Thermal conduction of one-dimensional isotopically disordered harmonic lattice.

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In the present communication we consider the one-dimensional (1D) isotopically disordered lattice with the harmonic potential. Our analytical method is adequate for any 1D lattice where potential energy can be presented as the quadratic form $U = \sum_{i,j} U_{ij} q(i) q(j)$, where $q(i)$ – coordinate or velocity of $i$-th particle. There are derived the closed system of equations for the temporal behavior of the correlation functions. The final expressions allow to calculate the kinetics and dynamics of the system – energy, temperature profile, thermal conduction and others. There is developed the method for the calculation of the evolution of the eigenvalues (frequencies) and eigenvectors (relaxation times) to their stationary values. Exact results are obtained for times $\approx 10^{14}$. The methods are suggested allowing to extend the range of the relaxation times upto $\approx 10^{28}$. The spectrum of relaxation times reaches it constant value starting from the number of particles $N$ in the lattice $N \geq 300$. Thermal conductance $\kappa$ has the non-monotonic character: for the number of particles $N < 300 \kappa$ increases as $\kappa \approx 2.4 \log N$, reaches the maximum value equal $\approx 4.0$ at $N \approx 300$ and then slowly decreases upto $N = 700$. The stationary state is unique and satisfies the Gibbs distribution. An excellent agreement between numerical simulations and analytical results is obtained where possible.

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At present, more attention is focused on statistical and transport properties of low-dimensional systems. Besides obvious achievements there exists few unresolved fundamental problems, e.g. if there exists the unique stationary state? If this state exists, then what is the time of relaxation to stationary state? Are some values self-averaged, i.e. if the thermodynamical limit really exists for these values? What are the sufficient conditions for the observation of finite value of thermal conductance in low-dimensional systems?

The diverging value of thermal conductance $\kappa \propto N^\alpha$ with $0.17 \leq \alpha \leq 0.5$ was obtained for certain model systems\textsuperscript{3,4,5,6,7}. Theoretical estimations for $\alpha$ give values $2/3$ or $1/3$ depending on the chosen model.

There was obtained the final value of thermal conductivity\textsuperscript{5,10,11,12}, and, moreover, numerical simulations predict even the "phase transition" from normal to diverging thermal conductivity when temperature and/or parameters vary. However some of these results were criticized\textsuperscript{13}.

Usually it is supposed that non-integrability is the necessary but not enough condition for the final value of thermal conduction in 1D systems\textsuperscript{14}. There was demonstrated\textsuperscript{15} that any 1D system
with the acoustical branch of excitation should have an infinite thermal conductivity in the limit of low temperatures. This statement is supported by the theorem that the one-dimensional system with momentum conservation and nonzero pressure have infinite thermal conductivity.\textsuperscript{15}

Many model lattices with different potentials of interaction were investigated. Important qualitative and quantitative results were obtained, though controversial results were observed for the same model systems. These and associated problems are thoroughly considered in the recent Review.\textsuperscript{1}

1D lattices are very useful prototypes for the (analytical and numerical) investigation of kinetic, dynamical and transport properties of more complex and practically interesting systems such as carbon nanotubes (see e.g.\textsuperscript{16,17,18,19}).

The problem of the dynamics of the disordered lattices was formulated over 50 years ago by F.Dyson\textsuperscript{20}, who gave the general formulation of the problem.

Dyson’s problem was chosen for the thorough investigation as this system meet most of the problems more or less common in the simulation of thermal conductance in low-dimensional systems. Small number of parameters allows to analyze their influence on the final results, and dynamical and transport properties.

We start from the quadratic hamiltonian with fixed boundary conditions (we are mainly interested in methodology, and the role of boundary conditions and other parameters will be considered and presented in a separate publication.)

\begin{equation}
H = \frac{1}{2} \sum_{i=1}^{N} m(i) v^2(i) - \frac{1}{2} \sum_{i=1}^{N} x(i) U_{ij} x(j),
\end{equation}

where in the considered case the matrix $\hat{U}$ has the form:

\begin{equation}
\hat{U} = \begin{pmatrix}
-2 & 1 & 0 & \cdots & 0 & 0 \\
1 & -2 & 1 & \cdots & 0 & 0 \\
0 & 1 & -2 & \cdots & 0 & 0 \\
\vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\
0 & 0 & \cdots & 1 & -2 & 1 \\
0 & 0 & \cdots & 0 & 1 & -2 \\
\end{pmatrix}.
\end{equation}

Recall that our approach is valid for the arbitrary quadratic Hamiltonians of the form

\begin{equation}
H = \sum q(i) H_{ij} q(j),
\end{equation}

giving rise to the linear equations of motion, where $q(i), q(j)$ – coordinates or velocities of the particles.

