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On the kinetic temperature of a one-dimensional crystal on the long-time scale

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ABSTRACT

We investigate the dynamics of the kinetic temperature of a finite one-dimensional harmonic chain, the evolution of which is initiated by a thermal shock. We demonstrate that the kinetic temperature returns arbitrarily close to its initial state (the one immediately following the thermal shock) infinitely many times, and we give an estimate for the time elapsed until the recurrence. This assertion is closely related to the Poincare recurrence theorem and we discuss their relation. To estimate the recurrence time we use its averaging along system's trajectory and provide a rigorous mathematical definition of the mean recurrence time. It turns out that the mean recurrence time exponentially increases with the number of particles in the chain. A connection is established between this problem and the local theorems of large deviations theory.

Previous studies have shown that in such a one-dimensional harmonic chain, at times of order N, a thermal echo phenomenon is observed — a sharp increase in the amplitude of kinetic temperature fluctuations. In the present work, we give a rigorous mathematical formulation to this phenomenon and estimate the amplitude of the fluctuations.

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1. Introduction

The study of certain properties of low-dimensional systems with simple interaction potentials can sometimes yield unexpected results. For instance, it is well known that heat propagates on a macro scale in accordance with Fourier's law. However, experimental research on nanowires and nanotubes shows a dependency of the thermal conductivity coefficient on the length of the sample [1–4], which contradicts Fourier's law. Theoretical research on ultra-pure materials demonstrates a ballistic character of heat propagation [5–7].

In addition to the violation of Fourier's law in ultra-pure materials, the existence of thermal waves [8], anisotropy of the thermal profile [9], non-monotonic damping of the sinusoidal temperature profile [10], and the phenomenon of ballistic resonance [11] can be observed.

For analytical research, the model of a one-dimensional harmonic crystal is often used as the simplest model of a solid body. In the works of A.M. Krivtsov [12,13], thermal processes in one-dimensional crystals were studied by analyzing the equations

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of dynamics of velocity covariances. The covariance approach generalizes classical concepts of kinetic and potential energy by introducing generalized energies, proportional to particle velocity covariances and deformation covariances of interparticle bonds. According to this approach, instead of one specific system, one must consider an ensemble of crystalline systems with identical statistical characteristics at the initial moment in time. The kinetic temperature of the crystal is the average over an ensemble of such systems.

The dynamics of kinetic temperature in a crystal are described by equations analogous to those describing the oscillations of a particle displaced from equilibrium at the initial moment in time in the same crystal. Due to this mechanical analogy and Poincaré's recurrence theorem, it can be claimed that there are infinitely many moments of kinetic temperature returning to a value arbitrarily close to its initial value in the system. The main result of the present paper is the rigorous derivation of lower and upper bounds for the average time of such a return. A consequence of our estimates is that the average time of the kinetic temperature return grows exponentially fast with the increase in the number of particles. In proving our statements, we use results from ergodic theory and large deviation theory. The problem of the mean recurrence time of a harmonic crystal close to its initial position was first considered in the work by Kac [14]. We use some of his ideas in the present work.

W. Hoover in his work [15] notes that although there are quite a few alternative definitions of temperature (kinetic, configurational, Langevin, etc.), in a state of equilibrium all these definitions of temperature are equivalent, and there is no ambiguity in the concept of temperature. Far from equilibrium, each of these temperatures differs from the others. However, besides the fact that the expression for kinetic temperature is simpler than the aforementioned definitions of temperature, it is proportional to one of the conserved quantities: energy. This partly explains the choice of kinetic temperature as the energetic characteristic of the system we study.

In the present work, we also study the effect of thermal echo specific to a one-dimensional harmonic crystal [16]. A thermal echo represents a quasi-periodic increase in the amplitude of kinetic temperature oscillations during a thermal transition process. Such a thermal process can be initiated by a thermal shock at the initial moment in time, where all the velocities of the particles in a one-dimensional crystal have random values, and the displacements of the particles are zero. Each new iteration of the thermal echo is realized through equal intervals of time, but the amplitude profile of the kinetic temperature oscillations around the thermal echo differs from the amplitude profiles of the kinetic temperature of neighboring temporal implementations of the thermal echo. Let us denote the number of particles in the system as N. In mathematical language, the thermal echo effect is expressed by the fact that the asymptotics for large N of the kinetic temperature fluctuations from the equilibrium state at times of order N has jumps of size $N^{-1/6}$ at moments multiple to the quasi-period. The latter statement will be rigorously proven in this work.

An alternative approach to studying the thermal properties of a harmonic crystal is based on a model of the crystal's interaction with an external reservoir. It first appeared in the 1940s in the works of Bogoliubov [17] and subsequently was actively studied by many authors. We note the classic works on studying Fourier's law and the propagation of heat in a crystal [5,18], and papers dedicated to convergence to thermal equilibrium [19–21].

Thus, the results of our study consist of the formulation and proof of two main theorems and numerical analyses of the dynamics of the kinetic temperature in one-dimensional crystal systems. The first theorem gives an asymptotic estimate of the amplitude of the kinetic temperature (see (8)). Theorem 2 specifies the upper and lower limits in which the mean return time lies (see (14)). Numerical results (see Table 1 and see graph in Fig. 3) extend the analytical study. We demonstrate that our theoretical conclusions that the return time grows exponentially with increasing particle number are qualitatively correct.

The paper is organized as follows. In Section 2 (''Thermal Echo''), we introduce the mathematical model and describe the phenomenon of thermal echo. In Section 3 (''Mean Recurrence Time''), we precisely define the mean recurrence time of the kinetic temperature and formulate theorems concerning its upper and lower bounds. Section 4 (''Numerical Simulation'') presents the results of computer modeling. In Section 5 (''Conclusion''), we provide final conclusions and share thoughts about further investigation. In Appendix A, we present the proof of Theorem 1 (on thermal echo), while Appendix B contains the proof of Theorem 2 (on mean recurrence time). In the final section, ''Auxiliary Lemmas'', we prove technical lemmas.

2. Thermal echo

We consider a model of a one-dimensional harmonic crystal consisting of N particles, described by a system of ordinary differential equations:

$$\dot{v}_n = \omega^2(u_{n-1} - 2u_n + u_{n+1}), \qquad v_n = \dot{u}_n \tag{1}$$

where u_n, v_n represent the displacement and velocity of the n^{th} particle, respectively. The elementary frequency $\omega = \sqrt{C/m}$, where C represents the stiffness of interparticle bonds, and m is the mass of the particle. The dot above the symbol denotes a derivative with respect to time, and $n = 1, \dots, N$. The system follows periodic boundary conditions:

$$u_n = u_{n+N}. \tag{2}$$

The initial conditions correspond to a thermal shock:

$$u_n(0) = 0, \quad v_n(0) = \sigma\xi_n, \tag{3}$$

where ξ_n are independent random variables with zero mean and unit variance, and σ^2 represents the variance of the initial velocities.

We introduce the kinetic temperature T as a measure of the kinetic energy of the system:

$$T = \frac{m}{k_B}\frac{1}{N}\sum_{k=1}^{N}\langle \tilde{v}_k^2\rangle, \tag{4}$$

where k_B denotes the Boltzmann constant, $\langle\cdot\rangle$ represents the mathematical expectation, and $\tilde{v}_n = v_n - \bar{v}$, where $\bar{v}$ is the average velocity defined as $\bar{v} = \frac{1}{N}\sum_{n=1}^{N} v_n$.

The kinetic temperature is related to the kinetic energy by the equation:

$$T = \frac{2}{N k_B}\left(\langle E_K\rangle - \frac{m\sigma^2}{2}\right),$$

where E_K is the kinetic energy defined as $E_K = \sum_{j=1}^{N}\frac{mv_j^2}{2}$.

This model is introduced and studied in works [8,12,13,22]. In particular, the temperature is given by the following expression:

$$T(t) = T_E\left(1 - \frac{1}{N} + \frac{1}{N}\sum_{k=1}^{N-1}\cos\left(4\omega t\sin\frac{\pi k}{N}\right)\right), \tag{5}$$

$$T_E = \frac{1}{2}\frac{m}{k_B}\sigma^2,$$

where T_E represents the equilibrium temperature.

