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===== TRANSLATIONS OF PUBLISHED ARTICLES =====

On Thermalization of One-Dimensional Lattices I. Microcanonical Ensemble

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Abstract. In numerical modeling of the properties of biomacromolecules, an important place is occupied by the problems of thermalization, i.e. the energy equipartition over the degrees of freedom. The paper considers some mechanisms of lattice thermalization: Chirikov resonances, wave turbulence, and some others. Thermalization in a microcanonical ensemble is considered, when the system is isolated from external influences and the total energy is conserved. Although microcanonical ensembles are rarely used in practical calculations, however, the basic ideas about the mechanisms of thermalization have been obtained specifically for these systems. The main attention is paid to the consideration of thermalization of lattices with Fermi-Pasta-Ulam-Tsingou potentials, since the main efforts to understand the basics of thermalization were made specifically for lattices of this type. The role of solitons and breathers in thermalization is discussed.

Key words: *thermalization, microcanonical ensemble, ergodicity, FPUT lattice*

INTRODUCTION

A large field of modern mathematical biology is modeling the thermodynamic and statistical properties of chain biomacromolecules [1, 2]. In molecular dynamics (MD) modeling of various properties of a system, the microcanonical and canonical ensembles are most widely used. In the former case, it is assumed that the system under study is isolated from the thermostat and the total energy is preserved in it. In the latter case, the system is put into interaction with the thermostat and a constant temperature is maintained in it in one way or another (on average). In the thermodynamic limit, when the number of particles is $N \rightarrow \infty$, both the approaches give the same results, but for a small number of particles this is not necessarily the case.

The advantage of modeling in a microcanonical ensemble is its relative simplicity and the ability to control the accuracy of computational methods, while ensuring that the total energy is preserved. However, this approach also has “inherent” problems. First, it is necessary to use a large number of different initial conditions in order, if possible, to cover a significant part of the phase space. Secondly, when modeling in a microcanonical ensemble, it is necessary to solve difficult issues related to ergodicity.

An important advantage of modeling in a canonical ensemble is the fundamental absence of the need to solve ergodicity problems, since the system from any initial state always reaches the Gibbs distribution at $t \rightarrow \infty$. Indeed, if the thermostat in the canonical ensemble is

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modeled by Langevin random forces with friction, then it follows directly from the Fokker-Planck equation that the equilibrium distribution is exactly the Gibbs distribution. And the agreement of the MD modeling results with exact thermodynamic expressions is achieved when thermodynamic equilibrium is reached. But this approach has its own problems. The first is a certain complication of the computational schemes due to the inclusion of additional forces simulating the thermostat in the right-hand side of Newton's equations. The second is the choice of a method for modeling the thermostat and determining the thermostat parameters.

The problem of thermalization, i.e. the equipartition of energy by the degrees of freedom, has been developed for a long time. The beginning was made by Boltzmann formulation of the famous ergodic hypothesis, which states that the time-averaged values of physical quantities are equal to their average statistical values. The ergodic hypothesis serves a justification for statistical physics [3].

It is important that Boltzmann's postulate eliminated the difficulties concerned with statistical description of multiparticle systems based on their dynamic evolution. For this purpose, a probabilistic interpretation was introduced in terms of (micro)canonical ensembles. Thus, the contradictions between the deterministic (classical dynamic) and probabilistic (statistical) approaches were eliminated [4].

It was also clear that the Boltzmann postulate is not satisfied for all systems. For example, systems with a harmonic interaction potential cannot be thermalized. The reason for the difference between thermalizable and non-thermalizable systems is the integrability/non-integrability of the corresponding dynamics. The integrability of a classical system is understood as a property of a specific model when it has solutions in a closed form, like a harmonic lattice, or in the form of quadratures (expressions in the form of ordinary integrals) like, for example, the Toda lattice with an exponential potential [5]. Integrable systems are also characterized by the property that any autocorrelation functions have constant values at $t \rightarrow \infty$.

The integrability/non-integrability property determines whether the system is ergodic or not. Integrability clearly indicates non-ergodicity. However, there are no algorithms for proving ergodicity for most models. And one can only rely on indirect evidence indicating ergodicity/non-ergodicity [6].

