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1992 J. Phys. A: Math. Gen. 25 3449

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# Energy transport and detailed verification of Fourier heat law in a chain of colliding harmonic oscillators

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Received 23 December 1991, in final form 6 March 1992

**Abstract.** We study a simple nonlinear classical Hamiltonian system with positive  $K$ -entropy, a model for heat conduction, and we find that it obeys the Fourier heat law. Numerical simulation of its dynamics can be performed very efficiently, so we are able to explore it in detail. We verify the Fourier heat law and calculate the coefficient of thermal conductivity  $K$  by three independent methods. The first is direct simulation, i.e. simulating the dynamics of the chain between two heat reservoirs. The second is Green–Kubo formalism which is derived in a self-contained manner. The third method—the one-sided heating of semi-infinite cold chain—is new and gives the best results. It yields the entire temperature dependence  $K(T)$  in a single numerical simulation and definitely demonstrates the validity of the Fourier heat law at all temperatures for the given system. We believe that this method can also be useful for other systems. We derive analytically the asymptotic behaviour of the coefficient of thermal conductivity at low temperatures  $T \rightarrow 0$  and observe that it agrees with numerical results obtained by the Green–Kubo formalism, which gives by far the best results at very low temperatures.

## 1. Introduction

### 1.1. History

Understanding macroscopic phenomena and their statistical laws in terms of deterministic microscopic dynamics has been one of the outstanding problems in the field of statistical physics ever since the pioneering works by Maxwell and Boltzmann and generally it is still a major challenge (Lebowitz and Spohn 1983). The fundamental question behind such studies is the understanding of the origin of the irreversibility and its compatibility with the time reversible deterministic microscopic dynamics (Peierls 1979). Among the problems of primary importance in this context are the transport phenomena, such as Fick's law of self-diffusion (Lebowitz and Spohn 1982, 1983) and the Fourier law of heat conduction (Lebowitz and Spohn 1978, Casati 1985). Microscopic understanding of heat conduction is still an open problem. In general, we are unable to derive the Fourier heat law from the microscopic equations of motion, which states that heat current is proportional to the negative gradient of the temperature.

However there is one important special case, namely the Lorentz gas in the Boltzmann–Grad limit, discussed by Lebowitz and Spohn (1978) in which an analytic theory and proof of the Fourier heat law has been successful. The Lorentz gas by definition consists of independent non-interacting point particles (wind particles)

moving freely among the randomly situated hard spherical scatterers of radius  $R$  and density  $\rho$ . (Upon hitting a scatterer a wind particle is specularly reflected.) The Boltzmann–Grad limit is defined by  $\rho \rightarrow \infty$ ,  $R \rightarrow 0$  but such that the mean free path  $1/(\rho R^2)$  is fixed and finite, whilst the volume  $\rho R^3$  occupied by the spherical obstacles goes to zero. Their approach is special in the sense that they actually look at an ensemble of statistically similar Lorentz gas systems, rather than analysing an individual deterministic dynamical system. Moreover, in the said Boltzmann–Grad limit the internal structure of the underlying Hamiltonian dynamical system becomes *infinitely complicated* ( $\rho \rightarrow \infty$ ), which obscures (what we feel to be) the essential point, namely that the Fourier heat law can be a consequence of a simply defined but non-integrable and chaotic dynamics. In this spirit the derivation of the Fourier heat law is still an open theoretical problem awaiting a general solution.

But on the other hand we can always solve the equations of motion numerically for systems, which consist of a sufficiently high number of particles, such that the thermodynamic limit is reached at least approximately. Even this is a very difficult task for reasons which we shall give later on. The first successful numerical simulations were performed only ten years ago. The reason for this is the following. Integrable systems (such as harmonic chains) which are the easiest to work with do not show any diffusive energy transport behaviour compatible with the Fourier heat law. The reason is that they possess indestructible normal modes which carry energy back and forth without any kind of dispersion because the energy stored in a given normal mode is a constant of motion. We need a mechanism which would destroy these constants of motion and therefore redistribute energy among the modes. Such a mechanism must also destroy the integrability of the system, because otherwise some other nonlinear normal modes would exist. Casher and Lebowitz (1971) showed analytically that a harmonic chain with randomly distributed masses seldom† obeys the Fourier heat law, which is in agreement with our argument.

It is not known what are the precise necessary and sufficient conditions for a system to obey the Fourier heat law. The numerical experiments by Casati (1985) on diatomic one-dimensional hard-point gas, which is a non-integrable system, were quite inconclusive because the thermodynamical limit was hardly reached. The chain of atoms and the observation time should be much longer. (This non-integrable system exhibits mixing but its  $K$ -entropy vanishes.)