For the modelling of the heat reservoir we use the Langevin random forces with friction, where in addition to dynamical equations the members $[-\gamma(i) \dot{x}(i) + \xi(i)]$ were added, and $\gamma(i), \xi(i)$ – the "friction" coefficient and random force, correspondingly. Lets consider first the most general case, when the Langevin sources acts on all particles of the lattice. Then the equation of motion in matrix form is

\begin{equation}
\dot{q} = (\hat{A} \hat{q} + \hat{E}),
\end{equation}
where time dependent vector of the state $\vec{q}$ is represented for convenience in the form

$$\vec{q}(t) = \left( \begin{array}{c} \vec{V} \\ \vec{X} \end{array} \right) = \{v(1), v(2), \ldots v(N); x(1), x(2), \ldots, x(N)\},$$

(5)

vector $\vec{\Xi}(i) = \{\xi(1), \xi(2), \ldots, \xi(N)\}$ in (4) is the vector of uncorrelated random forces, where random forces $\xi(i)$ obey the standard relations:

$$\langle \xi(i, t_1) \xi(j, t_2) \rangle = 2 \delta_{ij} \delta(t_1 - t_2) \frac{\gamma(i)}{m^2(i)}$$

(6)

Matrix $\hat{A}$ has the block form

$$\hat{A} = \begin{pmatrix} \hat{M}^{-1} \hat{U} & -\hat{M}^{-1} \hat{\Gamma} \\ \hat{I} & \hat{0} \end{pmatrix},$$

(7)

and matrix $\hat{U}$ namely this one that used in (1) and (2).

In equation (7) $\hat{M}(i, j) = \delta_{ij} m(i)$ is the diagonal matrix of random masses of particles, and $\hat{M}^{-1}$ – inverse matrix. We have chosen well known from literature the mass distribution such that randomly and with the equal probability masses have values 1 or 1/2. Matrix $\hat{\Gamma} = \delta_{ij} \gamma(i)$ – diagonal matrix of friction coefficients in Langevin forces for the corresponding particles, matrices $\hat{I}$ and $\hat{0}$, are, correspondingly, unit and null matrices.

Generally speaking, matrix $\hat{A}$ falls into a category of random matrices widely used in mathematics and physics (see, e.g. recent review).

Initial condition is chosen in the form $\vec{q}(t = 0) = \vec{0}$, i.e. initial temperature of all particles are equal to zero. Then the formal solution of equation (4) has the form

$$\vec{q}(t) = \int_0^t \hat{W}(t - \tau) \vec{\Xi}(\tau) d\tau$$

(8)

Note, that if the initial conditions are arbitrary, i.e. $\vec{q}(t = 0) = \vec{q}_0$, then there the solution of the inhomogeneous solution should be added to the r.h.s. of (8) and it has a form:

$$\vec{q}(t) = \hat{W}(t) \vec{q}_0 + \int_0^t \hat{W}(t - \tau) \vec{\Xi}(\tau) d\tau.$$

(9)

The time evolution operator $\hat{W}(t)$ satisfies the equation

$$\frac{d\hat{W}}{dt} = \hat{A} \hat{W}, \quad \hat{W}(t = 0) = \hat{I}$$

(10)

Define now the $2N \times 2N$ matrix of correlation functions (keeping in mind the definition )

$$\langle q(i, t) q(j, t) \rangle = \int_0^t \int_0^t d\tau_1 d\tau_2 W_{i,i_1}(t - \tau_1) W_{j,j_1}(t - \tau_2) \langle \xi_{i_1}(\tau_1) \xi_{j_1}(\tau_2) \rangle.$$ 

(11)

Using the expression (10), one can get:

$$C_{ij} \equiv \langle q(i, t) q(j, t) \rangle = \sum_p \frac{2 \gamma(p) T(p)}{m^2(p)} \int_0^t d\tau W_{ip}(\tau) W_{jp}(\tau).$$

(12)

where $p$ is the number of a particle in the lattice subjected to Langevin forces.
Expression for $W_{ip}(\tau)$ describes the evolution of the hole system, when at $t = 0$ the velocity of $p$-th particle is equal to unity, and displacement from the equilibrium position is zero. All other particles have zero displacements and velocities.

