Heat Conduction in One-Dimensional chain of Hard Discs with Substrate Potential

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9th January 2022

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Abstract

Heat conduction of one-dimensional chain of equivalent rigid particles in the field of external on-site potential is considered. Zero diameters of the particles correspond to exactly integrable case with divergent heat conduction coefficient. By means of simple analytical model it is demonstrated that for any nonzero particle size the integrability is violated and the heat conduction coefficient converges. The result of the analytical computation is verified by means of numerical simulation in a plausible diapason of parameters and good agreement is observed.

1 Introduction

Heat conductivity in one-dimensional (1D) lattices is a well known classical problem related to the microscopic foundation of Fourier’s law. The problem started from the famous work of Fermi, Pasta, and Ulam (FPU) \cite{1}, where an abnormal process of heat transfer was detected for the first time. Non-integrability of a system is a necessary condition for normal heat conductivity. As it was demonstrated recently for the FPU lattice \cite{2, 3, 4}, disordered harmonic chain \cite{5, 6, 7}, diatomic 1D gas of colliding particles \cite{8, 9, 10, 11}, and the diatomic Toda lattice \cite{12}, non-integrability is not sufficient in order to get normal heat conductivity. It leads to linear distribution of temperature along the chain for small gradient, but the value of heat flux is proportional to $1/N$, where $N$ is the number of particles of the chain, and number exponent $0 < \alpha < 1$. 

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Thus, the coefficient of heat conductivity diverges in the thermodynamic limit $N \rightarrow \infty$. Analytical estimations [4] have demonstrated that any chain possessing an acoustic phonon branch should have infinite heat conductivity in the limit of low temperatures.

From the other side, there are some artificial systems with on-site potential (ding-a-ling and related models) which have normal heat conductivity [13, 14]. The heat conductivity of the Frenkel-Kontorova chain was first considered in Ref. [15]. Finite heat conductivity for certain parameters was observed for Frenkel-Kontorova chain [16], for the chain with sinh-Gordon on-site potential [17], and for the chain with on-site potential [18, 19]. These models are not invariant with respect to translation and the momentum is not conserved. It was supposed that the on-site potential is extremely significant for normal heat conduction [18] and that the anharmonicity of the on-site potential is sufficient to ensure the validity of Fourier’s law [20]. A recent detailed review of the problem is presented in Ref. [21].

Probably the most interesting question related to heat conductivity of 1D models (which actually inspired the first investigation of Fermi, Pasta and Ulam [1]) is whether small perturbation of an integrable model will lead to convergent heat conduction coefficient. One supposes that for the one-dimensional chains with conserved momentum the answer is negative [22]. Still, normal heat conduction has been observed in some special systems with conserved momentum [23, 24, 25], but it may be clearly demonstrated only well apart from integrable limit.

The situation is not so clear in the systems with on-site potential. Although it was supposed that non-integrable system without additional integrals of motion would have convergent heat conductivity [22], no rigorous proof was presented. From the other side, recent attempt of numerical simulation of heat transfer in Frenkel-Kontorova model [26] demonstrated that because of computational difficulties no unambiguous conclusion can be drawn whether heat conduction is convergent for all finite values of perturbation of the integrable limit system (linear chain or continuous sine-Gordon system).

It seems that computational difficulties of investigation of heat conduction in a vicinity of integrable limit are not just issue of weak computers or ineffective procedures. In the systems with conserved momentum divergent heat conduction is fixed by power-like decrease of heat flux autocorrelation function with power less than unity. Still, for the systems with on-site potential exponential decrease is more typical [26]. For any fixed value of the exponent the heat conduction converges; if the exponent tends to zero with the value of the perturbation of the integrable case, then for any finite value of the perturbation the characteristic correlation time and length will be finite but may become very large. Consequently, they will exceed any available computation time or size of the system and still no conclusion on the convergence of heat conduction will be possible.

In this respect it is reasonable to mention the findings of our papers [24, 25, 26] concerning the transitions from infinite to finite heat conduction in the chain of rotators and Frenkel-Kontorova system. These findings were criticized in paper [27] by providing the computation results for larger systems. We agree with the authors that the results of papers [24, 25] do not prove the reality of the above transition. In fact, we have pointed it out in [26]. From the other side, it is clear that such more extended numerical simulations cannot prove that the transitions do not exist at all. Probably, such conclusion may be driven if, with the help of some not yet developed method, the simulation length or effective time will be extended by many orders of magnitude.