So far the only convincing results have been obtained for systems with positive  $K$ -entropy. (However, hard chaos is more likely a sufficient rather than necessary condition for the validity of the Fourier heat law.) The first positive results for such systems were given by Mokross and Büttner (1983) for a diatomic Toda chain. But their system is somehow inconvenient for numerical investigations and their results are not very accurate. The first really convincing and accurate demonstration of the Fourier heat law in a classical system was given by Casati *et al* (1984). They took a chain of fixed equidistant hard-point harmonic oscillators and put a free particle of the same mass between each pair of them. They have checked the Fourier heat law at a fairly low temperature and showed that at high temperatures the energy transport is no longer diffusive and therefore the Fourier heat law no longer holds. They argued that their ding-a-ling model (as they called it) approaches the limit of monoatomic hard-point gas at high temperatures, which is integrable. In this integrable limit it is not inconceivable to find a sharp transition such that at temperatures higher than

† The measure of the set of those mass distributions for which the Fourier heat law is obeyed is zero.

a certain well defined critical temperature the Fourier heat law definitely would not apply. The same qualitative argument also holds for our model, and yet we have established the validity of the Fourier heat law at higher temperatures as we will show and discuss later on. So we do not find any sharp 'phase transition'.

Casati *et al* (1984) have employed two independent methods: direct simulation of the chain between two stochastic heat reservoirs with different temperatures; and the Green-Kubo formalism. They found that the results of both were in agreement, which is quite convincing. We have used these two methods as well, and devised a new one which gives by far the best results. In this way we confirm the results by Casati *et al* (1984) and complement them by increasing the statistical significance and particularly by studying the temperature dependence of the heat conductivity.

## 1.2. Motivation

The motivation for our work is twofold. In the first place we want to show the validity of the Fourier heat law in the simplest possible dynamical system, realized as a one-dimensional chain which is chaotic and has positive  $K$ -entropy. Second, we want to explore the temperature dependence of the coefficient of thermal conductivity  $K(T)$ , and find out for which temperature intervals the Fourier heat law holds and where it possibly ceases to hold, and what kind of transition would occur between these two regimes. It turned out that there is no such transition for our model, as the Fourier heat law is obeyed at all temperatures. This is the most natural interpretation of our results and we will explain it later.

In section 2 we will present the definition of our model and describe the basic properties of its chaotic dynamics.

In section 3 we will present the first numerical method in studying the energy transport which we call the direct method. It is simply a simulation of a real physical experiment. We consider the chain of length  $N$  and couple the first particle to the stochastic heat reservoir with temperature  $T_L$  and the last particle to another heat reservoir with temperature  $T_R$ . Then we observe two quantities while simulating the dynamics of the system, namely the heat current  $J$  through the system and the temperature gradient  $\nabla T$  in the system. The transport coefficient  $K_N$  is defined as  $s - J/\nabla T$  and the Fourier heat law states that this must be asymptotically independent of  $N$  i.e. the limit  $\lim_{N \rightarrow \infty} K_N$  must exist and must be equal to  $K$  by definition. The results obtained by this method will be presented and the difficulties in using it will be explained.

In section 4 we will derive the Green-Kubo formula from first principles and then specialize to the one-dimensional discrete chains. The results of calculations using the Green-Kubo formula are compared with those of the direct method.

The new method is presented in section 5 and is based on one-sided heating of the semi-infinite cold chain. We are interested in the non-stationary problem—simulating the heating of initially cold semi-infinite chain on one side by a single stochastic heat reservoir with temperature  $T_L$ . We study the time development of the total energy and the temperature profile of the chain. We find the scaling exponents as predicted by the Fourier heat law. Using this data we can deduce the entire function  $K(T)$  for the whole temperature interval  $0 < T < T_L$  and demonstrate that the Fourier heat law holds in this temperature interval.

## 2. Basic properties of dynamics

Our model system is a simplification of Casati's ding-a-ling model. The difference is that in our chain of fixed harmonic hard-point oscillators which are allowed to collide there are no free hard-point particles in between. We think that the introduction of free particles in order to obtain an efficient mechanism for the redistribution of energy among oscillators is not necessary. Our chain consists of harmonically bound particles of only one kind with a hard-core interaction among them. Between the elastic collisions of hard-point particles, they behave just as independent oscillators. We call this system the *ding-dong* model due to the onomatopoeic analogy with the ding-a-ling model.

Formally, our ding-dong system is described by the Hamiltonian  $H = \sum_{k=1}^N \{p_k^2/2m + m\omega^2 q_k^2/2\}$  with *collision conditions*  $q_{k+1} + a \geq q_k$  where  $a$  is a lattice constant and  $q_k$  is the distance of the  $k$ th oscillator from its fixing point. We have three parameters,  $m, \omega$  and  $a$ , which can all be eliminated by the introduction of dimensionless variables  $q_k/a \rightarrow q_k, p_k/(m\omega a) \rightarrow p_k, H/(m\omega^2 a^2) \rightarrow H$ . Note that after introducing the energy unit the unit of temperature is  $m\omega^2 a^2/k_B$ , where  $k_B$  is the Boltzmann constant. Our model now has no free parameters and can be simply written as

$$H = \frac{1}{2} \sum_{k=1}^N \{p_k^2 + q_k^2\} \quad (1)$$

$$q_{k+1} + 1 \geq q_k. \quad (2)$$

This is one of the simplest many-body Hamiltonians that one can imagine but it shows highly irregular dynamics. Besides the energy it possesses only one additional constant of motion namely the centre-of-mass-motion energy

$$E^* = \frac{1}{2} \left\{ \left( \sum_{k=1}^N p_k \right)^2 + \left( \sum_{k=1}^N q_k \right)^2 \right\}. \quad (3)$$

The dynamics of the system is trivial if the total energy  $E$  is lower than the threshold energy  $E_c = \frac{1}{4}$ . In that case the oscillators are unable to collide and are therefore effectively independent. The threshold energy  $E_c$  is defined by the minimal energy that two oscillators must have in order to collide:  $q_k = -q_{k+1} = \frac{1}{2}, p_k = p_{k+1} = 0, \sum_k (q_k^2 + p_k^2)/2 = \frac{1}{4}$ . Above the threshold the dynamics becomes highly irregular and the so called stochastic transition occurs (see figure 1).

