Heat Conduction in a One-Dimensional Chain of Hard Disks with Substrate Potential

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Heat conduction in a one-dimensional chain of equivalent rigid particles in the field of the external on-site potential is considered. The zero diameters of the particles correspond to the integrable case with the divergent heat conduction coefficient. By means of a 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.

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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) [1], where an abnormal process of heat transfer was initially revealed. Nonintegrability of a system is a necessary condition for normal heat conductivity. As was recently demonstrated for the FPU lattice [2–4], disordered harmonic chain [5–7], diatomic 1D gas of colliding particles [8–11], and the diatomic Toda lattice [12], nonintegrability is not sufficient in order to get normal heat conductivity. It leads to the linear distribution of temperature along the chain for a small gradient, but the value of the heat flux is proportional to $1/N^{\alpha}$, where N is the number of particles of the chain, and the number exponent $0 < \alpha < 1$. Thus the coefficient of heat conductivity diverges in the thermodynamic limit $N \to \infty$. Analytical estimations [4] have suggested that any chain possessing an acoustic phonon branch should have infinite heat conductivity in the limit of low temperatures.

On the other hand, there are some systems with the on-site potential that have normal heat conductivity [13–19]. 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 inspired the first investigation of Fermi, Pasta, and Ulam [1]) is whether the small perturbation of an integrable model will lead to the convergent heat conduction coefficient. It seems that for 1D chains with conserved momentum the answer is negative [22]. Still, normal heat conduction has been observed in some special systems with conserved momentum [23–25], but it may be clearly demonstrated only well apart from the integrable limit.

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

It seems that computational difficulties of investigation of heat conduction in a vicinity of the integrable limit are not just a result of weak computers or ineffective procedures. In the systems with conserved momentum divergent heat conduction is fixed by a powerlike 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 concerning the convergence of the heat conduction coefficient will be possible.

A way to overcome this difficulty is to construct a model, which will be, at least to some extent, analytically tractable 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, to date no models besides pure harmonic chains were treated in such a way. A description of such a model is the scope of present Letter.

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

$$\mathcal{H} = \sum_n \left\{ \frac{1}{2} M \dot{x}_n^2 + V(x_{n+1} - x_n) + U(x_n) \right\}, \quad (1)$$

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where M is the mass of the particle, x_n is the coordinate of the center of the nth particle, $\dot{x}_n$ is the velocity of this particle, and $U(x)$ is the periodic on-site potential with period a [$U(x) \equiv U(x + a)$]. The interaction of absolutely rigid particles is described by the following hard-core potential: $V(r) = \infty$ if $r \leq d$ and $V(r) = 0$ if $r > d$, where d is the diameter of the particle. This potential corresponds to pure elastic impact with unit recovery coefficient.

It is well-known that the elastic collision of two equal particles in one dimension leads to the exchange of their velocities. An external potential 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 the external potential is a paradigm of the integrable nonlinear chain, since all interactions are reduced to the exchange of velocities. It is therefore natural to introduce quasiparticles associated with these individual values of velocities. They are characterized by a pair of parameters $(E_k, \mathbf{n}_k)$, where $E_k = v_k^2/2$ is an energy of the quasiparticle, and $\mathbf{n}_k$ 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 a simple exchange of parameters of the associated quasiparticles; therefore the quasiparticles themselves should be considered as noninteracting.

The situation changes if the external on-site potential is present. It is easy to introduce similar quasiparticles (E_k will be a sum of kinetic and potential energies). The unit vector $\mathbf{n}$ 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), depending on whether the energy of the quasiparticle exceeds the potential barrier. In every collision the particles exchange their velocity vectors but do not change their positions. Two quasiparticles then interact as follows:

$$E_1' = E_1 + U(x_c + d/2) - U(x_c - d/2), \qquad \mathbf{n}_1' = \mathbf{n}_1,$$
$$E_2' = E_2 - U(x_c + d/2) + U(x_c - d/2), \qquad \mathbf{n}_2' = \mathbf{n}_2.$$

The prime denotes the state after the collision; x_c is a point of contact between the particles. In the case of a 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 compensate each other and the energies of the quasiparticles are preserved in the collision. Therefore the interaction between the quasiparticles effectively disappears and the chain of equal particles with zero size subject to any on-site potential turns out to be a completely integrable system. Thus, contrary to some previous statements, it is possible to construct an example of a strongly nonlinear one-dimensional chain without momentum conservation, which will have divergent heat conductivity.