The other way to overcome this difficulty is to construct a model, which will be, at least to some extent, tractable analytically and will allow one to predict some characteristic features of the heat transfer process and the behavior of the heat conduction coefficient. Afterwards the numerical simulation may be used to verify the assumptions made in the analytic treatment. To the best of our knowledge, no models besides pure harmonic chains were treated in such a way to date. Introduction and investigation of a nontrivial model of this sort is a scope of present paper.

We are going to demonstrate that there exist models which have integrable system as their natural limit case, small perturbation of the integrability immediately leading to convergent heat conduction. The mechanism of energy scattering in this kind of systems is universal for any temperature and set of the
model parameters. The simplest example of such model is one-dimensional set of equal rigid particles with nonzero diameter \( (d > 0) \) subjected to periodic on-site potential. This system is completely integrable only if \( d = 0 \). It will be demonstrated that any \( d > 0 \) leads to effective mixing due to unequal exchange of energy between the particles in each collision. This mixing leads to diffusive mechanism of the heat transport and, subsequently, to convergent heat conduction.

### 2 Description of the model

Let us consider the one-dimensional system of hard particles with equal masses subject to periodic on-site potential. The Hamiltonian of this system will read

\[
H = \sum_n \left( \frac{1}{2} M \dot{x}_n^2 + V(x_{n+1} - x_n) + U(x_n)g; \right)
\]

where \( M \) – mass of the particle, \( x_n \) – coordinate of the center of the \( n \)-th particle, \( \dot{x}_n \) – velocity of this particle, \( U(x) \) – periodic on-site potential with period \( a \) \( U(x) = U(x+a) \). Interaction of absolutely hard particles is described by the following potential

\[
V(r) = \begin{cases} 1 & \text{if } r < d \\ 0 & \text{if } r > d; \end{cases}
\]

where \( d \) is the diameter of the particle. This potential corresponds to pure elastic impact with unit recovery coefficient. Sketch of the model considered is presented at Fig. 1.

It is well-known that the elastic collision of two equal particles with collinear velocity vectors leads to exchange of their velocities. An external potential present does not change this fact, since the collision takes zero time and thus the effect of the external force on the energy and momentum conservation is absent.

The one-dimensional chain of equivalent hard particles without external potential is a paradigm of the integrable nonlinear chain, since all interactions are reduced to exchange of velocities. In other words, the individual values of velocities are preserved and just transferred from particle to particle. It is natural therefore to introduce quasiparticles associated with these individual values of velocities. They will be characterized by a pair of parameters \( (E_k, n_k) \), where \( E_k = \sqrt{2} \) is an energy of the quasiparticle, \( n_k \) is a unit vector in a direction of its motion. Every particle in every moment ”carries” one quasiparticle. The elastic collision between the particles leads to simple exchange of parameters of the associated quasiparticles, therefore the quasiparticles themselves should be considered as non-interacting.
The situation changes if the external on-site potential is present. It is easy to introduce similar quasi-particles (\(E_k\) will be a sum of kinetic and potential energy). The unit vector \(n\) of each quasiparticle between subsequent interactions may be either constant (motion in one direction) or periodically changing (vibration of the particle in a potential well). In every collision the particles exchange their velocity vectors, but do not change their positions. Consequently two quasiparticles interact in a way described by the following relationships:

\[
\begin{align*}
E_0^1 &= E_1 + U (x_c + d=2) U (x_c - d=2); \\
E_0^2 &= E_2 U (x_c + d=2) + U (x_c - d=2); \\
n_0^1 &= n_1^1; \\
n_0^2 &= n_2^1.
\end{align*}
\]  

The values denoted by apostrophe correspond to the state after the collision, \(x_c\) is a point of contact between the particles. It should be mentioned that in the case of nonzero diameter the quasiparticles are associated with the centers of the carrying particles.

