\text{D.1})$$

where

$$\xi = \frac{x}{\mu}$$

$$\zeta = \begin{cases} \left(\frac{3}{2}\right)^{2/3} \left[\ln \left(\frac{1+\sqrt{1-\xi^2}}{\xi} \right) - \sqrt{1-\xi^2} \right]^{2/3}, & \text{if } 0 \leq \xi \leq 1; \\ -\left(\frac{3}{2}\right)^{2/3} \left[\sqrt{\xi^2-1} - \operatorname{arcsec} \xi \right]^{2/3}, & \text{if } \xi \geq 1, \end{cases}$$

and Ai is the Airy function [41].

In the case of the $\xi \rightarrow 1$, the representation (D.1) is reduced to the following one:

$$J_\mu(x) \approx \left(\frac{2}{\mu} \right)^{1/3} \operatorname{Ai} \left(2^{1/3} \mu^{2/3} (1-\xi) \right), \quad (\text{D.2})$$

where the approximation $\zeta \approx 2^{1/3}(\xi - 1)$ is used. The (D.2) is equivalent to representation (24), considered before.

Appendix E. Relative duration of the thermal echo

Let us denote by $\{x_i\}$ the set of points in which the Bessel function $J_\mu(x)$ has local maxima (x_1 is the first local maximum, x_2 is the second, etc). The approximate values of x_i are found from the condition that the argument of the Airy function in the expression (24) is equal to the values $-z_i$ (29):

$$x_i \approx \mu + z_i \left(\frac{\mu}{2} \right)^{1/3}, \quad J_\mu(x_i) \approx \left(\frac{\mu}{2} \right)^{-1/3} \operatorname{Ai}(-z_i). \quad (\text{E.1})$$

The value of the asymptotic period of the Bessel function is 2π as seen from the formula (26). Then the expression for the duration of the thermal echo becomes:

$$w_i \stackrel{\text{def}}{=} \frac{x_{i+1} - x_i}{2\pi} \approx \frac{z_{i+1} - z_i}{2\pi} \left(\frac{\mu}{2} \right)^{1/3}. \quad (\text{E.2})$$

ORCID iDs

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

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