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. After l collisions the energy of the quasiparticle will be

$$E(l) = E_0 + \sum_{j=1}^{l} \Delta E_j,$$
$$\Delta E_j = U\left(x_j + \frac{d}{2}\right) - U\left(x_j - \frac{d}{2}\right), \tag{2}$$

where jth collision takes place in point x_j, and E_0 is the initial energy of the quasiparticle. Now we suppose that the coordinates of subsequent contact points $\{\ldots, x_{j-1}, x_j, x_{j+1}, \ldots\}$, taken by the modulus of the period of the on-site potential, are not correlated. Such a proposition is equivalent to fast phase mixing [27].

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

$$\langle [E(l) - E_0]^2 \rangle = l \left\langle \left[U\left(x + \frac{d}{2}\right) - U\left(x - \frac{d}{2}\right) \right]^2 \right\rangle_x = lF(d). \tag{3}$$

The right-hand side of this expression depends only on the exact shape of the potential function $F(d) = \frac{1}{a}\int_0^a [U(x + d/2) - U(x - d/2)]^2 dx$. This 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 $\mathbf{n}$ is constant. Equation (3) describes random walks of the energy of the quasiparticle along the energy scale axis. Therefore, after a certain number of steps (collisions), the energy of the quasiparticle enters the zone below the potential barrier $E(l) < U_0$. In this case the behavior of the quasiparticle changes, as the constant vector $\mathbf{n}$ becomes oscillating, as described above. After some additional collisions the energy again exceeds U_0, but the direction of motion of the quasiparticle is arbitrary. It means that the only mechanism of energy transfer in the system under consideration is associated with the diffusion of the quasiparticles, which are trapped by the on-site potential and afterwards released in arbitrary direction.

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

$$\lambda \sim \frac{2a\langle (U_0 - E_0)^2 \rangle}{n_c F(d)} \sim \frac{2a[2(k_B T)^2 - 2U_0 k_B T + U_0^2]}{n_c F(d)}, \tag{4}$$

where n_c is a number of particles over one period of the

on-site potential (concentration). Coefficient 2 appears due to an equivalent probability of positive and negative energy shifts in any collision, T is the temperature of the system, and k_B is the Boltzmann constant.

The average absolute velocity of the quasiparticle may be estimated as $\langle|v|\rangle \sim a\sqrt{\pi k_B T/2}/(a - n_c d)$. Here the divisor takes into account the nonzero value of d and absolute rigidity of the particles. The dividend is due to the standard Maxwell distribution function for the 1D case.

The heat capacity of the system over one particle is unity, as the number of the quasiparticles is constant. Therefore the coefficient of heat conductivity may be estimated [27] as

$$\kappa \sim \lambda\langle|v|\rangle \sim \frac{2a^2[2(k_B T)^2 - 2U_0 k_B T + U_0^2]}{n_c(a - n_c d)F(d)}\sqrt{\frac{\pi k_B T}{2}}. \tag{5}$$

It is already possible to conclude that, according to (5), regardless of the concrete shape of the potential $U(x)$ in the limit $d \to 0$, we have $F(d) \to 0$ and therefore $\kappa \to \infty$, although for every nonzero value d the heat conductivity is finite. Therefore the small perturbation of the integrable case $d = 0$ immediately brings about convergent heat conductivity.

It is convenient to introduce the dimensionless variables for the following numerical simulation. Let us set the mass of each particle $M = 1$, the on-site potential period $a = 2$, its height $U_0 = 1$, and the 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 the periodic piecewise linear on-site potential: $U(x) = x$, if $0 \le x \le 1$; $U(x) = 2 - x$, if $1 \le x \le 2$ [$U(x + 2) \equiv U(x)$]. Then it follows from (5) that the nondimensional heat conduction coefficient is expressed as

$$\kappa = (2T^2 - 2T + 1)\sqrt{\pi T/2}/(2 - d)F(d), \tag{6}$$

where function $F(d) = d^2 - 2d^3/3$, for $0 < d \le 1$, and $F(d) = -4/3 + 4d - 3d^2 + 2d^3/3$, for $1 \le d < 2$.