If the diameter of the particles is zero, then the additives to the energies in the first two equations of system (3) compensate each other and the energies of the quasiparticles are preserved in the collision. Therefore effectively the interaction between the quasiparticles disappears and the chain of equal particles with zero size subject to any on-site potential turns out to be completely integrable system. Thus, contrary to some previous statements it is possible to construct an example of strongly nonlinear one-dimensional chain without momentum conservation, which will have clearly divergent heat conductivity (even linear temperature profile will not be formed).

The situation differs if the size of the particles is not zero, as the individual energies of the quasiparticles are not preserved in the collisions. In order to consider the effect of such interaction we propose simplified semi-phenomenological analytical model.

After 1 collisions the energy of the quasiparticle will be

\[
E (l) = E_0 + \sum_{j=1}^{x^1} E_j; \quad E_j = U (x_j + d=2) U (x_j - d=2); \quad j=1, \ldots, x^1
\]

where \(j\)-th collision takes place in point \(x_j\), \(E_0\) is the initial energy of the quasiparticle. Now we suppose that the coordinates of subsequent contact points \(x_1; x_2; \ldots; x_j; \ldots\), taken by modulus of the period of the on-site potential, are not correlated. Such proposition is equivalent to fast phase mixing in a system close to integrable one and is well-known in various kinetic problems \([28]\). The consequences of this proposition will be verified below by direct numerical simulation.

Average energy of the quasiparticle is equal to \(\langle E_0 \rangle\) over the ensemble of the quasiparticles, as obviously \(\langle E_j \rangle = 0\). Still, the second momentum will be nonzero:

\[
\langle E (l) \rangle = \langle E_0 \rangle^2 = \langle E_0 \rangle \langle U (x + d=2) U (x - d=2) \rangle
\]

The right-hand side of this expression will depend only on the exact shape of the potential function

\[
\langle E (l) \rangle = \langle E_0 \rangle^2 = \int F (d) \left( \frac{1}{a} \int_0^a U (x + d=2) U (x - d=2) \right) dx;
\]

where \(F (d) = \frac{1}{a} \int_0^a U (x + d=2) U (x - d=2) dx\).

The last expression is correct only at the limit of high temperatures; it neglects the fact that the quasiparticle spends more time near the top of the potential barrier due to lower velocity.

Let us consider the quasiparticle with initial energy \(E_0 > U_0\), where \(U_0\) is the height of the potential barrier. Therefore vector \(n\) is constant. Equations (5) and (6) describe random walks of the energy of the
quasiparticle along the energy scale axis. Therefore after certain number of steps (collisions) the energy of the quasiparticle will enter the zone below the potential barrier $E(l) < U_0$. In this case the behaviour of the quasiparticle will change, as constant vector $\mathbf{n}$ will become oscillating, as described above. After some additional collisions the energy will again exceed $U_0$, but the direction of motion of the quasiparticle will be arbitrary. It means that the only mechanism of energy transfer in the system under consideration is associated with diffusion of the quasiparticles, which are trapped by the on-site potential and afterwards released in arbitrary direction. Such traps-and-releases resemble Umklapp processes of phonon-phonon interaction [28], but occur in a purely classic system.

The diffusion of the quasiparticles in the chain is characterized by mean free path, which may be evaluated as

$$\frac{2a h (U_0 - E_0)^2}{n_c F'(d)} + \frac{2a [\mathbf{F}(d)]^2}{n_c F'(d)} + \frac{2U_b k_B T + U_0^2}{k_B T};$$

where $n_c$ is a number of particles over one period of the on-site potential (concentration). Coefficient 2 appears due to equivalent probability of positive and negative energy shift in any collision, $T$ – temperature of the system, $k_B$ – Boltzmann constant.

Average absolute velocity of the quasiparticle may be estimated as

$$\mathbf{v} = \frac{a}{n_c d} \frac{k_B T}{2};$$

Here the first multiplier takes into account the nonzero value of $d$ and absolute rigidity of the particles. The second one is due to standard Maxwell distribution function for 1D case.