In the general case the evolution operator $W_{ip}(t)$ for the $p$-th particle forecasts its temporary behavior at the initial condition $W_{ip}(t = 0) = \delta_{ip}$:

$$\frac{d W_{ip}}{dt} = \sum_j A_{ij} W_{jp}, \quad (13)$$

Generally speaking, one can solve the system of $2N$ equations (13) for every of Langevin particles $p$. As it can be seen from (12), the contributions from Langevin sources are also independent and additive. It also means the linearity of results on temperatures of Langevin sources.

The standard approach for the solving the system (13) consists in transformation to the problem for eigenvalues. Namely this approach was used in this communication. The solution will be searched as the series by eigenfunctions of operator $\hat{A}$.

Let’s consider the problem for the eigenvalues of relaxing vibrational states (vibrations relax because of an existence of friction in Langevin forces):

$$\hat{A} \bar{q}_k = \lambda_k \bar{q}_k, \quad (14)$$

where $k$ is the number of eigen solution (vibration). The complex value $\lambda_k$ can be represented in the form:

$$\lambda_k = -\frac{1}{\tau_k} + i \omega_k, \quad (15)$$

where $\tau_k$ and $\omega_k$ are, correspondingly, the relaxation time and eigen frequency of $k$-th mode. $\lambda_k$ is not purely imaginary because of the relaxation in Langevin forces, and formally because the matrix $\hat{A}$ is the unsymmetrical matrix and its eigenvalues in the general case are complex values.

Let’s expand $W_{ip}$ in the series over eigenvalues $q_k$:

$$W_{ip} = \sum_{k=1}^{2N} e^{\lambda_k t} c_{kp} q(i)_k \quad (16)$$

Actually we have $N$ equations for all Langevin particles with still unknown coefficients $c_{kp}$, which can be determined from the same equation (16) at $t = 0$ and the initial condition $W_{ip}(t = 0) = \delta_{ip}$:

$$\delta_{ip} = \sum_{i=1}^{2N} c_{kp} q(i)_k, \quad (17)$$

what in the symbolic form can be rewritten as

$$\hat{B} = \hat{A} \hat{x}, \quad \hat{B} = \delta_{ip}, \quad \hat{x} = c_{kp}, \quad \hat{A} = q_k(i). \quad (18)$$

Substituting the solution of the equation (16) in (12), one finally gets

$$C_{ij} = \sum_{p=1}^{N} \frac{2 \gamma(p) T(p)}{m^2(p)} \sum_{k_1, k_2=1}^{2N} \frac{1 - e^{(\lambda_{k_1} + \lambda_{k_2}) t}}{\lambda_{k_1} + \lambda_{k_2}} q(i)_{k_1} q(j)_{k_2} \quad (19)$$
At \( t \to \infty \) the fraction in (19) reduces to \( 1/(\lambda_{k_1} + \lambda_{k_2}) \).

One can check, that our results (12) and (19) satisfies the equation for the correlation function, which can be obtained from the Fokker-Planck equation for the distribution function \( P(\vec{q}) \) with the initial condition \( P(\vec{q}, t = 0) = \delta(\vec{q}) \).

An expression (12) is easily generalized for the correlation functions taken at different instants of time:

\[
\langle q(i, t) q(j, t + \Delta) \rangle = \sum_{p=1}^{N} \frac{2 \gamma(p) T(p)}{m^2(p)} \int_{0}^{t} d\tau W_{ip}(\tau) W_{jp}(\tau + \Delta) \tag{20}
\]

The generalization of expression (19) for correlation functions taken at different times is also obvious.

Further particular calculations will be done for the case, when the Langevin forces acts only on extreme 1-st and N-th particles and we’ll present some results for this case. We also consider for the definiteness that \( \gamma(1) = \gamma(N) = 1 \). The solution of this problem we find as the solution of the problem for eigenvalues (14) and the system of linear equations (17).

Note, that the standard matrix calculus with double precision (at the diagonalization of matrix (7) give the relaxation times only of the order \( \tau \simeq 10^{14} \). Really, as the result we get the complex value, and if the imaginary part (frequencies) \( \simeq 1 \), then it is impossible to ”catch” the real part \( 1/\tau < 10^{-14} \). This fact becomes obvious if one returns back to the expression (19). There stands a value of the type \( e^{i\omega t} \) in the nominator, and if \( \omega \) is defined with the precision \( \simeq 10^{-14} \), then it is not possible to use times greater then \( t > 10^{14} \). Nevertheless we can use \( t = \infty \), because of the damping the phase terms becomes to be zero.