The next important step in the problem of thermalization of classical systems was the first numerical simulation of the problem of energy equipartition (thermalization) in a lattice with interactions between neighboring particles by means of potentials $U_\alpha(y) = \frac{1}{2}y^2 + \frac{\alpha}{3}y^3$ and

$U_\beta(y) = \frac{1}{2}y^2 + \frac{\beta}{4}y^4$ on the first computer MANIAC-I (y is the difference in deviations of neighboring particles from their equilibrium positions). This work was initiated by E. Fermi during his frequent visits to the Los Alamos laboratory in the early 1950s and is a continuation of his early interests in this field [7]. The results were published in 1955 in the Los Alamos report [8] after E. Fermi death in November 1954.

Fermi was convinced that, despite their simplicity and idealization, lattices with potentials U_α and U_β could be extremely useful models in statistical mechanics, solid state physics, and computational physics. And so it happened. And for many years, these lattices became a "testing ground" where numerous ideas from the field of nonlinear physics were worked out, and these lattices themselves became useful models for studying transfer phenomena in physics, chemistry and biology.

A lattice with rigid boundary conditions with the number of particles $N = 32$ or $N = 64$ was studied numerically. The initial condition was the excitation of the longest-wave mode. It was expected that due to nonlinearity the energy would be uniformly distributed between all oscillatory modes. However, unexpectedly, recurrence was observed: after some time of dynamic evolution, all the energy (with an accuracy of better than 3 %) was again

concentrated in the initial mode. This result, called the “FPU paradox”, contradicted the ideas of that time that the nonlinearity of the potential should lead to thermalization of the system.

The fate of the results published in the report [8] is curious. Due to limited access to the report, it was almost unknown to researchers working in the field of nonlinear dynamics and statistical physics. And only 10 years later, after the publication of the collected scientific works of E. Fermi [9], the results became known to a wide range of researchers. And after that, the number of publications related to this topic grew extraordinarily quickly.

In honor of the 50th anniversary of the publication of the report, large collections of papers were published where the ideas formulated over the past period were summarized [10, 11]. Until 2005, the models formulated in the report [8] for lattices with potentials U_α and U_β were called “FPU models” after the authors’ names (E. Fermi, J. Pasta, S. Ulam). However, in 2005, a proposal was made to call this problem “the FPUT problem” taking into account the contribution made by Mary Tsingou to the numerical modeling of the formulated problem [12]. And this name for the model is currently accepted.

Of course, the set of models with nonlinear interaction potentials is not limited to FPUT lattices. However, the expansion of almost any nonlinear potential into a series yields FPUT potentials as the first terms. This is why these potentials have acquired such significance in the theory of lattice thermalization.

The α -FPUT system exhibits a complex quasi-periodic motion called “FPU recurrence”. This quasi-periodicity has stimulated research in the field of integrability [13] and soliton physics [14]. It is usually assumed that integrability is related to the closeness of the real interaction potential to the exactly integrable Toda potential [5]. Recently, works have appeared in which the FPUT model is considered in great detail and some refinements of the thermalization mechanisms have appeared (see, for example, [15–17]).

In this paper we will limit ourselves to considering the problem of thermalization of 1D lattices in a microcanonical ensemble. It is the microcanonical ensemble of 1D lattices that was the object for which the main theoretical results were obtained, attempting to explain the mechanisms of thermalization.

For isolated systems with a finite number of particles, it sometimes happens that the temperature of the system, determined in various ways (e.g. from the average kinetic energy of the particles, or the energy of the vibrational modes), is not the same [18]. Then the definition of “thermalization” as applied to an isolated system with a finite number of particles can be quite vague. Therefore, “thermalization” is sometimes understood in a broader sense, as statistical relaxation to a stationary distribution.

Below we will consider some mechanisms that provide thermalization of nonlinear one-dimensional lattices.

CHIRIKOV'S RESONANCES

One of the first mechanisms explaining thermalization was the resonant exchange of energy between vibrational modes [19, 20]. To understand the mechanism, it is necessary to define the concept of an oscillatory mode for a system with an arbitrary potential of particle interaction. At some point in time, a system of N particles with masses m can be represented as an N -dimensional vector of particle displacement from equilibrium positions $\mathbf{x}(t) \equiv \{x_1(t), x_2(t), \dots, x_N(t)\}$ and N -dimensional vector of velocities $\mathbf{v}(t) \equiv \{v_1(t), v_2(t), \dots, v_N(t)\}$.