Heat capacity of the system over one particle is unity, as the number of degrees of freedom (i.e. the number of quasiparticles) coincides with the number of the particles and does not depend on the temperature and other parameters of the system. Therefore the coefficient of heat conductivity may be estimated [28] as

$$\frac{8(2T^2 \mathbf{F}(d) + 2T + 1)}{2T + 1} F(d);$$

It is already possible to conclude that according to (9) regardless the concrete shape of potential $U(x)$ in the limit $d \to 0$ we have $\mathbf{F}(d) \to 0$ and therefore $\to 1$, although for every nonzero value $d$ the heat conductivity will be finite. Therefore unlikely known models with conserved momentum the small perturbation of the integrable case $d = 0$ immediately brings about convergent heat conductivity.

4 Numerical simulations

It is convenient to introduce the dimensionless variables for the following numerical simulation. Let us set the mass of each particle $M = 1$, on-site potential period $a = 2$, its height $U_0 = 1$, and Boltzmann constant $k_B = 1$ in all above relationships. We suppose that the chain contains one particle per each period of the potential, i.e. that $n_c = 1$, and the particle diameter $0 < d < 2$.

Let us consider periodic piecewise linear on-site potential

$$U(x) = \begin{cases} x & \text{if } x \in [0;1]; \\ 2 & \text{if } x \in [1;2]; \\ U(x + 2l) & \text{if } x \in [0;2); \text{ for } l = 0; 1; 2; \ldots \end{cases};$$

(the shape of the potential is presented at Fig. 1). Then it follows from (9) that the non-dimensional heat conduction coefficient is expressed as

$$= \frac{8(2T^2 \mathbf{F}(d) + 2T + 1)}{2T + 1} F(d);$$

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where function \[ F(d) = \begin{cases} d^2 & \text{for } 0 < d < 1 \\ 4 = 3 + 4d & 3d^2 + 2 = 3d^2 & \text{for } 1 < d < 2 \end{cases} \] \hspace{1cm} (12)

The numerical scheme for solving the equations of motion describing the dynamics of the 1D hard-point gas has been developed in a series of papers [29, 8, 30].

Dynamics of the system of particles with potential of the nearest-neighbor interaction (2) and piecewise linear on-site potential (10) may be described exactly. Between the collisions each particle moves under constant force with sign dependent on the position of the particle. Therefore the coordinate of each particle depends on time as piecewise parabolic function which may be easily computed analytically. If the particle centers are situated at distance equal to \( d \), then elastic collision occurs. The particles exchange their momenta as described above and afterwards the particle motion is again described by piecewise parabolic functions until the next collision.

Let us consider finite chain of \( N \) particles with periodic boundary conditions. Let at the moment \( t = 0 \) one particle be at each potential minimum and let us choose Boltzmann's distribution of the initial velocity. Solving the equations of motion, we find a time \( t_1 \) of the first collision between some pair of the adjacent particles, next a time \( t_2 \) of the second collision, in general between another pair of the adjacent particles, and so on. As a result, we obtain a sequence \( t_1, t_2, \ldots, t_{I_k} \), where \( t_k \) is the time of the \( k \)th collision in the system, and \( n_1 \) and \( n_1 + 1 \) are the particles participating in this collision. Since we need to implement numerical simulations as long as possible, in order to find the time asymptotic of the heat flux autocorrelation function entering the Green-Kubo formula, we use the numerical scheme of paper [9]. First, we incorporate the energy change of the \( n \)th particle during the \( k \)th collision as

\[ E_{n_k} = \frac{1}{2} (v_{n_k}^2 - v_{n_k + 1}^2) \]

Next, we introduce a time step \( \tau \), which is significantly less than the simulation time, but satisfies the inequality \( \tau < \tau_0 \), where \( \tau_0 = \frac{1}{\ln I_k} \), (\( t_k = 0 \)) is the mean time between successive collisions. Then, for each \( k = 0; 1; \ldots \), we define the local energy flow as a piecewise constant (in time) function

\[ j_k(t) = a \frac{\tau}{I_k}, k \tau < (k + 1) \tau \]

where the integer sets \( I_k \)'s are defined by

\[ I_k = fi j k t \tau < (k + 1) \tau; n_1 = ng \]

The set \( I_k \) takes into account those collisions that occur between particles \( n \) and \( n + 1 \) during the time interval \( k \tau < (k + 1) \tau \). Equilibration times were typically occurring in the system of the order \( 10^6 \). After these times have passed, we define the time-averaged local thermal flow

\[ J_n = \frac{1}{Z} \frac{1}{t_0} \lim \frac{1}{t} j_k(t) \]

and the temperature distribution \( T_n = \frac{1}{Z} \frac{1}{t_0} \lim \frac{1}{t} j_k(t) \). To find these averaged quantities, we have used times up to \( 10^7 \).