Namely these long-living states correspond to highly localized states. It follows from the well known fact, that there are localized states with eigen frequencies \( \sim 1 \) and very small damping in long disordered chains. Analogous localized states were discovered by P.Anderson in the diffusion problem (see also review23).

Actually, in double summation (19) the most dangerous is the case, when in denominator \( \lambda_{k_1} = \lambda_{k_2}^* \), what is the very small number for the localized vibrational modes \( \sim -2\tau_p \).

But it turns out that the order of computations can be doubled. Namely, from the equation \( \hat{A} \vec{q} = \lambda \vec{q} \), rewritten in components, it follows

\[
m(p) x_k(p) \lambda_k^2 = x_k(p - 1) - 2 x_k(p) + x_k(p + 1) - \gamma(p) \lambda_k x_k(p). \tag{21}
\]

From the equation (21) one can get (multiplying on complex conjugated, summing and dividing real and imaginary parts) expression (valid only at \( \gamma(1) = \gamma(N) = 1 \):

\[
\frac{1}{\tau_k} = - \frac{|x_k(1)|^2 + |x_k(N)|^2}{2 \sum_{i=1}^{N} m_i |x_i|^2} \tag{22}
\]

Thus there stands a value of the order of unity in denominator. If eigenvector is known with the precision of the order of \( 10^{-14} \), then the relaxation times can be calculated with the precision \( \sim 10^{-28} \), i.e. \( \tau \sim 10^{28} \). It means that using the standard PC one can investigate the kinetics of
FIG. 1: The dependence of normalized distribution function for relaxation times for different number of particles in the lattice. Solid curve – \( N = 100 \), dashed line – \( N = 200 \). Points of different forms correspond to \( N \) from \( N = 320 \) to \( N = 700 \).

isotopically disordered chains for the times much greater then it is available at any direct numerical simulation.

Thus, the limiting (by precision) stages of computations are the matrix operations (7) and (18).

Below we shall demonstrate some of the most essential results.

The spectrum of relaxation times depending on the chain length \( N \) at \( N \geq 100 \) is shown in Fig. 1. As we mainly interested in the long-time kinetics, then the calculation of the relaxation times we’ve performed starting from \( \lg \tau > 7.5 \) (up to this value the spectrum is irregular and it is approximately the end point of relaxation times for the regular harmonic chain). One can see, that the spectrum depends on \( N \) for \( N < 300 \). Starting from \( N = 300 \) the spectrum takes the constant value, as in the thermodynamical limit this spectrum should be the constant value.

The "tails" of relaxation times were approximated by several functional dependencies \( f(\lg(\tau)) \), and the mean of logarithm of relaxation time in all cases was calculated according to

\[
\langle \lg \tau \rangle = \frac{\int_{7.5}^{\infty} \lg \tau f(\lg(\tau)) d\lg \tau}{\int_{7.5}^{\infty} f(\lg(\tau)) d\lg \tau}
\]

(23)

It turned out that at this approach and the different choices of approximating functions \( \langle \lg \tau \rangle \approx 17 \). Naturally, we supposed that the relaxation law is valid for larger times, therefor the upper limit in (23) is chosen to be the infinity.

For \( N > 300 \) the probability that \( \lg \tau > 7.5 \) is large then \( 1/3 \). i.e. area of the tail is large then \( 1/3 \) from the total area under the curve of the distribution function.

The largest time have vibrational modes, localized in the center of the chain. It is connected with the fact that the corresponding vibrational wave functions have negligibly small amplitudes at the Langevin sources (ends of the chain), and these sources too long "drive" these modes. Naturally, that the maximum relaxation times \( \tau_{max} \) should grow with the growth of \( N \). But the law of growth of \( \tau_{max} \) with \( N \) is still unknown.
The temperature profiles along the chain for different boundary temperatures are shown in Fig. 2 for $N = 70$, where our results are exact, for arbitrary times. The profiles are shown for $\tau = 4, 6, 10, 14, \infty$ time units.