The energy of the k -th vibrational mode in the harmonic approximation is defined as the expansion in vibrational modes of the harmonic lattice:

$$E^k(t) = \frac{m}{2} \left\{ \left[\omega^k \mathbf{q}^k \mathbf{x}(t) \right]^2 + \left[\mathbf{q}^k \mathbf{v}(t) \right]^2 \right\}, \quad (1)$$

where the first and second terms are potential and kinetic energies, while $\mathbf{q}^k$ and ω^k are the k -th eigenvector and frequency of the corresponding eigenvalue problem in the harmonic approximation. $\mathbf{q}^k \mathbf{x}(t)$ means the scalar product of vectors: $\mathbf{q}^k \mathbf{x}(t) \equiv \sum_j q_j^k x_j(t)$ and j is the number of the lattice mode. The total exact energy can be calculated, for example, like this: $E^{\text{exact}}(t) = \sum_j \left[\frac{m}{2} v_j^2 + U(x_j, x_{j-1}) \right]$ where $U(x_j, x_{j-1})$ – potential of neighbor particle interaction.

The total energy obtained from the harmonic expansion $E^{\text{harm}}(t) = \sum_k E^k(t)$ and the exact energy $E^{\text{exact}}(t)$ for nonlinear problems usually do not coincide. The value $\Delta E = (E^{\text{exact}} - E^{\text{harm}}) / E^{\text{exact}}$ can be considered a measure of the nonlinearity of the system under study. The value of ΔE increases with increasing nonlinearity of the potential and temperature.

Let us note another result of the lattice dynamics analysis: a relation was obtained between the temperature and frequencies of the oscillatory modes: $T \propto \sqrt{\prod_{k=1}^N \omega^k}$ that is, the temperature is proportional to the geometric mean of the frequencies of the vibrational modes.

Normal modes can also be defined as the solution of the problem of eigenvalues (squared frequencies ω^2) and eigenvectors $\mathbf{q}$ of the dynamic matrix (Hessian):

$$G_{i,j} = \frac{1}{m} \frac{\partial^2 U(x_i, x_j)}{\partial x_i \partial x_j}, \quad (2)$$

where $U(x_i, x_j)$ is a potential energy functional.

It may turn out that the frequencies of some modes are in resonance. Then energy exchange between these modes is possible. Using the example of a lattice with a Morse potential, it can be clearly shown that energy exchange due to resonances between modes is actually realized [21]. One end of the lattice of $N = 10$ particles is rigidly fixed, the other end is free. The longest-wave mode with some energy was excited. In the initial state, there is no resonance between the vibrational modes. Then the lattice begins to slowly stretch adiabatically by the free end. The stretching was carried out as follows: for a lattice of N particles, the leftmost particle has a coordinate $x_1 = 0$, and the coordinate of the N -th particle varies according to the law $x_N(t) = vt$ and $v \ll 1$.

When stretching, the bond stiffnesses in the Morse potential soften and the oscillation frequencies decrease (Fig. 1). With very slow stretching, it is possible to simulate adiabatic cooling under tension. The interaction potentials between neighboring particles are chosen randomly: $U(y_i) = \xi_j [1 - \exp(y_i)]^2$ and ξ_j is a random variable chosen from the interval $[0.5 - 1.5]$ and $y_i = x_i - x_{i-1}$. The sets of random values $\{\xi_j\}$ are determined independently for each sample. Random potentials are used to ensure that the mode frequencies are also random. This allows one to study the dynamics for different samples and collect statistics. It can be expected that for some samples, resonances between varying frequencies of oscillation modes will randomly occur during stretching.

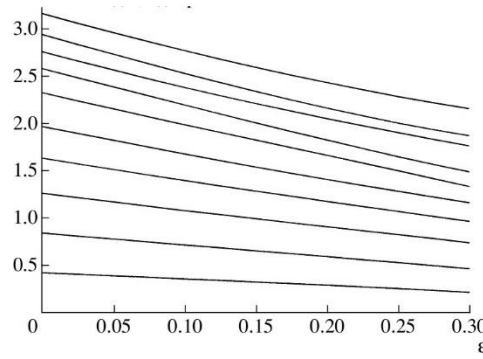


Fig. 1. Dependence of the frequencies of oscillatory modes on the relative elongation ε . $N = 10$.