The phenomenon of thermal echo is introduced and studied in the work [16]. Thermal echo is observed on time scales of the order of N for sufficiently large N and mathematically follows from Theorem 1. To formulate it, we consider the relative fluctuation of temperature from the equilibrium state as:

$$\delta(t) = \frac{T(t) - T_E}{T_E},$$

and define the quasiperiod as:

$$t_N \overset{\text{def}}{=} \frac{N}{2\omega}.$$

Theorem 1 (*Thermal Echo Theorem*). *In the limit $N \to \infty$, for any integer number $k \geqslant 0$ and all $x \in (0,1)$, the following asymptotic relations hold:*

$$\delta((k+x)t_N) \sim \frac{b_k^{(N)}(x)}{\sqrt{N}}, \tag{6}$$

$$\delta((k+1)t_N) \sim \frac{a(k)}{\sqrt[3]{N}}, \tag{7}$$

where the bounded functions are introduced:

$$a(k) = \frac{1}{\sqrt[3]{k+1}}\frac{\Gamma\left(\frac{1}{3}\right)}{2\pi\cdot\sqrt[6]{3}} \sim \frac{0.355}{\sqrt[3]{k}},\ \ k > 0,$$

$$b_k^{(N)}(x) = \sqrt{\frac{2}{\pi}}\left[\frac{1}{\sqrt{k+x}}\cos\left(2(k+x)N - \frac{\pi}{4}\right) + 2\sum_{p=1}^{k}\frac{1}{\sqrt[4]{x_p^2-1}}\cos\left(2pNg(x_p) + \frac{\pi}{4}\right)\right],$$

$$g(x) = \arccos\frac{1}{x} - \sqrt{x^2-1}, \quad x_p = \frac{k+x}{p} > 1.$$

If $k = 0$, then the sum in the expression for $b_k^{(N)}(x)$ is absent. Furthermore, the following inequality holds:

$$|b_k^{(N)}(x)| \leqslant c_1 + c_2 k + c_3\sqrt[4]{\frac{k}{x}}, \tag{8}$$

$$c_1 = 3.6, \qquad c_2 = 2.8, \qquad c_3 = 1.4,$$

for all N, x, and $k \geqslant 1$. The symbol $\sim$ denotes the asymptotic equivalence of two functions according to the definitions in the book [23].

Referring to the book [23] we can express the asymptotic equalities (6)–(7) using o-notations as follows:

$$\delta((k+x)t_N) = \frac{b_k^{(N)}(x)}{\sqrt{N}} + \bar{\bar{o}}\left(\frac{1}{\sqrt{N}}\right), \tag{9}$$

$$\delta((k+1)t_N) = \frac{a(k)}{\sqrt[3]{N}} + \bar{\bar{o}}\left(\frac{1}{\sqrt[3]{N}}\right), \tag{10}$$

as $N \to \infty$.

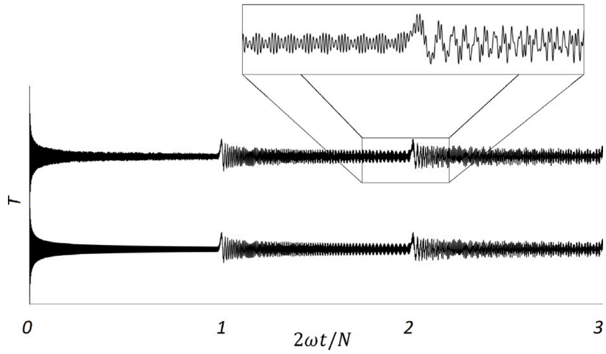

Fig. 1. Fluctuations of the kinetic temperature T in a finite crystal. Numerical (top) and analytical (bottom) solutions. Averaging is performed using 100 numerical experiments. The number of particles is $N = 10^3$, t is time, and ω is the elementary frequency.

From this theorem, it follows that at times that are multiples of the quasiperiod, fluctuations exhibit jumps of the order of $N^{-1/6}$. This is the thermal echo effect. Fig. 1 shows a comparison of the analytical solution (bottom) and computer simulation of the dynamics of crystal particles (top). The considered crystal contains 10^3 particles. The analytical solution is described by the formula (5). The computer simulation performs the central difference method to numerically solve a system of 10^3 differential equations of crystal chain dynamics (1) with an integration step of $0.02/\omega$. The final result is obtained by averaging over 100 realizations and all particles of identical crystal chains.

It can be seen that the fluctuations of the kinetic temperature decrease with increasing N [16], meaning that on time scales of the order of N, the fluctuations tend to zero. Studying the harmonic crystal on time scales of the order of N is equivalent to studying the hydrodynamic limit of the corresponding particle system. The hydrodynamic limit in the purely deterministic case for a one-dimensional harmonic crystal has been investigated in works [24,25]. More precisely, the mentioned works derive the hydrodynamic Euler equations under suitable scaling of initial conditions and the frequency ω, but it can be easily shown that this is equivalent to the transition to the hydrodynamic limit.

Due to Poincaré's recurrence theorem and the invertibility of the system, at some point in time, the fluctuations of the kinetic temperature must return sufficiently close to their initial value $\delta(0) = 1 - \frac{2}{N}$. However, it is not necessary that this return occurs at the moment of realization of the next thermal echo. Furthermore, we will estimate the time of return and show that it is of exponentially large order in N. The return to the initial position can be easily established without referring to Poincaré's theorem, simply by using the explicit formula (5).

3. Mean recurrence time

Let us consider the function

$$h(t) = \frac{1}{N-1}\sum_{k=1}^{N-1}\cos\left(4\omega t \sin\frac{\pi k}{N}\right) \tag{11}$$

The function h is related to the relative fluctuation of the kinetic temperature $\delta(t)$ as follows:

$$\delta(t) = -\frac{1}{N} + \frac{N-1}{N}h(t)$$

At the initial time $h(0) = 1$. We define the time when the function h returns to values close to its initial value. Let us fix some $x > 0$ and divide the entire time axis into two sets:

$$A = A(x) = \{p \geqslant 0 : h(p) > x\}, \qquad A' = \{p \geqslant 0 : h(p) \leqslant x\}.$$

Next, we consider the consecutive moments of transition from one set to the other:

$$0 < t_1 < s_1 < t_2 < s_2 < \cdots, \tag{12}$$

where t_k represents the moment of transition from A to A', and S_k represents the moment of transition from A' to A (see Fig. 2).

We define the mean recurrence time to set A by the formula:

$$\tau(x) \stackrel{\text{def}}{=} \lim_{L\to\infty}\frac{1}{L}\sum_{k=1}^{L}(s_k - t_k) \tag{13}$$

Theorem 2 (*Mean Recurrence Time*). *For all $x \in (0,1)$, the limit in (13) exists, and for $N \geqslant 7$, the following estimate holds:*

$$r_N(x)\frac{b_1^N(x)}{\omega} < \tau(x) < \frac{b_2^N(x)}{\omega} \tag{14}$$

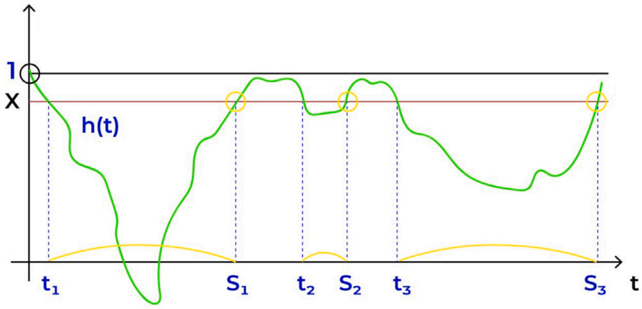

Fig. 2. Schematic representation of the evolution of kinetic temperature at long times. t_k represents the moment of transition of the kinetic temperature from A to A', and S_k represents the moment of transition from A' to A.

where the following functions are introduced:

$$b_1(x) \overset{def}{=} \frac{\alpha_1}{\sqrt[4]{1-x}}, \qquad \alpha_1 \overset{def}{=} \sqrt{\frac{2}{\sqrt{\pi e}}} \approx 0.83$$

$$b_2(x) \overset{def}{=} \frac{\alpha_2}{\sqrt[4]{1-x}}, \qquad \alpha_2 \overset{def}{=} \sqrt{\frac{\pi}{\sqrt{2}}} \approx 1.49$$

$$r_N(x) \overset{def}{=} \frac{(1-x)^{\frac{7}{2}} x^2}{N^{\frac{3}{2}}} \cdot 10^{-9}.$$

The theorem shows that the mean recurrence time of the kinetic temperature exponentially increases with the number of particles in the system N. Indeed, for x close to 1, the values of functions b_1 and b_2 are greater than 1, and the remainder term r_N is of the order of $N^{-3/2}$, significantly smaller in comparison to $b_1^N(x)$.