One can easily show that the ding-dong model possesses interesting types of motion which can be called quasi-solitons. If we have all oscillators initially at rest  $q_k = p_k = 0$  and then hit the first oscillator to reach momentum  $p_1 > 1$  we observe that we get a *non-destructive localized pulse* which propagates through the 'cold' chain and leaves the cold chain behind for some discrete values of initial momentum  $p_1^{(n)} = 1/\cos(\pi/(2(n+1)))$  (Prosen 1991). Figure 2 shows the contrast between chaotic motion and regular motion of a quasi-soliton in a ding-dong chain.

Here we shall dedicate a few words to the numerical method and its efficiency analysis. Between two subsequent collisions the dynamics of the ding-dong chain remains trivial—the simple unfolding of equal-frequency sines. It takes only a small

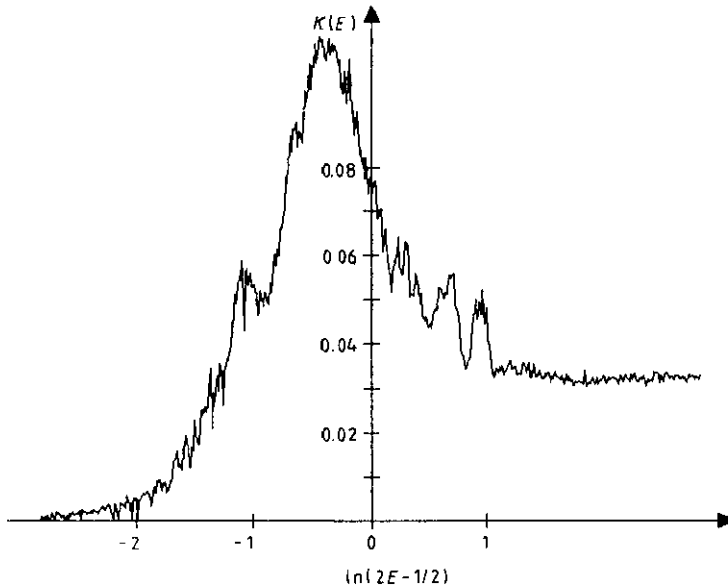


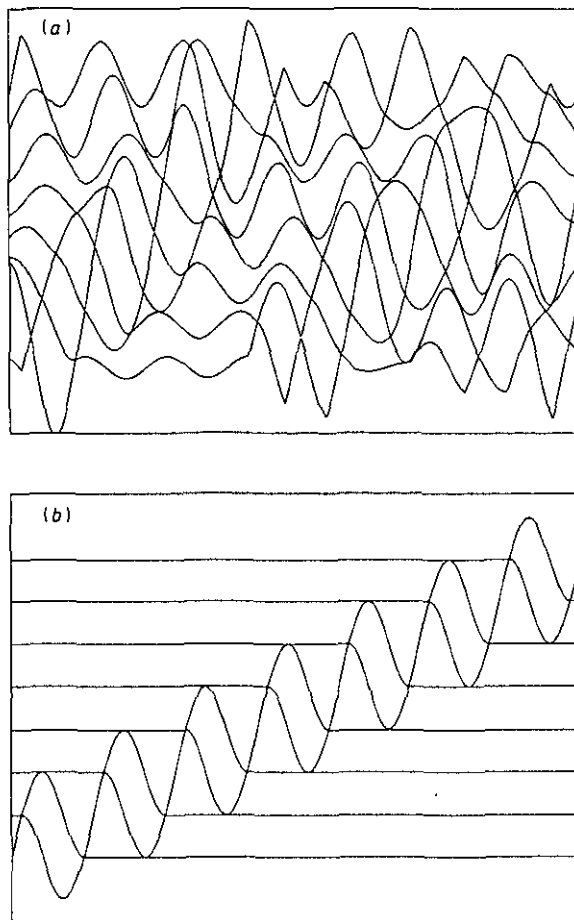
Figure 1. The  $K$ -entropy (i.e. the average maximal Lyapunov exponent) is plotted against the logarithm of energy  $E - E_c$  for the three-particle cyclic chain. The centre-of-mass motion was eliminated by setting  $E^* = 0$ , so the system has essentially two degrees of freedom. We have investigated the  $K$ -entropy for longer chains too but we have not observed any qualitative changes.