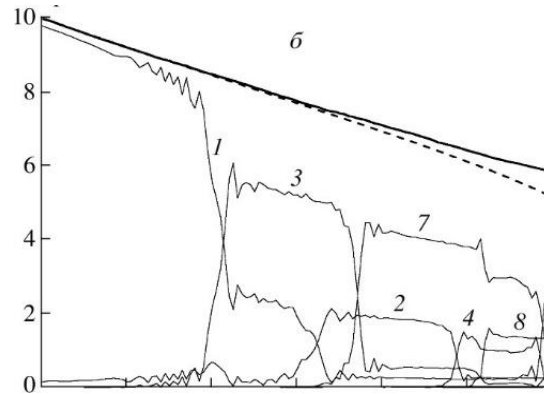


Fig. 2. Evolution of the energies of the modes (numbers are shown as digits) during stretching of one Morse lattice sample with random potentials, $N = 10$. The solid line is the exact total energy, the dotted line is the energy obtained from the harmonic expansion.

Figure 2 shows the change in the energies of individual vibrational modes depending on the relative elongation ε . Resonances are clearly visible. For example, the first resonant energy exchange occurs between the first and third vibrational modes, then between the third and seventh modes, and so on. A detailed analysis shows that in addition to double resonances, there are triple resonances.

The conditions for the feasibility of energy exchange due to Chirikov resonances are facilitated by an increase in the number of particles due to an increase in the density of levels in the frequency spectrum and a greater probability of commensurability of frequencies leading to resonances.

Chirikov resonances and their role in thermalization for the β -FPUT model are considered in detail in [22], and for the α -FPUT model – in [23]. For the β -FPUT lattice, it is analytically shown that the thermalization of the lattice is carried out due to complex resonances between six vibrational modes [24].

An alternative opinion was also expressed [25] that lattices with paired nonlinear particle interaction potentials of the general form $V(\mathbf{q}) = \sum_{i < j} V(|q_i - q_j|)$ are not ergodic. This category

includes all potentials of the FPUT with even powers of θ : $V(y) = \frac{1}{2}y^2 + \frac{1}{\theta}y^{\theta}$.

Wave turbulence

New ideas related to the so-called theory of wave turbulence have recently emerged in the problem of thermalization [26, 27]. This approach has made it possible to consider many issues from a different point of view and to solve some previously unsolved problems.

The fundamentals of the theory of wave turbulence relate to the statistical mechanics of a large number of interacting waves (oscillatory modes) in the limit of weak nonlinearity. The

approach is based on the wave kinetic equation (for more information about the theory of wave turbulence, see the review [28]).

The developed theory of wave turbulence made it possible to further clarify the main mechanisms of lattice thermalization, as well as to explain the power-law dependence of the time to achieve complete thermalization on the nonlinearity parameters, observed in numerical experiments. Resonances play a major role in the dynamics of thermalization. And the theory allows us to naturally predict the shift and broadening of oscillation frequencies caused by nonlinearity. This allows us to predict the overlap of Chirikov resonances, which is the basis of thermalization. The theory of wave turbulence also makes it possible to find out the causes of anomalous thermal conductivity of one-dimensional lattices.

Lyapunov exponent

In classical mechanics, one of the answers to the question of the causes of the equidistribution of energy is the concept of local instability of motion, leading to chaotic dynamics, although the equations of motion themselves are quite deterministic.

In [29], the FPUT model $V(y) = \frac{1}{2}y^2 + \frac{1}{\theta}y^\theta$ was studied for $\theta = 4$ and $\theta = 6$. The approach first proposed by A. Poincare was used, which consists in considering dynamics from a geometric point of view. The connection between the dynamic basis of statistical mechanics and Riemann differential geometry is substantiated in [30, 31].