Note that the lower estimate for $\tau(x)$ is nontrivial (i.e., the value on the left is greater than 1) for sufficiently large N and $x > 1 - \frac{4}{\pi e} \approx 0.53$. For example, for $\omega = 3 \cdot 10^{14}$ s^{-1} (we assume time unit is second) [16], for $x = 0.9999$ and $N = 50$, the lower estimate gives a mean recurrence time $\tau(x)$ of about 10^7 seconds.

In the work by Kac [14], the mean recurrence time of the entire harmonic crystal system to the vicinity of the initial position is studied. Using his ideas and results, we obtain the upper estimate in Theorem 2 for the recurrence time.

From Theorem 2, it follows that

$$\ln b_1(x) \leqslant \liminf_{N\to\infty} \frac{\ln(\tau(x))}{N} \leqslant \limsup_{N\to\infty} \frac{\ln(\tau(x))}{N} \leqslant \ln b_2(x)$$

Using more sophisticated methods in the proof, it can be shown that for all $x > 0.5$, the following limit exists:

$$\lim_{N\to\infty} \frac{\ln(\tau(x))}{N} = I(x),$$

where $I(x)$ is a smooth function called the action functional. More details on how to improve the results see the end of Appendix B.

From Theorem 2, it follows that

$$I(x) \sim -\frac{1}{4}\ln(1-x)$$

as $x \to 1$.

If we define the mean recurrence time differently, for example, as:

$$\hat{\tau}(x) = \lim_{k\to\infty} \frac{S_k}{k},$$

it can be similarly proved that $\hat{\tau}(x)$ exponentially increases with increasing N.

4. Numerical simulation

In this section, we present the results of numerical simulation of the dynamics of kinetic temperature in finite harmonic crystals. Three experiments were conducted for crystals containing 7, 10, and 13 particles. In the computer simulation, the analytical solution of the relative temperature fluctuation (11) was computed with a time discretization step of $\frac{1}{500\omega}$. The number of numerical steps was 2^{42}. In each experiment, the number of system returns $h(t) \geq x$ was calculated for three different levels: $x = 0.99$, $x = 0.999$, and $x = 0.9999$. From the table, it can be seen that as the number of particles increases, the number of returns within a fixed time interval exponentially decreases, while the mean recurrence time and the standard deviation exponentially increase.

Table 1
Results of numerical experiments. Table displays numerical results for the dynamics of kinetic temperature in harmonic crystals with 7, 10, and 13 particles. It shows the number of returns, mean recurrence time, and standard deviation for three levels of x.

Level x	Number of returns	Mean recurrence time ωt	Standard deviation
Number of particles in the crystal: 7			
0.99	98,339	335.13	485.12
0.999	12,737	2,523.00	2,792.96
0.9999	722	41,921.45	27,085.77
Number of particles in the crystal: 10			
0.99	4,124	7,187.19	11,153.59
0.999	189	155,981.86	103,893.16
0.9999	3	10,386,721.06	8,189,677.18
Number of particles in the crystal: 13			
0.99	57	455,021.73	446,265.25
0.999	1		
0.9999	1		

It can be observed that the standard deviation and the mean recurrence time are of the same order of magnitude, indicating that the recurrence time values deviate significantly from the mean value.

Fig. 3 contains graphs constructed based on calculations performed with data that is more extensive compared to what is presented in the table. The graphs allow for a more vivid demonstration of the dependence of the number of returns, the mean return time, and the standard deviation of the mean return time on levels of x.

According to Theorem 2, applied to the parameters from Table 1, we obtain an estimate of the recurrence time that approaches zero from below and significantly exceeds this value from above compared to the data obtained in the numerical experiments. Such a discrepancy may be caused by the roughness of the upper estimate, which was calculated based on the assumption of the entire system returning to a state close to the initial state, rather than just the return of the kinetic temperature.

In the course of the simulations, it has been found that the computation of the recurrence time in systems encompassing a more substantial quantity of particles necessitates an exponential augmentation in computational duration. This observation retrospectively justifies the selection of the particle count employed in the modeling. In the current computational analyses, we examine the period requisite for the system's return to a state where the kinetic temperature deviates by less than 1% from its initial value. Such a threshold is sufficiently substantial to observe a notable quantity of returns, particularly in systems comprising a lesser number of particles. Concurrently, it is relatively small to ensure that the observable differences in the system's dynamics post-return are negligibly insignificant.

At the same time, the analytical results for the lower estimate of the recurrence time are of particular value. For a small number of particles in the system, this value is close to zero, but it exponentially increases as the number of particles increases. For $x = 0.99$, the expression for the lower estimate of the dimensionless recurrence time $r_N(x)b_1^N(x)$ only becomes greater than one for $N > 44$.

5. Conclusion

The present paper investigates the dynamics of kinetic temperature in a one-dimensional harmonic crystal. It builds upon previous studies dedicated to exploring the phenomenon of thermal echo. The main focus of this paper is on the investigation of the average interval between the recurrence times of the kinetic temperature to its initial value, known as the mean recurrence time.

Analytical and numerical methods have been employed to study the recurrence time and its relation to the size of the crystal. Theorems describing the properties of the recurrence time have been presented, and numerical simulations have been conducted to confirm the theoretical findings.

The main result of this research lies is the rigorous proof that the mean recurrence time exponentially increases with the number of particles in the crystal. This observation holds fundamental significance for a deeper understanding of the dynamics of crystalline systems and can find broad applications in various fields related to heat transfer and thermal processes.

Further investigations can be directed towards extending the model and considering various factors that influence the dynamics of kinetic temperature, such as nonlinearities or quantum–mechanical aspects. The studies referenced in [11] and [26] indicate that in the regime of weak nonlinearity, the harmonic theory remains effectively applicable over short time scales. The impact of pronounced nonlinearity remains unexplored; however, it can be conjectured that the findings regarding the average return time are likely to retain their validity. It is anticipated that the average return time will continue to increase exponentially with the number of particles, with the primary variation being in the exponent of this growth. The analytical results for the upper bound estimation of the mean recurrence time have been found to be overestimated compared to the results of numerical simulations. Therefore, the search for more accurate analytical estimations is also of interest for future research. Particularly, finding the function $I(x)$, introduced above. Additional research could focus on estimating the standard deviation of the recurrence time.

This study contributes to the understanding of the thermal echo phenomenon in harmonic crystals and the dynamics of kinetic temperature. The research findings can be valuable for various applications related to heat transfer and crystalline systems and can stimulate further research in this field.

CRediT authorship contribution statement

A.A. Lykov: Writing – review & editing, Writing – original draft, Formal analysis, Conceptualization. **A.S. Murachev:** Writing – review & editing, Writing – original draft, Visualization, Software, Investigation, Conceptualization.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Data availability

No data was used for the research described in the article.

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Appendix A. Proof of Theorem 1 on thermal echo

For all real z, the equality is valid [27]:

$$\frac{1}{N}\sum_{k=0}^{N-1}\cos(z\sin\frac{\pi k}{N}) = J_0(z) + 2\sum_{p=1}^{\infty} J_{2pN}(z),$$

where $J_n(z)$ is the Bessel function of the first kind.