As was shown above, because of extremely long life time of vibrational modes, localized in the center of the lattice and having the relaxation times greater than $> 10^{28}$ for $N > 100$, the temperature in the center of the lattice is calculated not very exactly. For the lattice of any size we can guarantee only the results for $\sim 30 - 40$ particles from every end. It also means that the numerical simulations (e.g., temperature distribution along the chain) for large lattices are incorrect as the states localized in the center of the lattice have no enough time to relax to the stationary state during the period of time of the numerical simulation.

Because of the thermal flow in the stationary state is a constant value along the length of all the lattice, then it can be calculated in the vicinity of ends, where, as was stated above, all our calculations are exact. It is obvious that the system may not reach its stationary state. The specific coefficient of thermal conductance $\kappa$ as dependent on the chain length is shown in Fig. 3. $\kappa$ depends only on the temperature difference on the chain ends and doesn’t depend on the absolute temperature ($(T(1) + T(N))/2$), what is obvious from \cite{12}. Really, if the Langevin sources acts at extreme atoms (1-st and $N$-th), then the expression \cite{12} can be rewritten

\[ C_{ij} = \frac{2T(1)}{m_1^2(1)} \int_0^t W_{i1}(\tau) W_{j1}(\tau) d\tau + \frac{2T(N)}{m_1^2(N)} \int_0^t W_{iN}(\tau) W_{jN}(\tau) d\tau. \quad (24) \]

Let’s change the temperature at the ends in the same manner: $T(1) \rightarrow T(1) + T, \ T(N) \rightarrow T(N) + T$. Then the change in correlation functions \cite{24} has the form of the correlator for equal temperatures at the ends of the lattice:

\[ C_{ij} = \frac{2T}{m_1^2} \int_0^t W_{i1}(\tau) W_{j1}(\tau) d\tau + \frac{2T}{m_N^2} \int_0^t W_{iN}(\tau) W_{jN}(\tau) d\tau, \quad (25) \]
FIG. 3: The dependence of the coefficient of thermal conductance on the chain length. The linear fitting of the initial part of the curve corresponds to $\kappa \approx 2.4 \log N$.

and it is obvious, that any changes in the thermal flow and other additives, depending on the temperature difference become zero.

As it is seen from Fig. 3, for not too long lattices, $\kappa$ grows as $\kappa \approx 2.4 \log N$ upto $N \sim 300$, and then slowly decreases. (Calculations for $N > 1000$ we couldn’t perform because of computational limitations).

Note, that all phonon states are localized for the 1D lattice\cite{24,25}. It was proven for the electroconductance problem\cite{24} that the electroconductivity tends to zero as the absolute temperature also tends to zero. As to our knowledge, there is no such a statement for the thermal conductance of disordered 1D systems. But in the weak coupling approximation, i.e. at $\gamma \ll 1$ it was supposed that for the rigid boundary conditions $\kappa \sim 1/\sqrt{N}$, i.e. tends to zero\cite{24}. (Recall the strange result that at free boundary conditions thermal conduction diverges as $\kappa \sim \sqrt{N}$).

It is probable that the slow decreasing of $\kappa$ for $N > 300$ observed in Fig. 3 is the manifestation of the tendency of $\kappa$ to zero when $N \to \infty$. We couldn’t check this fact because of computational limitations.

The thermal conduction was calculated according to $\kappa = -J \Delta T$, where $\Delta T$ was defined as the temperature difference on the lattice ends (it is impossible to determine the temperature in the vicinity of a lattice center, because of an existence of localized modes with extremely long time of life). Therefore we restricted ourselves by such a simple expression which is valid by the order of magnitude.

In Conclusion we say that the solved problem partially continues the classical works of Libowitz with co-workers\cite{26,27} on the dynamics of 1D disordered systems. We investigated the kinetic, dynamical and transport properties of 1D isotopically disordered harmonic lattice. The accuracy of our computations for all values, except the relaxation times, is limited by values of the order of $10^{-14}$. We’ve succeeded to calculate the relaxation times with the precision $10^{-28}$. Our precision...
of solution is determined by standard matrix operations performed on PC with double precision. Relaxation times calculated by us many orders of magnitude exceed any value obtained in direct numerical simulations. We’ve got non-monotonic dependence of thermal conduction which is dependent on \( N \) with maximum at \( N \sim 300 \). The stationary state is unique but times of its achievement grow with the increase in chain length. Because of additivity of all results on temperature \( \Theta \), the detailed calculations can be done at single chosen temperature at the chain ends.

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