In [29], the "Lyapunov time" was determined, which is the inverse of the largest Lyapunov exponent. Lyapunov time is directly related to the nonlinearity parameter, which is responsible for the degree of non-integrability of the system. Moreover, it is shown that the well-known universal law of thermalization $t_{eq} \sim \gamma^{-2}$ (γ is a certain parameter of nonlinearity) is directly related to the value of the maximum Lyapunov exponent.

Solitons and breathers

One of the most important problems of biophysics is to clarify the mechanisms of self-focusing and energy transport, which occurs, for example, during photosynthesis. This is an important bioenergetic process that is very fast (less than a picosecond) and very efficient (about 95 %). Bioenergetics also requires that energy transfer take place over long distances, as is realized, for example, by hydrolysis of adenosine triphosphate. In this process, energy is transferred over relatively long distances with virtually no losses and ensures subsequent conformational changes in biological macromolecules. These and some other features of energy transfer led A.S. Davydov to the assumption that solitons may be responsible for energy transfer in biological systems [32].

Solitons are solutions of some continuum equations. For example, using the Korteweg–de Vries equation, Zabusky and Kruskal showed the possibility of recursion, i.e., the return of a dynamical system to its initial state [14]. And to explain this phenomenon, the concept of "soliton" was formulated. They also explained the reasons for the strange behavior of the FPUT model. The stability of soliton solutions is explained by the exact integrability of the corresponding equations.

Although energy transfer via solitons seems to be a very attractive mechanism of energy transfer in bioenergetics, there are some doubts about its actual feasibility [33, 34].

An alternative and more general principle has been proposed, which can be applied to a wide range of physical, chemical and biological phenomena and which is related to the concept of discrete breathers (DB).

The necessary conditions for the existence of breathers are the nonlinearity of the Hamiltonian and the discreteness of the lattice [35–37]. S. Aubry called these conditions "anticontinuity" [38]. There are sufficient reasons to believe that for some nonlinear systems that do not have an exact solution, nevertheless, there are trajectories in the phase space that

are very close to the trajectories related to special periodic solutions in time – DB. These localized states can exist for a very long time.

The existence of breathers is explained as follows. In the continuous case (continuity), for the equation $U_{tt} - U_{xx} = 0$ the spectrum is usually linear (the ratio $\omega^2 \propto k^2$ holds in the dispersion relation). However, for a similar equation in the discrete case $U(l)_{tt} - [U(l-1) + U(l+1) - 2U(l)]$, where $l \in \mathbb{Z}$, the dispersion relation becomes nonlinear: $\omega^2 = 2[1 - \cos(k)]$. It can be shown that the vibrational modes outside the linear part of the spectrum do not have a significant spatial extent, i.e. they are localized.

The existence of DB is known for many types of potentials: α - and β -FPUT, Klein–Gordon potential and many others. This property is not limited to some exceptional integrable models, but is rather general.

The results of numerical modeling of discrete non-integrable systems show that the existence of a large number of such solutions is possible for many types of potentials.

One of the problems of biophysics is to clarify the possible mechanisms of self-focusing and energy transport in biopolymers. Localization and energy transfer are of vital importance in nature. Such processes are usually explained by solitons [39].

An alternative mechanism for effective targeted energy transfer (targeted energy transfer) using breathers was proposed in relation to solitons [40]. The implementation of this mechanism implies resonant energy transfer.

Let us consider the simplest case of two coupled harmonic oscillators. If the oscillator frequencies are in resonance, then any amount of energy transferred to one of the oscillators begins to be periodically redistributed between the oscillators with a frequency proportional to the coupling energy of the oscillators. This picture changes dramatically in the case of anharmonic oscillators due to the fact that their frequencies depend on the amplitude.

Let some energy be transferred to one of the oscillators. Then, if the initial frequencies are in resonance, then a small part of the energy transferred to another oscillator violates the resonance conditions and energy is no longer transferred from one oscillator to another. However, there are exceptions to this rule, when resonance still continues to exist and full energy transfer is possible. This can be done by fine-tuning the nonlinear lattice in such a way that targeted energy transfer (TET) can be realized. The authors of the work [40], where the criteria for implementing TET are considered in detail, understand that it is practically impossible to implement this scenario in a randomly selected lattice. However, they suggest that in the process of evolution it is possible to adjust the system parameters in such a way that this mechanism can play a significant role in bioenergetics.