Due to this equality and the formula (5) we can write

$$\delta(t) = -\frac{1}{N} + \sum_{p=0}^{\infty}\alpha_p J_{2pN}(4\omega t),$$

where we introduced the notation:

$$\alpha_p = \begin{cases} 1, & p = 0, \\ 2, & p > 0. \end{cases}$$

First, Let us prove formula (6). Let us split the sum for $\delta((k+x)t_N)$ into two terms

$$\delta((k+x)t_N) = \sum_{p=0}^{k}\alpha_p J_{2pN}(2(k+x)N) + \sum_{p=k+1}^{+\infty}\alpha_p J_{2pN}(2(k+x)N) - \frac{1}{N} = S_1 + S_2 - \frac{1}{N}. \tag{A.1}$$

Let us estimate the first sum, using the first two statements of Lemma 1:

$$S_1 = \sum_{p=0}^{k}\alpha_p J_{2pN}(2(k+x)N) = J_0(2(k+x)N) + 2\sum_{p=1}^{k} J_{2pN}(2pNx_p), \quad \text{where } x_p = \frac{k+x}{p}.$$

For $N\to\infty$ we have the following approximation:

$$S_1 = \frac{1}{\sqrt{N}}\left[\sqrt{\frac{2}{\pi(k+x)}}\cos\left(2(k+x)N - \frac{\pi}{4}\right) + 2\sum_{p=1}^{k}\sqrt{\frac{2}{\pi\sqrt{x_p^2-1}}}\cos\left(2pNg(x_p) + \frac{\pi}{4}\right)\right] + O\left(\frac{1}{N}\right)$$

Let us estimate the second sum in (A.1), relying on the fourth inequality of Lemma 1:

$$|S_2| = \left|\sum_{p=k+1}^{+\infty}\alpha_p J_{2pN}(2(k+x)N)\right| = \left|\sum_{p=k+1}^{+\infty}\alpha_p J_{2pN}(2pNx_p)\right| \leqslant 2\sum_{p=k+1}^{\infty}\frac{e^{-2pNf(x_p)}}{(1-x_p^2)^{\frac14}\sqrt{2\pi 2pN}} \leqslant \frac{1}{(1-x_{k+1}^2)^{\frac14}\sqrt{kN}}\sum_{p=k+1}^{\infty} e^{-2pNf(x_{k+1})}$$
$$= \frac{1}{(1-x_{k+1}^2)^{\frac14}\sqrt{kN}}\frac{e^{-2(k+1)Nf(x_{k+1})}}{1-e^{-2Nf(x_{k+1})}} = O\left(q^{-N}\right), \quad \text{where } x_p = \frac{k+x}{p}.$$

for some $q > 1$. Thus, the second statement is proven. The formula (7) is checked similarly using the third item of Lemma 1.

Next, Let us prove inequality (8) for $b_k^{(N)}(x)$. We have estimates:

$$|b_k^{(N)}(x)| \leqslant \sqrt{\frac{2}{\pi}}\left(\frac{1}{\sqrt{k+x}} + 2\sum_{p=1}^{k}\frac{1}{\sqrt[4]{(\frac{k+x}{p})^2-1}}\right) \leqslant \sqrt{\frac{2}{\pi}}(1+2A),$$

where we denoted the sum by A. Let us continue estimating A:

$$A \stackrel{\text{def}}{=} \sum_{p=1}^{k} \frac{1}{\sqrt[4]{(\frac{k+x}{p})^2 - 1}} = \sum_{p=1}^{k} \sqrt[4]{\frac{p^2}{(k+x)^2 - p^2}} = \sum_{p=1}^{k-1} \sqrt[4]{\frac{p^2}{(k+x)^2 - p^2}} + \sqrt[4]{\frac{k^2}{(k+x)^2 - k^2}} = A_1 + A_2.$$

For A_1 from previous equation we have inequalities:

$$A_1 = \sum_{p=1}^{k-1} \sqrt[4]{\frac{p^2}{(k+x)^2 - p^2}} \leqslant \int_1^k \sqrt[4]{\frac{u^2}{(k+x)^2 - u^2}} du \leqslant \int_0^{k+x} \sqrt[4]{\frac{u^2}{(k+x)^2 - u^2}} du = (k+x) \int_0^1 \sqrt[4]{\frac{v^2}{1 - v^2}} dv = (k+x)\beta.$$

Let us calculate β :

$$\beta = \int_0^1 \sqrt[4]{\frac{v^2}{1 - v^2}} dv = \frac{1}{2} \int_0^1 y^{-1/4}(1-y)^{-1/4} dy = \frac{1}{2} B\left(\frac{3}{4}, \frac{3}{4}\right),$$

where B denotes the beta function. Using known properties of the beta function, we get:

$$\beta = \frac{1}{2} \frac{(\Gamma\left(\frac{3}{4}\right))^2}{\Gamma\left(\frac{3}{2}\right)} = \frac{2\pi^2}{\frac{1}{2}\sqrt{\pi}(\Gamma\left(\frac{1}{4}\right))^2} = \frac{4\pi^{3/2}}{(\Gamma\left(\frac{1}{4}\right))^2}$$

Let us estimate A_2:

$$A_2 = \sqrt[4]{\frac{k^2}{(k+x)^2 - k^2}} = \sqrt[4]{\frac{1}{(1+\frac{x}{k})^2 - 1}} = \sqrt[4]{\frac{1}{\frac{x}{k}\left(2 + \frac{x}{k}\right)}} \leqslant \sqrt[4]{\frac{k}{x}} \sqrt[4]{\frac{1}{2}}.$$

Finally, we obtain inequalities:

$$|b_k^{(N)}(x)| \leqslant \sqrt{\frac{2}{\pi}} \left(1 + 2\beta(k+1) + 2\sqrt[4]{\frac{1}{2}}\sqrt[4]{\frac{k}{x}}\right)$$
$$\leqslant c_1 + c_2 k + c_3 \sqrt[4]{\frac{k}{x}},$$

where

$$c_1 = 3.6, \quad c_2 = 2.8, \quad c_3 = 1.4.$$

The statement is thus fully proven.

Lemma 1. *The following statements are true for the Bessel function:*

1. *as* $x \to +\infty$
$$J_0(x) = \sqrt{\frac{2}{\pi x}} \cos\left(x - \frac{\pi}{4}\right) + O\left(\frac{1}{x}\right)$$
2. *as* $\nu \to +\infty,\ x > 1$
$$J_\nu(\nu x) = \sqrt{\frac{2}{\pi\nu\sqrt{x^2-1}}} \cos\left(\nu g(x) + \frac{\pi}{4}\right) + O\left(\frac{1}{\nu}\right)$$
where
$$g(x) = \arccos\frac{1}{x} - \sqrt{x^2 - 1}$$
3. *as* $\nu \to +\infty$
$$J_\nu(\nu) = \frac{\Gamma\left(\frac{1}{3}\right)}{2^{\frac{2}{3}}\pi \cdot \sqrt[6]{3}\nu^{\frac{1}{3}}} + O\left(\frac{1}{\nu^{\frac{2}{3}}}\right)$$
4. *for* $0 < x \leqslant 1$
$$|J_\nu(\nu x)| \leqslant \frac{e^{-\nu f(x)}}{(1-x^2)^{\frac{1}{4}}\sqrt{2\pi\nu}},$$
where function $f(x)$ *is a strictly decreasing function and* $f(1) = 0$.

Proof. All statements are well known and can be found in the book [27]. □

It should be noted that Bessel functions of the first kind often arise in harmonic crystal models. For example, in the paper by Klein and Prigogine [28], based on the solution obtained by Schrödinger [29], it was shown that in an infinite one-dimensional harmonic crystal with random initial conditions, the oscillations of kinetic and potential energy are described by the Bessel function of the first kind and zero order, and tend to equal equilibrium values.

In the works [30,31], the non-trivial properties of Bessel functions were required to prove the uniform boundedness of the solutions of the infinite harmonic crystal.

Appendix B. Proof of Theorem 2 on mean recurrence time

Let us outline the proof strategy. First, we will reduce the problem to computing the mean recurrence time in a subset $\hat{A}$ of a classical dynamical system, which is a shift on a torus. These shifts on the torus define a strongly ergodic dynamical system with an invariant Lebesgue measure. Therefore, we can use the Smoluchowski–Katz formula, which expresses the mean recurrence time (Lemma 3) in terms of the invariant measure. The upper bound follows almost immediately if we apply it to a set that is a rectangle on the torus contained in $\hat{A}$.

To obtain the lower bound, we reduce the problem to estimating the density of the sum of independent identically distributed random variables in the domain of large deviations. Local theorems for large deviations has been known since the 1950s [32,33] and is well described, for example, in the book [34]. However, the mentioned sources have restrictions on the random variables that do not hold in our case. It is also quite difficult to extract all the necessary constants from those works. Therefore, we had to reprove some local theorems of large deviations, relying on techniques and ideas from [32–34].