number of floating point operations to determine the time of the next collision if the coordinates at the previous collision are known. We call such a procedure a *one-step integration*. One can observe that almost any other non-trivial model of a chain of colliding particles requires solving the transcendental equation at each such one-step. In the case of the ding-a-ling model (Casati *et al* 1984) one must solve a transcendental equation of type  $at + b = \sin(t)$  at each step. Now we shall determine how many floating point operations are required in the one-step. Determination of the time of the next collision takes only one evaluation of the arctangent. Then we must transform the coordinates  $(q_k, p_k)$  to the time of next collision. One might think at first sight that this should take  $\mathcal{O}(N)$  floating point operations. But we can do much better. We do not need to transform the coordinates of all oscillators but only these of the participants in the collision. We must also know where the next collision will occur so we must know the *predicted time of collision* for each pair of particles. We shall not go into details here but we only mention that we managed to develop an algorithm that takes only  $\mathcal{O}(\log(N))$  operations per one-step by careful book-keeping of predicted times and by transforming only what is necessary at each step (Prosen 1991), which is an application of searching methods in sophisticated data structures (heaps). For technical details the reader is referred, for example, to Knuth (1968).

### 3. Direct simulation method

#### 3.1. Preparation of the numerical experiment

The direct method is the most natural experiment that one can imagine in this context.



**Figure 2.** The figure shows a typical chaotic trajectory (a) of the eight-particle cyclic chain. Time increases in horizontal direction and the distinct lines correspond to the distinct oscillators. A very atypical trajectory is the quasi-soliton (b) which represents the only type of non-diffusive low-energy transport.

Take the chain of  $N$  particles and put it between two heat reservoirs. Then wait until the conditions become stationary. Then measure the average heat current through the system and the temperature gradient, divide them and the result is the coefficient of thermal conduction  $K_N$ . If it is independent of  $N$  when  $N$  is large enough then we may say that the Fourier heat law holds for a given system.

But there are some technical questions which occur when one wants to prepare such a numerical experiment: What is a heat reservoir and how to implement the coupling of edges of the system to the heat reservoirs? We used the same recipe which has been used in almost all previous numerical simulations (Jackson *et al* 1968, Casati *et al* 1984). Imagine that the reservoir is modelled by the ideal gas of hard-point particles with the same mass as the mass of the particles of our system and is placed behind the wall of contact. When an edge particle crosses this wall it collides instantly with one gas particle, takes on its momentum (because they have equal masses) and returns back to the other side of the wall. This interaction looks like a collision after which the particle 'forgets' its velocity prior to the collision, and its

new velocity is distributed according to the Maxwell-like distribution

$$\frac{dP(v)}{dv} = \frac{|v|}{T} \exp\left(-\frac{v^2}{2T}\right) \tag{4}$$

where  $T$  is an effective temperature of the heat reservoir. The velocity after collision must be positive when interacting with the left reservoir, and negative when interacting with the right one. Formula (4) can be derived very easily. Factor  $|v|$  is a consequence of the fact that an edge particle bounces more frequently to the fast free-gas particles than to the slow ones (see Jackson *et al* 1968, Casati 1985).

Models other than free-gas particles for the heat reservoir would yield distributions that would differ from the Maxwell-like (4), and we leave it as an open problem to investigate in detail what the consequences are of such other choices. For example, a reservoir made up of harmonic oscillators in thermodynamic equilibrium would give rise to a Gaussian distribution rather than the Maxwell-like (4). However, we expect that, ultimately, the stationary state would be independent of the model of the heat reservoir, so we proceed with assumption (4).

We still need a proper definition of local temperature in the chain. We are studying quasi-equilibrium statistical mechanics which defines *local temperature* as twice the kinetic energy

$$T_k = \langle p_k^2 \rangle. \tag{5}$$

$\langle \dots \rangle$  represents the thermodynamical average or time average which must coincide by assumption. Numerical simulation proceeds as follows. We start with the chain of  $N$  particles with initial condition  $q_k = 0, p_k = 0$  and two heat reservoirs at both edges with effective temperatures  $T_L$  and  $T_R$ , where we can assume  $T_L > T_R$ . We leave the system to relax to the stationary state for about  $N_{\text{relax}}$  collisions after the simulation begins. It is easy to show that  $N_{\text{relax}} = \mathcal{O}(N^3)$ . Due to the random walk the time needed for thermal excitations to fill the whole chain is proportional to  $N^2$  if one assumes the validity of the Fourier heat law, and the number of collisions per unit time is proportional to  $N$  so the product is proportional to  $N^3$ . After the stationary state is established we start to measure the time average of interesting quantities. These are the temperature field  $T_k$ , the average heat current from the left reservoir to the chain  $\langle J_L \rangle$  and from the chain to the right heat reservoirs  $\langle J_R \rangle$  and perhaps several others such as  $\langle q_k \rangle$  and  $\langle q_k^2 \rangle$ . We calculate the time average of each of these quantities, say  $p_k^2$ , as the average over the discrete set of times  $t_n = n\tau, n = 1, 2 \dots$

$$T_k = \frac{1}{M} \sum_{n=1}^M p_k^2(n\tau) \tag{6}$$

with an effective statistical error

$$\delta T_k = \frac{\sigma_k}{\sqrt{M}} \quad \sigma_k^2 = \frac{1}{M} \sum_{k=1}^M p_k^4(n\tau) - \left( \frac{1}{M} \sum_{n=1}^M p_k^2(n\tau) \right)^2 \tag{7}$$

where  $M\tau$  is the total time of simulation. We have found that the best choice for  $\tau$  is of the order of the average time between two collisions of a fixed pair of particles. If



$\tau$  is much larger, then too much of the generated information would be lost. On the other hand, a much smaller  $\tau$  means too much computer time spent calculating sums (6) and (7) on account of actual simulation (performing the one-step procedure).