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 [8,28,29] based on the exact analytical solution of the equations of motion between collisions and reconsidering the initial conditions after each collision. In order to increase the simulation time, the numerical scheme of paper [9] is used. To find the heat flux autocorrelation function $C(t)$ numerically, we calculated the time mean $\langle J(\tau)J(\tau - t)\rangle_\tau/NT^2$, where $J(t)$ is the total heat flow through the gas/chain system consisting of $N = 500$ particles and T is the temperature of the system, averaged over 10^4 realizations of initial thermalization.

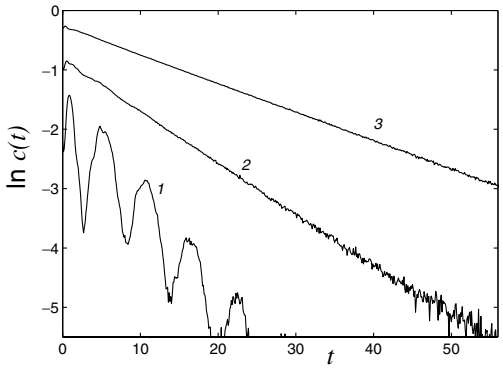

FIG. 1. Correlation function of the system of particles with $d = 0.5$ under temperatures $T = 0.24$, 0.45, and 0.75 (curves 1, 2, and 3).

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

The dependence of α and κ on particle diameter d is presented in Fig. 2. The maximum of α and the minimum of κ are attained at $d = 1.4$. As the temperature grows, α decreases and heat conduction κ increases.

A theoretical analysis of the heat conductivity presented above allows one only an approximate (although rather reliable; see Fig. 2) prediction of the numerical value of the heat conduction coefficient κ. Still, the other

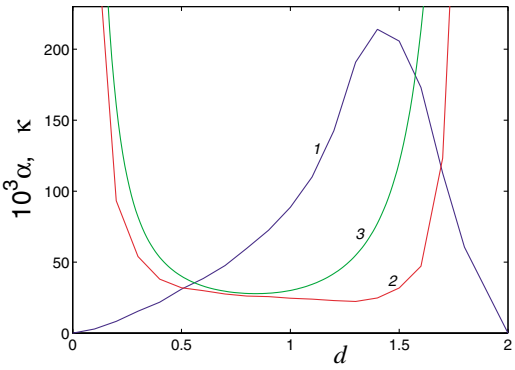

FIG. 2 (color online). Dependence of the coefficient of the exponential decrease of the autocorrelation function α (curve 1) and the coefficient of the heat conduction κ (curve 2) on the particle diameter d of 1D gas at $T = 1$. Curve 3 represents theoretical predictions according to formula (6).

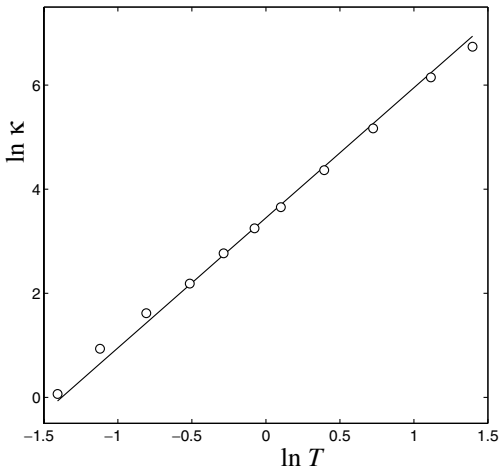

FIG. 3. Dependence of the heat conduction coefficient on the temperature. The markers correspond to numerical results ($\ln\kappa$ versus $\ln T$); the straight line is $\ln\kappa = 2.5\ln T + 3.45$, corresponding to estimations $\kappa \sim T^{5/2}$ (diameter $d = 0.5$).

question of interest is the asymptotic dependence of the heat conduction on the parameters of the model. Formula (6) leads to the following estimation for the temperature dependence of the heat conduction coefficient: $\kappa \sim T^{5/2}$, for $T \to \infty$. Figure 3 demonstrates that this analytical estimation perfectly corresponds to the numerical simulation data.

We have considered the heat conduction process in the 1D lattice of hard particles with the periodic on-site potential. An analytical treatment predicts that for zero diameter of the particles the system will be completely integrable regardless of 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 the 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 case of high temperatures.

It should be stressed again that the behavior of the heat conduction coefficient described above cannot be revealed only by numerical simulation, unlike the systems with conserved momentum. 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. This is why the analytical approach is also necessary.

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