Let us proceed with a detailed proof.

Without loss of generality, we can assume that N is an odd number given by $N = 2n + 1$. From the condition $N \geqslant 7$, it follows that $n \geqslant 3$. Let us rewrite the formula for $h(t)$ as follows:

$$h(t) = \frac{1}{n}\sum_{k=1}^{n}\cos\left(4\omega t \sin\frac{\pi k}{2n+1}\right) = \frac{1}{n}\sum_{k=1}^{n}\cos\left(t\omega_k\right),$$

where we introduced the notation

$$\omega_k = 4\omega \sin\frac{\pi k}{2n+1},\ \ k = 1,\dots,n.$$

Consider the n-dimensional torus

$$T_n = \{(\varphi_1,\dots,\varphi_n):\ \ \varphi_k \in [0,2\pi]\}$$

and the shifts on it

$$g^t(\varphi_1,\dots,\varphi_n) = (\varphi_1+\omega_1 t,\dots,\varphi_n+\omega_n t),\quad t \geqslant 0,$$

where addition is taken modulo 2π. Then the following obvious equality holds:

$$h(t) = H(g^t(\bar{0})),\ \ \bar{0} = (0,0,\dots,0) \in T_n,$$

$$H(\varphi_1,\dots,\varphi_n) = \frac{1}{n}\sum_{k=1}^{n}\cos(\varphi_k)$$

The Lindemann–Weierstrass theorem implies that the numbers $\omega_1,\dots,\omega_n$ are linearly independent over the rationals. Thus, the flow g^t is strong ergodic [35] with the invariant measure μ given by:

$$\mu(B) = \left(\frac{1}{2\pi}\right)^n |B|,$$

where $|\cdot|$ denotes the Lebesgue measure of a set $B \subset T_n$. Clearly, $t \in A(x)$ if and only if

$$g^t(\bar{0}) \in \hat{A}(x) = \{\bar{\varphi} \in T_n:\ \ H(\bar{\varphi}) > x\}$$

Hence, the time $\tau(x)$ is the mean recurrence time of the trajectory of the flow g^t to the set $\hat{A}(x)$ and therefore, due to strong ergodicity, $\tau(x)$ is well-defined. For a set $B \subset T_n$, let τ_B be the mean recurrence time to B, defined in a similar manner, if it exists. Then

$$\tau(x) = \tau_{\hat{A}(x)}.$$

Next, using this representation, we will estimate $\tau(x)$.

Notice that if $\cos\varphi_k \geqslant x$ for all $k = 1,\dots,n$, then $(\varphi_1,\dots,\varphi_n) \in A(x)$. Therefore,

$$\tau(x) \leqslant \tau_I,$$

where $I = \{(\varphi_1,\dots,\varphi_n) \in T_n:\ \cos\varphi_k \geqslant x\}$. From the paper [36], we easily obtain the following formula:

$$\tau_I = \frac{2\pi}{\Delta}\frac{\Delta^{n-1}-1}{\sum_{k=1}^{n}\omega_k},\quad \Delta = \frac{\pi}{\arccos(x)}.$$

Hence, we have the estimate:

$$\tau_I \leqslant \frac{\pi}{2\omega} \frac{1}{\sum_{k=1}^{n} \sin \frac{\pi k}{2n+1}} \Delta^n = \frac{\pi}{2\omega} \frac{1}{\frac{1}{2} \cot \frac{\pi}{2n+1}} \Delta^n \leqslant \frac{1}{\omega} \Delta^{N/2}.$$

It is easy to see that

$$\arccos(x) \geqslant \sqrt{2(1-x)}$$

for $x \in (0,1)$. Thus, the upper bound is established.

Let us prove the lower bound. We will use the Smoluchowski–Katz formula for the mean recurrence time (Lemma 3). This yields the equality:

$$\tau(x) = \lim_{\varepsilon \to 0+} \varepsilon \frac{1-\mu(\hat{A}(x))}{\mu(\hat{A}(x)^\varepsilon)} = \frac{1-\mu(\hat{A}(x))}{\pi_n(x)}, \tag{B.1}$$

where we define

$$\pi_n(x) = \lim_{\varepsilon \to 0+} \frac{1}{\varepsilon} \mu(\hat{A}(x)^\varepsilon) = \lim_{\varepsilon \to 0+} \frac{1}{\varepsilon} \int_{\varphi \in T_n:\ H(\varphi) \geqslant x,\ H(g^\varepsilon(\varphi)) < x} \mu(d\varphi).$$

Refer to Lemma 3 for the definition of $\hat{A}(x)^\varepsilon$.

First, let us estimate $\mu(\hat{A}(x))$. Suppose $U_1, \dots, U_n$ are independent random variables uniformly distributed on the interval $[0, 2\pi]$. Then,

$$\mu(\hat{A}(x)) = \mathrm{P}\left(\frac{1}{n} \sum_{k=1}^{n} \cos U_k \geqslant x \right),$$

where $\mathrm{P}(\cdot)$ denotes the probability of the corresponding event. By applying Hoeffding's inequality, we obtain the estimate:

$$\mathrm{P}\left(\frac{1}{n} \sum_{k=1}^{n} \cos U_k \geqslant x \right) \leqslant e^{-\frac{nx^2}{2}}.$$

Therefore, we have shown that

$$\tau(x) \geqslant \frac{1-e^{-\frac{nx^2}{2}}}{\pi_n(x)}.$$

Using simple calculus we obtain the bounds:

$$\tau(x) \geqslant \frac{1-e^{-\frac{n}{2}}}{\pi_n(x)} x^2 \geqslant \frac{1-e^{-\frac{3}{2}}}{\pi_n(x)} x^2 \tag{B.2}$$

Let us prove the following lemma:

Lemma 2. *The formula holds:*

$$\pi_n(x) = \left(\frac{1}{2\pi}\right)^n \int_{\varphi \in T_n:\ H(\varphi)=x} [(\bar{\omega}, \nu)]^+ d\sigma,$$

where $[x]^+ = \max\{x, 0\}$, $\bar{\omega} = (\omega_1, \dots, \omega_n)$, $(,)$ *is the Euclidean scalar product,* $d\sigma$ *is the standard volume element on the surface* $S(x) = \{\varphi \in T_n : H(\varphi) = x\}$, ν *is the unit normal vector to the surface* $S(x)$ *directed outward from* $A(x)$*:*

$$\nu = -\frac{1}{|\nabla H|} \nabla H.$$

Proof. The formula is obtained by covering the surface $S(x)$ with small neighborhoods and locally tracking the volume element on this surface. □

From Lemma 2, we obtain the representation:

$$\pi_n(x) = \left(\frac{1}{2\pi}\right)^n \int_{S(x)} [\bar{\omega}, -\nabla H]^+ \omega_H,$$

where $\omega_H = \frac{1}{|\nabla H|} d\sigma$ is the Gelfand–Leray differential form. Using the Cauchy–Bunyakovsky–Schwarz inequality, we obtain the estimate:

$$\pi_n(x) \leqslant \left(\frac{1}{2\pi}\right)^n |\bar{\omega}| \int_{S(x)} \omega_H \leqslant 4\omega\sqrt{n} \left(\frac{1}{2\pi}\right)^n \int_{S(x)} \omega_H.$$

Let $U_1, \dots, U_n$ be the random variables defined above. It is easy to see that the random variable

$$W_n = H(U) = \frac{1}{n} \sum_{k=1}^{n} \cos U_k \tag{B.3}$$

has density $p_{W_n}(\cdot)$ and

$$p_{W_n}(x) = \left(\frac{1}{2\pi}\right)^n \int_{S(x)} \omega_H.$$

Thus, we have proven the inequality:

$$\pi_n(x) \leqslant 4\omega\sqrt{n} p_{W_n}(x).$$

Hence, by Lemma 4, we conclude that

$$\pi_n(x) \leqslant 4\omega n^{\frac{3}{2}} \left(\frac{2\beta}{1-x}\right)^3 \left(\frac{\sqrt{1-x}}{\gamma}\right)^n.$$