To find the heat flux autocorrelation function \( C(t) \) numerically, we calculated the time mean \( h \mathcal{J}(\tau) = \int_0^\infty J(t) T^2 \), with \( J(t) = \frac{1}{N} \sum _n j_k(t) \) being the total heat flow through the gas/chain system consisting of \( N = 500 \) particles and temperature \( T = \frac{1}{N} \sum _n T_n \) averaged over \( 10^6 \) realizations of initial thermalization.

Numerical simulation of the dynamics demonstrates exponential decrease of the autocorrelation \( C(t) \) for all values of the diameter \( 0 < d < 2 \) and temperature \( T > 0 \) where the simulation time is
plausible from technical viewpoint. For low temperatures however the exponential decrease is accompanied by oscillations with period corresponding to the frequency of the vibrations near the potential minima (Fig. 2). The reason is that if the temperatures are low, the concentration of transient particles decreases exponentially and majority of the particles vibrates near the potential minima. It means that the 1D gas on the on-site potential has finite heat conductivity. Coefficient of the exponential decrease of the autocorrelation function

$$\lim_{t \to 1} \frac{\ln C(t)}{t}$$

(15)

and coefficient of the heat conduction

$$z \int_0^\infty C(t)dt;$$

(16)

are computed numerically.

Dependence of and on particle diameter $d$ is presented at Fig. 3. Maximum of and minimum of is attained at $d = 1 \pi$. As the temperature grows, decreases [Fig. 4 (a)], and heat conduction increases [Fig. 4 (a)].

Theoretical analysis of the heat conductivity presented above allows only approximate [although rather reliable, see Figs. 3(b), 5] prediction of the numerical value of the heat conduction coefficient $\lambda$. Still, the other question of interest is the asymptotic dependence of the heat conduction on the parameters of the model. Formulae (11), (12) lead to the following estimations:

$$T^{5/2}; \quad \text{for } T \to 1;$$

(17)

$$d^2; \quad \text{for } d \to 0;$$

(18)
Figure 3: Dependence of the coefficient of the exponential decrease of the autocorrelation function (a) and the coefficient of the heat conduction (b) on the particle diameter $d$ of 1D gas at $T=1$. Curves 1 and 2 correspond to piecewise linear on-site potential (10), curve 3 represent theoretical predictions according to formula (11).
Figure 4: Temperature dependence of exponent coefficient (a) and heat conduction coefficient (b) for particle diameter \( d = 0.5 \).
Figure 5: Dependence of heat conduction coefficient on the temperature. The markers correspond to numerical results ($\ln \kappa$ versus $\ln T$), the straight line is $\ln \kappa = 2.5 \ln T + 3.45$, corresponding to (17). Particle diameter $d = 0.5$.

These estimations should be compared to numerical results.

In order to check estimation (17) we consider the dependence of the logarithm of the heat conduction $\ln \kappa$ on the logarithm of the temperature $\ln T$. From Fig. 5 it is clear that in accordance with (17) $\ln \kappa$ grows as $2.5 \ln T$ as $T \to 1$. Fig. 6 (a) demonstrates that as $d \to +0$, the logarithm $\ln \kappa$ grows as $2 \ln d$, in accordance with (18). Fig. 6 (b) demonstrates that as $d \to 2 - 0$, the logarithm $\ln \kappa$ grows as $3 \ln (2 - d)$, in accordance with (19). So, it is possible to conclude that analytical estimations (17), (18) and (19) fairly correspond to the numerical simulations data.