We expect the temperature profile  $T_k$  far away from the edges  $k \gg 1, N - k \gg 1$  to be linear  $T_k - T_l = \nabla T(k - l)$ . If the stationary state during the simulation is reached the averages of currents  $\langle J_L \rangle$  and  $\langle J_R \rangle$  must be equal within the statistical error. To improve the accuracy we take their average  $\langle J \rangle = (\langle J_L \rangle + \langle J_R \rangle)/2$  and divide it by  $-\nabla T$  which gives the coefficient of thermal conduction  $K$  by definition.

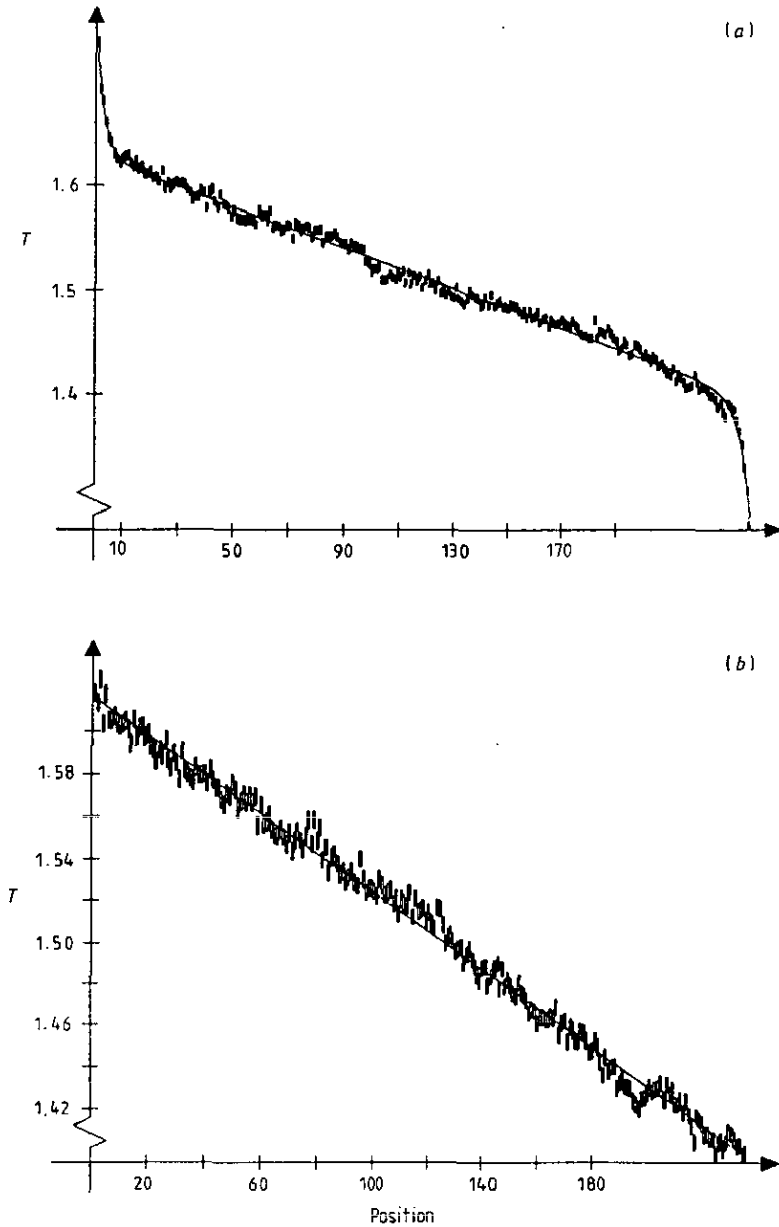
The question that remains is where to put the walls of the heat reservoirs. We tried to put them at the fixing points of the edge oscillators. The first oscillator must therefore always be on the right side of its fixing point and *vice versa* for the last:  $\langle q_1 \rangle > 0, \langle q_N \rangle < 0$ . This makes edges very special because  $\langle q_k \rangle = 0$  does not apply. These edge effects have turned out to be very annoying at large temperatures (see figure 3). The edges behave effectively like thermal resistors whose resistivity increases with temperature, so that almost the entire temperature fall  $T_L - T_R$  goes on account of the edges. The temperature gradient far away from the edges that goes into the definition of  $K$  is therefore very small and subject to large errors.

One might argue that reservoir walls expose a kind of pressure on the system and that we ought to move them a bit, the left one to the left and the right one to the right. But then the system can lose contact with the thermal reservoirs for some initial conditions.