The constants β and γ are defined in Lemma 4. Substituting this estimate into inequality (B.2), we obtain:

$$\tau(x) \geqslant \frac{1-e^{-\frac{3}{2}}}{4\omega n^{\frac{3}{2}} \left(\frac{2\beta}{1-x}\right)^3 \left(\frac{\sqrt{1-x}}{\gamma}\right)^n} x^2 \geqslant \frac{1}{\omega} \frac{1-e^{-\frac{3}{2}}}{4(2\beta)^3} \frac{(1-x)^3 x^2}{n^{\frac{3}{2}}} \left(\frac{\gamma}{\sqrt{1-x}}\right)^n \geqslant \frac{1}{\omega} \frac{1-e^{-\frac{3}{2}}}{4(2\beta)^3} \frac{(1-x)^3 x^2}{(N/2)^{\frac{3}{2}}} \left(\frac{\gamma}{\sqrt{1-x}}\right)^{N/2} \left(\frac{\gamma}{\sqrt{1-x}}\right)^{-1/2}$$

$$= \frac{1}{\omega}\theta \frac{(1-x)^{\frac{7}{2}} x^2}{N^{\frac{3}{2}}} \left(\frac{\alpha_1}{\sqrt[4]{1-x}}\right)^N,$$

where

$$\alpha_1 = \sqrt{\gamma}, \quad \theta = \frac{1-e^{-\frac{3}{2}}}{4(2\beta)^3} 2^{3/2} \frac{1}{\sqrt{\gamma}} > 10^{-9}.$$

Thus, the theorem is completely proven.

At the end of Appendix B, we provide a hint on improving the estimates for $\tau(x)$. The key idea involves employing a probability interpretation for the quantity π_n defined in Formula (B.1). Now we formulate it in more details. Let us consider random variables $(\xi_1, \dots, \xi_n) \in T_n$ with the joint density function

$$p_\xi(\varphi) = \frac{1}{Z}[\bar{\omega}, -\nabla H]^+ = \frac{1}{Z}\left[\frac{1}{n}\sum_{k=1}^n \omega_k \sin\varphi_k\right]^+,$$

where Z is the normalized factor defined by the condition:

$$\int_{T_n} p_\xi(\varphi) d\mu(\varphi) = 1.$$

Next introduce the random variable $\eta = H(\xi) = \frac{1}{n}\sum_{k=1}^n \cos\xi_k$. It is evident that η has a density function $p_\eta(x)$. From Lemma 2, follows the equality

$$\pi_n(x) = p_\eta(x) Z.$$

By the central limit theorem (Lyapunov's formulation), it follows that $Z \sim c/\sqrt{n}$ for some absolute constant $c > 0$, independent of n. Therefore, the estimation of the asymptotic for $\pi_n(x)$ is reduced to determining the asymptotic for $p_\eta(x)$. The asymptotic for $p_\eta(x)$ pertains to a local theorem for large deviation of dependent random variables $\xi_1, \dots, \xi_n$. We hypothesize that employing more advanced techniques in large deviation theory will result in an explicit asymptotic expression for $p_\eta(x)$.

Auxiliary lemmas

Lemma 3. *For an ergodic flow g^t, the Smoluchowski–Kac formula holds for the mean recurrence time τ_B to a set B:*

$$\tau_B = \lim_{\varepsilon\to 0+} \varepsilon \frac{1-\mu(B)}{\mu(B^\varepsilon)},$$

where μ is the normalized invariant measure of the flow, $B^\varepsilon = B \setminus (g^\varepsilon B)$ represents the points in B that leave B after the transformation g^ε.

Proof. This formula can be found in [36]. For the sake of completeness, we provide a proof for the case of an ergodic discrete-time dynamical system. Let T denote the corresponding transformation, and let μ be the invariant measure. We will use the notation introduced in (12) by replacing the set A with B. According to the ergodic theorem, we have:

$$\lim_{N\to\infty} \frac{N}{t_N} = \mu(\hat{B}),$$

where $\hat{B} = B \setminus (T(B))$ represents the points in B that leave B after the transformation T. Furthermore, due to the ergodic theorem, we have the relation:

$$\lim_{N\to\infty} \frac{1}{s_N} \sum_{k=1}^N (S_k - t_k) = \mu(B')$$

where B' denotes the complement of the set. We can then write:

$$\tau_B = \lim_{N\to\infty} \frac{1}{N}\sum_{k=1}^{N}(S_k - t_k) = \lim_{N\to\infty} \frac{s_N}{N}\frac{1}{s_N}\sum_{k=1}^{N}(S_k - t_k) = \frac{\mu(B')}{\mu(\hat{B})}.$$

We used the fact that

$$\lim_{N\to\infty} \frac{s_N - t_N}{N} = 0.$$

Thus, the Smoluchowski–Kac formula for discrete dynamical systems is established. The transition to continuous time is straightforward since our main dynamical system on the torus is smooth. □

Lemma 4. *Let $U_1, \dots, U_n$ be independent random variables uniformly distributed on the interval $[0, 2\pi]$. Consider the random variable:*

$$W_n = \frac{1}{n}\sum_{k=1}^{n}\cos U_k.$$

Then, for all $0 < x < 1$ and $n \geqslant 3$, the density p_{W_n} of the random variable W_n satisfies the following estimate:

$$p_{W_n}(x) \leqslant n\left(\frac{2\beta}{1-x}\right)^3\left(\frac{\sqrt{1-x}}{\gamma}\right)^n,$$

where

$$\beta = 95, \quad \gamma = \frac{2}{\sqrt{\pi e}}$$

Proof. This statement can be regarded as a local inequality of large deviations (see [32,33]). To prove the statement, we will use ideas from [32].

Consider the generating functions of the random variables W_n and $\cos U_1$:

$$M_n(z) = \mathrm{E}e^{zW_n} = \int_{\mathbb{R}} e^{zx}p_{W_n}(x)dx,$$
$$u(z) = \mathrm{E}e^{z\cos U_1} = \frac{1}{2\pi}\int_0^{2\pi} e^{z\cos x}dx.$$

Since W_n and $\cos U_1$ are bounded, $M_n(z)$ and $u(z)$ are well-defined for any $z \in \mathbb{C}$. We have the obvious equality:

$$M_n(z) = \left(u\left(\frac{z}{n}\right)\right)^n. \tag{B.4}$$

By the stationary phase method (see [23]), it follows that for large $|t|$ and all $a \in \mathbb{R}$, the following asymptotic holds:

$$u(a+it) = \frac{1}{2\pi}\int_0^{2\pi} e^{a\cos x}e^{it\cos x}dx \sim \frac{c_1(a) + c_2(a)e^{-it}}{\sqrt{|t|}},$$

where c_1 and c_2 are functions depending only on a, but not on t. Therefore, for $n \geqslant 3$ and all $a \in \mathbb{R}$, the function $M_n(a+it)$ is absolutely integrable with respect to t on $\mathbb{R}$, and the inversion formula holds:

$$p_{W_n}(x) = \frac{1}{2\pi i}\int_{a-i\infty}^{a+i\infty} M_n(z)e^{-zx}dz.$$

The value of a will be chosen later to obtain the best upper bound for the density. Using formula (B.4), we obtain:

$$p_{W_n}(x) = \frac{1}{2\pi}\int_{-\infty}^{+\infty} u^n\left(\frac{a+it}{n}\right)e^{-(a+it)x}dt = \frac{ne^{-anx}}{2\pi}\int_{-\infty}^{+\infty} u^n(a+it)\,e^{-itnx}dt. \tag{B.5}$$

In the last equality, we made the substitution $a \to an,\ t \to tn$. Note that $|u(a+it)| \leqslant u(a)$ for all $a, t \in \mathbb{R}$. Therefore,

$$\left|\int_{-\infty}^{+\infty} u^n(a+it)\,e^{-itnx}dt\right| = \left|\int_{-1}^{1} u^n(a+it)\,e^{-itnx}dt + \int_{|t|\geqslant 1} u^n(a+it)\,e^{-itnx}dt\right| \leqslant 2u^n(a) + \left|\int_{|t|\geqslant 1} u^n(a+it)\,e^{-itnx}dt\right|.$$