Speed of sound in nonlinear lattices

There are some issues that are not directly related to thermalization problems, but are important in practical applications. One of them is thermal expansion. For a harmonic potential, thermal expansion is absent. However, for lattices with nonlinear potentials, thermal expansion is possible.

When solving problems about dynamics (solving the corresponding differential equations), the question arises about the choice of boundary conditions. There are two types of boundary conditions. The first type is free boundary conditions. In this case, the total length of the lattice is not limited by anything and can vary in accordance with the internal dynamics of the lattice. The second type of boundary conditions are cyclic boundary conditions or rigidly fixed ends of the lattice. In this case, the total length of the lattice is rigidly fixed by the initial conditions.

For nonlinear asymmetric potentials (α -FPUT, Morse, and some others), the existence of thermal expansion is obvious: with increasing temperature, the length of the lattice with free ends also increases. In this case, the potential energy of the interaction corresponds to its

minimum. At the same time, the rigidity of the bonds is preserved and therefore the speed of sound does not change. For lattices with cyclic boundary conditions or rigidly fixed ends, the total length of the lattice remains unchanged. Then, in this case, unrealized thermal expansion will lead to the occurrence of internal stresses of the bonds and to an increase in the effective rigidity of the bonds. Therefore, the speed of sound increases.

It is natural to expect that lattices with symmetric potentials should not experience thermal expansion. However, it turns out that some lattices with such potentials do experience thermal expansion. Let us demonstrate this using the example of the potential potential β -FPUT:

$U(y) = \frac{ky^2}{2} + \frac{\beta y^4}{4}$ [41]. Let us dimensionalize the problem, i.e. numerically set $k = \beta = m = k_B = 1$.

Then the β -FPUT potential can be rewritten as

$$U(y) = \left(1 + \frac{y^2}{2}\right) \frac{y^2}{2} \quad (3)$$

and the expression in brackets can be replaced by the effective rigidity of the harmonic coupling

$$U(y) = k_{\text{eff}} \frac{y^2}{2}. \quad (4)$$

The problem is to find k_{eff} . This problem can be solved using the mean field approximation (MF). The average value of the potential energy is

$$\langle U_p(y) \rangle = k_{\text{eff}} \frac{1}{2} \langle y^2 \rangle \quad (5)$$

where $\langle y^2 \rangle$ – average value y^2 .

In the harmonic approximation (4), according to the virial theorem, the average values of kinetic and potential energies are equal to $U_p = U_k$. For one-dimensional systems, the dimensionless equality $U_k \equiv T/2$ holds and T is the dimensionless temperature. Then:

$$k_{\text{eff}} \frac{1}{2} \langle y^2 \rangle = \frac{T}{2} \quad (6)$$

The self-consistency condition in the MF approximation (the expression in brackets in (3) is equal to k_{eff} :

$$1 + \frac{1}{2} \langle y^2 \rangle = k_{\text{eff}} \quad (7)$$

From (3) it follows that $\langle y^2 \rangle = T/k_{\text{eff}}$ and substituting $\langle y^2 \rangle = T/k_{\text{eff}}$ into equation (7) gives a self-consistent solution for k_{eff} :

$$1 + T/(2k_{\text{eff}}) = k_{\text{eff}} \quad (8)$$

with the solution

$$k_{\text{eff}} = \frac{1}{2} + \sqrt{\frac{1}{4} + \frac{T}{2}} \quad (9)$$

Thus, the effective (“nonlinear”) speed of sound

$$v_{\text{eff}} = \sqrt{k_{\text{eff}}} = \sqrt{\frac{1}{2} + \sqrt{\frac{1}{4} + \frac{T}{2}}}, (m=1). \quad (10)$$

is greater than the speed of sound $v^{\text{harm}} = 1$ in the harmonic approximation. For example, expression (10) gives the value $v_{\text{eff}} = 1.27$ for $T = 2$.

The speed of sound in a lattice with potential (3) can be calculated numerically using a general-form correlator $\langle \Delta x_k(t) \Delta x_{k+m}(t+\tau) \rangle$, where $\Delta x_k(t)$ is the deviation of the k -th site from the equilibrium position at time t . Autocorrelators of this type are used to find the correlation between some event and its “copy” in another place with a time delay. In practical implementations of the method, one can fix, for example, τ and search for a copy by scanning over the lattice sites m . Alternatively one can fix m and scan for τ . Instead of Δx deviations, one can use Δx velocity deviations and use velocity-velocity and coordinate-velocity correlators.