Fortunately, we managed to eliminate these annoying effects. We have slightly modified our model by adding two free particles of unit mass between each of the reservoirs and the corresponding edge particle. Now we are able to displace reservoir walls because free particles always maintain contact between heat reservoirs and the chain. By  $a$  we denote the distance from the edge particle's fixing point and reservoir wall. The optimal choice for  $a(T)$  is determined by the condition that the average position of the edge harmonic particle is zero.  $a$  is a function of temperature  $T$  of the corresponding reservoir. When we found out that this idea works, we realized that the free particles in Casati's ding-a-ling model play a similar role. With this modification we have to solve a transcendental equation each time two near-edge particles collide. Although it takes much more computer time than the evaluation of the arctangent, it happens only once in typically  $N$  normal collisions and is therefore negligible in the limit  $N \rightarrow \infty$  and even in practice when  $N \approx 10^2$ . We call this method the *improved direct method* in contrast to the simple *direct method*. In table 1 we show the optimal values of the wall-edge distance  $a(T)$  for a few most frequently used temperatures. The behaviour of  $a(T)$  is very smooth and so it can be interpolated for values of  $T$  that are not in table 1. We have not investigated  $a(T)$  for lower temperatures because the edge effects occur at about  $T \approx 0.3$  and higher and become severe at about  $T \approx 2$ .

### 3.2. Results

We have performed many numerical experiments for various lengths  $N$  and temperatures  $T$  (where  $T = \frac{1}{2}(T_L + T_R)$ , and  $(T_L - T_R)/T$  small). There are some serious difficulties at very low and very high temperatures. At very low temperatures most of the computer time is spent due to the bouncing of the edge oscillators at the walls, because most of the time they have not enough energy to collide with the neighbouring oscillator. This results in very large fluctuations of the heat current and the temperature which makes simulation practically impossible beyond  $T < 0.1$ . But



**Figure 3.** The two kinds of energy profiles are plotted. The first (a) is a result of simple direct method where one can easily see the edge effects. The temperature profile  $T_k$  can be fitted with the ansatz of the form  $T_k = A \exp(-\alpha(k-1)) + B \exp(-\beta(N-k)) + Ck + D$  in this case. The edge effects therefore fall exponentially. The edge effects are completely eliminated in the second temperature profile (b) which is a result of the improved direct method. The height of the bars is the estimated statistical error. Reservoir temperatures, lengths of the chain and the times of simulation are the same for both profiles:  $T_L = 1.75$ ,  $T_R = 1.25$ ,  $N = 240$ ,  $M = 300\,000$ .

on the other hand the convergence of  $K_N$  with  $N$  is becoming drastically slower with increasing temperature, which is not surprising because here we approach the

**Table 1.** The values of the optimal edge-wall distance  $a(T)$  for a few temperatures  $T$ .

$T$	$a(T)$
0.5	$2.40 \pm 0.03$
1.0	$2.07 \pm 0.02$
2.0	$1.95 \pm 0.01$
3.0	$1.92 \pm 0.01$
4.0	$1.91 \pm 0.01$

integrable case of free particles where the Fourier heat law (asymptotically) does not apply (Casati 1985). Table 2 illustrates the convergence of  $K_N$  for some typical temperatures. One can see that  $K_N(T = 0.1)$  has already converged at  $N = 10$  and on the other hand  $K_N(T = 4.0)$  does not converge even for  $N = 420$ . The present computer capabilities did not allow us to prove the convergence of  $K_N$  (i.e. Fourier heat law) for  $T > 3$  with the direct method but we are able to prove it indirectly as we will show in section 5.

**Table 2.** The convergence of the coefficient of thermal conduction for finite chains  $K_N(T)$  with  $N$ . One can easily see that the rate of convergence rapidly decreases with temperature.

$N$	10	20	30	40	50	60	Error (%)
$K(T = 0.10)$	0.36	0.38	0.36	0.39	0.36	0.38	$\sim 8$
$K(T = 0.25)$	0.74	0.92	1.08	1.11	1.26	1.19	$\sim 7$
$N$	70	140	210	280	350	420	Error (%)
$K(T = 2.50)$	128	173	215	209	197	209	$\sim 4$
$K(T = 4.00)$	—	363	400	453	—	486	$\sim 5$

All useful data from our numerical simulations using the direct method are summarized in table 3 which gives the function  $K(T)$ . The last column suggests that except for low temperatures  $K(T) \propto T^2$ .

**Table 3.** The function  $K(T)$  as obtained by the direct method at all temperatures for which the convergence of  $K_N$  with  $N$  was clearly observed. For major part of the table  $T \geq 0.5$  the improved direct method was used.

$T$	$K(T)$	$K(T)/T^2$
0.1	$0.037 \pm 0.002$	3.7
0.25	$1.24 \pm 0.05$	19.2
0.5	$6.6 \pm 0.3$	26.4
1.0	$30 \pm 1$	30.0
1.5	$74 \pm 2$	32.9
1.8	$103 \pm 3$	31.8
2.0	$128 \pm 5$	32.0
2.5	$207 \pm 6$	33.1
3.0	$295 \pm 7$	32.8

4. Green-Kubo formalism

In this section we derive the Green-Kubo formula for the transport of energy along a general *homogeneous one-dimensional lattice of colliding particles*. The first steps of the derivation will follow Visscher (1974) in a modified version and the last few will specialize to discrete lattices. Our derivation is self-contained unlike Visscher's (1974) and does not refer to quantum mechanics. The derivation is unperturbative and is exact up to the final step when we use the assumption of constant temperature gradient (15).