Applying Lemma 6, we obtain inequalities for the last integral:

$$\left|\int_{|t|\geqslant 1} u^n(a+it)\,e^{-itnx}dt\right| = \left|\int_{|t|\geqslant 1} u^{n-3}(a+it)\,u^3(a+it)e^{-itnx}dt\right| \leqslant u^{n-3}(a)\int_{|t|\geqslant 1}\frac{\beta^3e^{3a}}{|t|^{\frac{3}{2}}}dt = 4\beta^3e^{3a}u^{n-3}(a) = 4\left(\frac{\beta e^a}{u(a)}\right)^3 u^n(a).$$

Thus, we have proved the inequality:

$$\left|\int_{-\infty}^{+\infty} u^n(a+it)\,e^{-itnx}dt\right| \leqslant \left(2 + 4\left(\frac{\beta e^a}{u(a)}\right)^3\right)u^n(a).$$

Substituting this estimate into formula (B.5), we obtain:

$$p_{W_n}(x) \leqslant c_n(a)e^{n\lambda(a,x)}, \tag{B.6}$$

where

$$c_n(a) = \frac{n}{2\pi}\left(2 + 4\left(\frac{\beta e^a}{u(a)}\right)^3\right), \quad \lambda(a,x) = -ax + \ln u(a).$$

From Lemma 5, it follows that:

$$\lambda(a,x) \leqslant -ax + a + \ln\delta - \frac{1}{2}\ln a = (1-x)a + \ln\delta - \frac{1}{2}\ln a = f(a).$$

Let us find the derivative of f:

$$f'(a) = 1 - x - \frac{1}{2a}.$$

Therefore, the minimum of the function f is attained at the point $\frac{1}{2(1-x)}$. Taking this point as a, we have:

$$a = a(x) = \frac{1}{2(1-x)}.$$

We obtain the inequalities:

$$\lambda(a(x),x) \leqslant f(a(x)) = \frac{1}{2} + \ln\delta - \frac{1}{2}\ln\frac{1}{2} + \ln\sqrt{1-x} = \ln\frac{\sqrt{1-x}}{\gamma},$$

where

$$\gamma = \frac{1}{\sqrt{2e\delta}} = \frac{2}{\sqrt{\pi e}}.$$

Substituting the obtained estimate into (B.6), we have:

$$p_{W_n}(x) \leqslant c_n(a(x))\left(\frac{\sqrt{1-x}}{\gamma}\right)^n.$$

Next, we estimate $c_n(a(x))$ based on Lemma 5:

$$c_n(a) \leqslant \frac{n}{2\pi}\left(2 + 4\left(\frac{\beta e^a a}{e^a - 1}\right)^3\right) \leqslant \frac{n}{\pi}\left(1 + 2\beta^3\left(a + \frac{a}{e^a - 1}\right)^3\right) \leqslant \frac{n}{\pi}\left(1 + 2\beta^3(a+1)^3\right).$$

Using the fact that $a = a(x) = \frac{1}{2(1-x)} > \frac{1}{2}$, we obtain:

$$c_n(a) \leqslant \frac{n}{\pi}\left((2a)^3 + 2\beta^3(a+2a)^3\right) = \frac{n}{\pi}(2^3 + 2\beta^3\cdot 3^3)a^3 \leqslant \frac{n}{\pi}\frac{1 + 2\beta^3(1.5)^3}{(1-x)^3} \leqslant n\frac{3\beta^3}{(1-x)^3} \leqslant n\left(\frac{2\beta}{1-x}\right)^3. \quad \square$$

Lemma 5. *For all $a > 0$, the following inequalities hold:*

$$\frac{e^a - 1}{a} \leqslant u(a) \leqslant \delta\frac{e^a}{\sqrt{a}}, \tag{B.7}$$

where $\delta = \frac{1}{2}\sqrt{\frac{\pi}{2}}$.

Proof. We have the equality:

$$u(a) = \frac{1}{\pi}\int_0^\pi e^{a\cos x}dx.$$

First, we prove the upper bound. Using the inequality $\sin x \geqslant \frac{2}{\pi}x$ valid for $x \in [0, \frac{\pi}{2}]$ and the equality $\cos x = 1 - 2\sin^2\frac{x}{2}$, we obtain that for all $x \in [0, \pi]$ the following estimate holds:

$$\cos x \leqslant 1 - 2\left(\frac{2}{\pi}\frac{x}{2}\right)^2 = 1 - \frac{2}{\pi^2}x^2.$$

Therefore, for $u(a)$ we have the inequalities:

$$u(a) \leqslant \frac{1}{\pi}\int_0^\pi e^{a(1-\frac{2}{\pi^2}x^2)}dx \leqslant \frac{e^a}{\pi}\int_0^{+\infty} e^{-a\frac{2}{\pi^2}x^2}dx = \frac{e^a}{\pi}\frac{1}{2}\sqrt{\frac{\pi^3}{2a}} = \delta\frac{e^a}{\sqrt{a}}.$$

Next, we check the left inequality in (B.7). Using the inequality $\cos x \geqslant 1 - \frac{2}{\pi}x$, we have:

$$u(a) \geqslant \int_0^{\frac{\pi}{2}} e^{a\cos x}dx \geqslant \int_0^{\frac{\pi}{2}} e^{a(1-\frac{2}{\pi}x)}dx = \frac{\pi}{2}\frac{e^a - 1}{a} \geqslant \frac{e^a - 1}{a}. \quad \square$$

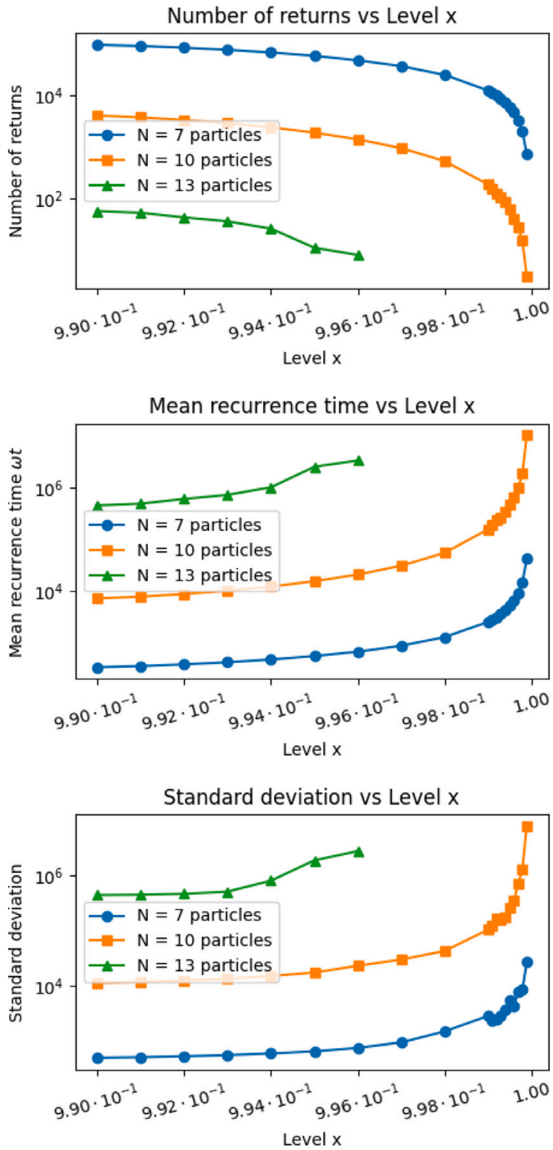

Fig. 3. The graphs presented in logarithmic scale illustrate the number of returns, mean, and standard deviation of the repetition time $h(t) \geq x$ for systems of 7, 10, and 13 particles. The graphs show that as the number of particles increases, the system return frequency decreases, while the mean and standard deviation of the repetition time increase.

Lemma 6. *For all* $a > 0$ *and* $|t| > 1$*, the following inequality holds:*

$$|u(a + it)| \leqslant \beta \frac{e^a}{\sqrt{|t|}},$$

where $\beta = 95$.