The above analytical estimations imply that the type of dependence of characteristic exponent and heat conductivity on diameter $d$ and temperature $T$ does not depend on the concrete shape of on-site potential $U(x)$ — actually, only its finiteness and periodicity do matter. Piecewise linear periodic potential (10) was chosen since it allowed essential simplification of the numerical procedure. For comparison we have considered also the smooth sinusoidal periodic potential

$$U(x) = \left\lfloor \cos(u) \right\rfloor_{-2}$$

with period 2 and amplitude $U_0 = 1$, similarly to potential (10).
Figure 6: Dependence of the heat conduction coefficient on the particle diameter (logarithmic coordinates, $\ln \kappa$ versus $\ln d$ (a) and versus $\ln (2 - d)$ (b), curves 1 and 3). Lines $\ln \kappa = 2 \ln d$ (curve 2) and $\ln \kappa = 3 \ln (2 - d)$ (curve 4) correspond to relationships (18) and (19). Temperature $T = 1$.
Figure 7: Dependence of the coefficient of the exponential decrease of the autocorrelation function (a) and the coefficient of the heat conduction (b) on the particle diameter $d$ of 1D gas at $T=1$. Curves 1 and 2 correspond to smooth on-site potential (20), curve 3 represent theoretical predictions according to formula (11).
Potential (20) does not allow exact integration and requires standard numerical procedures. Therefore it is convenient also to change rigid wall potential (2) by smooth Lennard-Jones potential

\[
V (r) = \frac{1}{r} - \frac{1}{2d} r^2 \quad : \quad \text{(21)}
\]

Parameter \( \sigma > 0 \) characterizes rigidity of the potential, the hard-particle potential being the limit case:

\[
V (r) = \lim_{T \to +0} V (r) : \quad \text{(22)}
\]

Methods of computing of the autocorrelation function \( C(t) \) and the heat conduction coefficient in 1D chain with analytic potentials of interaction are described in [26] in detail. It should be mentioned that in order to get close to the limit of the hard particles we should use small values of \( T = 1 \) value \( = 0.01 \) was used). It implies rather small value of the integration step. (We used standard Runge-Kutta procedure of the fourth order with constant integration step \( t = 0.0001 \)). Therefore for the case of hard (or nearly hard) particles the simulation with smooth on-site potential (20) is far more time-consuming than the simulation with piecewise linear potential (2).

In the case of hard particles with smooth on-site potential the autocorrelation function \( C(t) \) decreases exponentially as \( t \to +0 \) for all range \( 0 < d < 2 \), \( T > 0 \), i.e. the heat conduction converges. Fig. 7 demonstrates that the type of dependence of of and on parameters \( d \) and \( T \) is similar for piecewise linear potential (2) and sinusoidal potential (20) (although numerical values and vary slightly). For this potential function \( F (d) = \frac{1}{2} \sin^2 (d=2) \). It confirms that type of heat conduction does not depend on concrete choice of on-site potential function.

5 Conclusion

We have considered the heat conduction process in the 1D lattice of hard particles with periodic on-site potential. Analytical treatment predicts that for zero diameter of the particles the system will be completely integrable regardless the exact shape of the on-site potential. Therefore the heat conductivity will be infinite. For any nonzero size of the particles the heat transfer is governed by diffusion of quasiparticles giving rise to finite heat conductivity. The value of the heat conduction coefficient computed by the analytical treatment is in line with numerical simulation data. This coincidence is very profound if speaking about the asymptotic scaling behavior of the heat conduction coefficient in the cases of small and large particle sizes, as well as for the case of high temperatures. The characteristic behavior of the heat conduction coefficient does not depend on the exact shape of the on-site potential function.

The above results mean that there exists a new class of universality of 1D chain models with respect to their heat conductivity. The limit case of zero-size particles is integrable, but the slightest perturbation of this integrable case by introducing the nonzero size leads to drastic change of the behavior – it becomes diffusive and the heat conduction coefficient converges. It should be stressed that this class of universality, unlikely the systems with conserved momentum, cannot be revealed by sole numerical simulation. The reason is that the correlation length (as well as the heat conduction coefficient) diverges as the system approaches the integrable limit; therefore any finite capacity of the numerical installation will be exceeded. That is why the analytical approach is also necessary.

The authors are grateful to Russian Foundation of Basic Research (grant 01-03-33122) and to RAS Commission for Support of Young Scientists (6th competition, grant No. 123) for financial support. O.V.G. is grateful to Russian Science Support Foundation for the financial support.

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