First we have to define the local heat current from the site  $k$  to  $k + 1$ . We denote it by  $j_k$ . In order to satisfy the discrete continuity equation

$$\frac{d}{dt} E_k(t) + \nabla j_k(t) = 0 \quad E_k = \frac{1}{2}(p_k^2 + q_k^2) \quad \nabla j_k = j_k - j_{k-1} \quad (8)$$

we obtain the following expression for the heat current

$$j_k = \frac{1}{2}(p_{k+1} - p_k)(p_{k+1}^2 - p_k^2)\delta(q_{k+1} - q_k + 1). \quad (9)$$

We can prove the last relation by inserting it into continuity equation (8) and integrating it over a small time interval which covers one collision.

In the beginning, at time  $t_0$  we take a very specially chosen ensemble of initial conditions  $(q(t_0), p(t_0))$ . Their distribution will be locally canonical

$$\rho_0(q, p) = Z^{-1} \exp\left(-\sum_{k=1}^N \frac{p_k^2 + q_k^2}{2T_k}\right) = Z^{-1} \exp\left(-\sum_{k=1}^N \frac{E_k}{T_k}\right). \quad (10)$$

From now on in this section we denote by  $\langle \rangle$  a locally canonical average  $\langle A \rangle = \int dq dp A(q, p) \rho_0(q, p)$  of any quantity  $A$ . Each particle is in local equilibrium at temperature  $T_k$  but globally this cannot represent stationary distribution. We may easily verify this fact by calculating  $\langle j_k \rangle$  for an arbitrary *temperature profile*  $T_k$ . After using formula (9) and performing a few Gaussian integrals one finds

$$\langle j_k(t_0) \rangle = 0. \quad (11)$$

This is surprising because one would naively expect  $\langle j_k \rangle > 0$  if  $T_{k+1} > T_k$ . But the fact (11) simply implies that we have to wait for distribution  $\rho_0$  to relax into a stationary one. In other words, we have to compute  $\langle j_k(\infty) \rangle$ . It is the famous Green-Kubo formula that enables us to do this.

Let us take arbitrary observable  $A = A(q, p)$  which is not an explicit function of time,  $\partial A / \partial t = 0$ . Time evolution of  $A$  can most elegantly be written by means of Poisson bracket

$$\frac{d}{dt} A = \frac{dq}{dt} \frac{\partial A}{\partial q} + \frac{dp}{dt} \frac{\partial A}{\partial p} = \frac{\partial H}{\partial p} \frac{\partial A}{\partial q} - \frac{\partial H}{\partial q} \frac{\partial A}{\partial p} = \{H, A\}. \quad (12)$$

The goal is to calculate  $\langle A(t) \rangle$  at some later time  $t \gg t_0$ . Now we are able to do this almost directly

$$\begin{aligned}
\langle A(t) \rangle &= \langle A(t_0) \rangle + \int_{t_0}^t dt' \left\langle \frac{d}{dt'} A(t') \right\rangle \\
&= \langle A(t_0) \rangle + \int_{t_0}^t dt' \langle \{H, A\} \rangle \\
&= \langle A(t_0) \rangle + \int_{t_0}^t dt' \int dq \int dp \rho_0 \left\{ \frac{\partial H}{\partial p} \frac{\partial A(t')}{\partial q} - \frac{\partial H}{\partial q} \frac{\partial A(t')}{\partial p} \right\} \\
&\quad \text{(per partes)} \\
&= \langle A(t_0) \rangle - \int_{t_0}^t dt' \int dq \int dp A(t') \left\{ \frac{\partial}{\partial q} \left( \rho_0 \frac{\partial H}{\partial p} \right) - \frac{\partial}{\partial p} \left( \rho_0 \frac{\partial H}{\partial q} \right) \right\} \\
&= \langle A(t_0) \rangle - \int_{t_0}^t dt' \int dq \int dp A(t') \left\{ \frac{\partial H}{\partial p} \frac{\partial \rho_0}{\partial q} - \frac{\partial H}{\partial q} \frac{\partial \rho_0}{\partial p} \right\} \\
&= \langle A(t_0) \rangle - \int_{t_0}^t dt' \int dq \int dp A(t') \frac{d}{dt'} \rho_0 \\
&\quad \text{(derivative of (10) with respect to } t) \\
&= \langle A(t_0) \rangle + \int_{t_0}^t dt' \left\langle A(t') \sum_k \frac{\dot{E}_k(t_0)}{T_k} \right\rangle \quad \text{(continuity equation)} \\
&= \langle A(t_0) \rangle - \int_{t_0}^t dt' \left\langle A(t') \sum_k \frac{\nabla j_k(t_0)}{T_k} \right\rangle.
\end{aligned}$$