Proof. To prove the lemma, we will use the results from the paper [37]. We have the equality:

$$u(a + it) = \frac{1}{\pi} \int_0^\pi e^{a \cos x} e^{it \cos x} dx = I\left(0, \frac{\pi}{4}\right) + I\left(\frac{\pi}{4}, \frac{3\pi}{4}\right) + I\left(\frac{3\pi}{4}, \pi\right),$$

where

$$I(p, q) = \frac{1}{\pi} \int_p^q e^{a \cos x} e^{it \cos x} dx.$$

We estimate the integral $I\left(0, \frac{\pi}{4}\right)$ using Corollary 2, page 6 of [37] (an analogue of van der Corput's lemma):

$$\left|I\left(0, \frac{\pi}{4}\right)\right| \leqslant \frac{1}{4} e^{a} \min\{1, \frac{48}{\sqrt{|t|(\frac{\pi}{4})^{2} \frac{1}{2\pi} \frac{1}{\sqrt{2}}}}\} \leqslant 46 \frac{e^{a}}{\sqrt{|t|}}.$$

A similar estimate holds for the third integral:

$$I\left(\frac{3\pi}{4}, \pi\right) \leqslant 46 \frac{e^{a}}{\sqrt{|t|}}.$$

To estimate the second integral, we perform integration by parts:

$$I\left(\frac{\pi}{4}, \frac{3\pi}{4}\right) = \frac{1}{\pi} e^{a\cos x} \frac{e^{it\cos x}}{-it\sin x}\Bigg|_{\frac{\pi}{4}}^{\frac{3\pi}{4}} + \frac{1}{it\pi} \int_{\frac{\pi}{4}}^{\frac{3\pi}{4}} e^{it\cos x} \frac{d}{dx}\left(\frac{e^{a\cos x}}{\sin x}\right) dx.$$

Thus, we obtain the inequality:

$$\left|I\left(\frac{\pi}{4}, \frac{3\pi}{4}\right)\right| \leqslant \frac{e^{a}}{|t|}\left(\frac{2}{\pi\frac{1}{\sqrt{2}}} + \frac{1}{2}(1 + \frac{1}{\frac{1}{2}})\right) \leqslant 3\frac{e^{a}}{|t|} \leqslant 3\frac{e^{a}}{\sqrt{|t|}}.$$

By summing up the inequalities for all three integrals, we obtain the statement of the lemma. □

References

[1] R. Anufriev, S. Gluchko, S. Volz, M. Nomura, Quasi-ballistic heat conduction due to levy phonon flights in silicon nanowires, ACS Nano 12 (12) (2018) 11928–11935.
[2] R. Anufriev, S. Gluchko, S. Volz, M. Nomura, Probing ballistic thermal conduction in segmented silicon nanowires, Nanoscale 11 (28) (2019) 13407–13414.
[3] C.W. Chang, D. Okawa, H. Garcia, A. Majumdar, A. Zettl, Breakdown of Fouriers law in nanotube thermal conductors, Phys. Rev. Lett. 101 (2008) 075903.
[4] C.W Chang, Experimental probing of non-Fourier thermal conductors, in: S. Lepri (Ed.), Thermal Transport in Low Dimensions from Statistical Physics to Nanoscale Heat Transfer, Vol. 921, 2016, pp. 305–338.
[5] Z. Rieder, J.L. Lebowitz, E. Lieb, Properties of a harmonic crystal in a stationary nonequilibrium state, J. Math. Phys. 8 (5) (1967) 1073–1078.
[6] S. Lepri, R. Livi, A. Politi, Thermal conduction in classical low-dimensional lattices, Phys. Rep. 377 (1) (2003) 1–80.
[7] A. Dhar, Heat transport in low-dimensional systems, Adv. Phys. 57 (5) (2008) 457–537.
[8] V.A. Kuzkin, A.M. Krivtsov, Fast and slow thermal processes in harmonic scalar lattices, J. Phys.: Condens. Matter. 29 (50) (2017) 505401.
[9] S.N. Gavrilov, A.M. Krivtsov, Steady-state kinetic temperature distribution in a two-dimensional square harmonic scalar lattice lying in a viscous environment and subjected to a point heat source., Contin. Mech. Thermodyn. 32 (1) (2020) 41–61.
[10] A.A. Sokolov, A.M. Krivtsov, W.H. Müller, E.N. Vilchevskaya, Change of entropy for one-dimensional ballistic heat equation — sinusoidal initial perturbation, Phys. Rev. E 99 (2019) 042107.
[11] V.A. Kuzkin, A.M. Krivtsov, Ballistic resonance and thermalization in the Fermi-Pasta-Ulam-Tsingou chain at finite temperaturen, Phys. Rev. E 101 (2020) 042209.
[12] A.M. Krivtsov, Energy oscillations in a one-dimensional crystal, in: Doklady Physics, Vol. 59, Pleiades Publishing, 2014, pp. 427–430.
[13] A.M. Krivtsov, Heat transfer in infinite harmonic one-dimensional crystals, in: Doklady Physics, Vol. 60, Springer, 2015, pp. 407–411.
[14] M. Kac, Remark on recurrence times, Phys. Rev. E 115 (1) (1959) 1.
[15] W.G. Hoover, C.G. Hoover, Nonequilibrium temperature and thermometry in heat-conducting ϕ 4 models, Phys. Rev. E 77 (4) (2008) 041104.
[16] A.S. Murachev, A.M. Krivtsov, D.V. Tsvetkov, Thermal echo in a finite one-dimensional harmonic crystal, 31, (9) IOP Publishing, 2019, 095702,
[17] N.N. Bogolubov, On the influence of random force on a harmonic vibrator (in Russian), Uch. zap. MSU 77 (1945) 51–73.
[18] F. Bonetto, J.L. Lebowitz, J. Lukkarinen, Fourier's law for a harmonic crystal with self-consistent stochastic reservoirs, J. Stat. Phys. 116 (2004) 783–813.
[19] A. Lykov, V. Malyshev, Role of the memory in convergence to invariant gibbs measure, Dokl. Math. 88 (2013) 513–515.
[20] A. Lykov, V. Malyshev, Convergence to gibbs equilibrium — Unveiling the mystery, Markov Process. Related Fields 19 (2013) 643–666.
[21] A. Lykov, V. Malyshev, Liouville ergodicity of linear multi-particle Hamiltonian system with one marked particle velocity flips, Markov Process. Related Fields 21 (2015) 381–412.
[22] A.M. Krivtsov, The ballistic heat equation for a one-dimensional harmonic crystal, in: Dynamical Processes in Generalized Continua and Structures, Springer, 2019, pp. 345–358.
[23] A. Erdelyi, Asymptotic Expansions, 1954.
[24] A. Lykov, V. Malyshev, From the N-body problem to Euler equations, Russ. J. Math. Phys. 24 (95) (2017) 79–95.
[25] V. Malyshev, Zamyatin A., Regular dynamics and collisions inside classical closed string, Markov Process. Related Fields 28 (95) (2022) 489–525.
[26] V.A. Kuzkin, S.D. Liazhkov, Equilibration of kinetic temperatures in face-centered cubic lattices, Phys. Rev. E 102 (4) (2020) 042219.
[27] G. Watson, A Treatise on the Theory of Bessel Functions, Cambridge, 1922.
[28] G. Klein, I. Prigogine, Sur la mécanique statistique des phénomènes irréversibles III, Physica 19 (1–12) (1953) 1053–1071.
[29] E. Schrödinger, Zur dynamik elastisch gekoppelter punktsysteme, Ann. Phys., Lpz. 349 (14) (1914) 916–934.
[30] A. Lykov, V. Malyshev, How smooth should be the system initially to escape unbounded chaos, Markov Process. Related Fields 26 (2020) 233–286.
[31] A. Lykov, V. Malyshev, Uniformly bounded initial chaos in large system often intensies infinitely, Markov Process. Related Fields 26 (2020) 213–231.
[32] W. Richter, Local limit theorems for large deviations, Theory Probab. Appl. 2 (1) (1957) 206–220.
[33] L. Saulis, V. Statulevicius, Limit Theorems for Large Deviations, Kluwer Academic Publishers, 1991.
[34] A.A. Borovkov, Asymptotic Analysis of Random Walks. Light-Tailed Distributions, Cambridge University Press, 2020.
[35] I. Cornfeld, Ya. Sinai, S. and Fomin, Ergodic Theory, Springer, 1982.
[36] M. Kac, Remark on recurrence time, Phys. Rev. 115 (1) (1959).
[37] G. Arhipov, A. Karatsuba, V. Chubarikov, Trigonometric integrals, Math. USSR-Izv. 15 (2) (1980) 211–239.