To find the speed of sound, the correlator $\langle \Delta x_{50}(t) \Delta x_{50+m}(t+20) \rangle$ was used on a lattice of $N = 101$ sites with rigid boundary conditions at a thermalized lattice temperature of $T = 2$. The lattice was heated using a Langevin thermostat. The thermostat was switched off; the system was maintained for some time until thermalization was achieved, which was checked from the equidistribution of energies; the correlator was calculated. The number of MD trajectories was 10^5 , the trajectory length was $t = 50$.

Determining the speed of sound using an autocorrelator is a rather resource-intensive and time-consuming procedure. However, this is probably the only reliable method for determining the speed of sound.

Figure 3 shows the result of the correlation function calculation. The correlator has two peaks at $m = \pm 25$ and time $t = 20$, which corresponds to the speed of sound $v \approx 1.25$, which is very close to the result obtained above $v \approx 1.27$ in the mean field approximation.

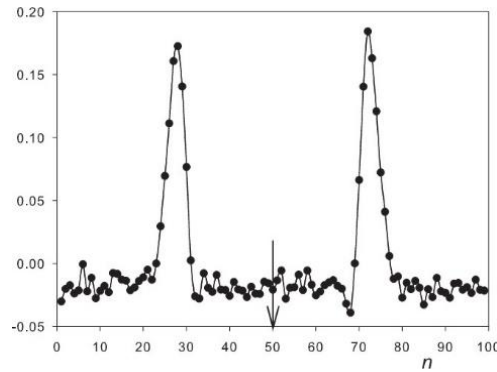


Fig. 3. Values of the coordinate-to-coordinate autocorrelator $\langle \Delta x_{50}(t) \Delta x_{50+m}(t+20) \rangle$ depending on the coordinate on the lattice. The lattice β -FPUT, $N = 101$, $T = 2$. The arrow points to the coordinate $n = 50$.

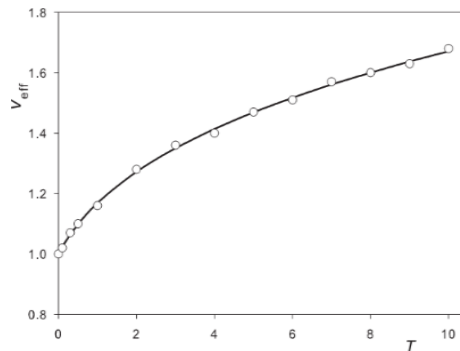


Fig. 4. The speed of sound calculated in the mean field approximation (solid line) and in the calculation of the correlator (circles) depending on temperature.

The Figure 4 shows a comparison of the speed of sound calculated in the mean field approximation and the calculations of the correlator depending on temperature.

Note that the SP method turns out to be applicable up to very high temperatures $T = 10$, although initially it was focused on use at low temperatures. It should also be noted that the increase in the speed of sound with increasing temperature is quite significant: the speed of sound at $T = 8$ is more than 50 % higher than the speed of sound in the harmonic approximation.

Even more surprising is the effect of boundary conditions on the thermal conductivity of one-dimensional lattices: the thermal conductivity coefficient $\kappa \propto 1/\sqrt{N}$ for rigid boundary conditions and an anomalous dependence on the lattice length $\kappa \propto \sqrt{N}$ for free boundaries [42]. The reason of this effect of boundary conditions on the physically calculated quantity is still unclear.

CONCLUSIONS

The paper considers some problems of thermalization of lattices with different particle interaction potentials in a microcanonical ensemble, when there is no interaction with a thermal reservoir. This consideration was carried out, since it is the microcanonical ensemble that makes it possible to accurately study most thermalization problems.

The presentation provides an opportunity to get acquainted with some basic principles of thermalization.

The authors of this paper avoided providing complicated mathematical calculations. If necessary, details can be found in the cited literature.

In the next paper, some practical issues of thermalization in the canonical ensemble will be considered, when the system is brought into interaction in one way or another with an external heat reservoir.

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