We define the gradient of inverse temperature as  $\nabla(1/T_k) = 1/T_{k+1} - 1/T_k$ , and perform a kind of *discrete per-partes*

$$\sum_k \frac{\nabla j_k}{T_k} = \sum_k \frac{j_k - j_{k-1}}{T_k} = \sum_k \left( \frac{j_k}{T_k} - \frac{j_k}{T_{k+1}} \right) = - \sum_k \nabla \left( \frac{1}{T_k} \right) j_k \quad (13)$$

and the required result is

$$\langle A(t) \rangle = \langle A(t_0) \rangle + \sum_k \nabla(1/T_k) \int_{t_0}^t dt' \langle j_k(t_0) A(t') \rangle. \quad (14)$$

The next step is to substitute a general observable  $A$  with a special one, namely the average heat current  $J = N^{-1} \sum_{k=1}^N j_k$ . We might take any local current  $j_k$  instead because in stationary state they are all equal  $\langle j_k(\infty) \rangle = \langle J(\infty) \rangle$  but the fluctuations in  $J$  are the smallest. The first term  $\langle A(t_0) \rangle$  vanishes by (11) and finally we obtain the Green-Kubo formula for thermal conduction

$$\begin{aligned}
\langle J(t) \rangle &= \sum_{k=1}^N \nabla(1/T_k) \int_{t_0}^t dt' \langle j_k(t_0) J(t') \rangle \\
&= - \nabla T \frac{N}{T^2} \int_{t_0}^t dt' \langle J(t_0) J(t') \rangle + \mathcal{O}((\nabla T)^2) \quad (15)
\end{aligned}$$

$$K = - \lim_{t \rightarrow \infty} \frac{J(t)}{\nabla T} = \frac{N}{T^2} \int_{t_0}^{\infty} dt' \langle J(t_0) J(t') \rangle. \quad (16)$$

The coefficient of thermal conduction is proportional to the integral of the heat current autocorrelation function. At the right most part of equation (15) we have used the fact that far away from the edges the inverse temperature gradient is constant, so  $\nabla(1/T_k) = \nabla(1/T) = -\nabla T/T^2$ .

By the so called discrete *per-partes* summation we have neglected the problem of edges where  $k = 1, N$ . The formulae (14) and (15) are therefore exact only for infinite and cyclic ( $N + 1 \equiv 1$ ) chains, but for finite chains they hold for times  $t - t_0$  shorter than the *sound transit time* across the lattice. In the numerical study we considered the cyclic chain. The temperature gradient in the cyclic chain must be zero and so is the stationary value of the heat current  $\langle J(\infty) \rangle$  but  $K$  remains well defined and finite by (16) because  $\nabla T$  cancels out.

**Table 4.** The table shows the function  $K(T)$  at moderate and low temperatures as obtained by the Green-Kubo formula. The last column suggests the asymptotic behaviour (22) which is also confirmed analytically in the appendix.

$T$	$K(T)$	$K(T) \exp(1/4T)$
0.020	$(1.2 \pm 0.7) \times 10^{-6}$	0.349
0.030	$(9.5 \pm 2.0) \times 10^{-5}$	0.395
0.040	$(6.0 \pm 0.5) \times 10^{-4}$	0.311
0.050	$(2.45 \pm 0.1) \times 10^{-3}$	0.364
0.060	$(6.0 \pm 0.3) \times 10^{-3}$	0.387
0.075	$(1.36 \pm 0.05) \times 10^{-2}$	0.381
0.100	$(3.8 \pm 0.2) \times 10^{-2}$	0.463
0.250	$1.1 \pm 0.1$	3.0
0.500	$6.3 \pm 0.3$	10.4
1.000	$29.5 \pm 1.5$	37.9
2.000	$120 \pm 10$	136

The formula (16) is the final result but for numerical study it still needs some modifications. We observe that the heat current is defined through the  $\delta$ -function (9) and might therefore look nicer in integrated form. Let us define its integral  $\Delta Q(t_1, t_2) = N \int_{t_1}^{t_2} dt' J(t')$ , which is equal to the integrated total energy flow† in cyclic chain between times  $t_1$  and  $t_2$ . We retain the dependence on initial and final time in  $K$

$$K(T, t_0, t) = \frac{1}{T^2} \langle J(t_0) \Delta Q(t_0, t) \rangle. \tag{17}$$

$K(T, t_0, t)$  depends only on the difference  $t - t_0$  and practically reaches its limiting value for  $t - t_0 > t_c$  where  $t_c$  is a *characteristic relaxation time*. We may approximate the limit  $K(T)$  by an average over  $t_0$ ,  $K(T) \approx (1/t) \int_0^t dt_0 K(T, t_0, t)$  where the error is of order  $t_c/t$ . Thus, the limit

$$K(T) = \lim_{t \rightarrow \infty} \frac{1}{t} \int_0^t dt_0 K(T, t_0, t) \tag{18}$$

is exact. Now we insert (17) into (18) and perform integration over  $t_0$ .  $J(t_0)$  in (17) differs from zero only at times of collisions and  $\Delta Q(t_0, t)$  is always a finite and well

† It is the sum of the energy exchanges in all collisions.

behaved function. By  $\nu(t)$  we denote the number of collisions between times 0 and  $t$  and enumerate them with integers  $1, 2, \dots, \nu(t)$ . Let  $\Delta Q_j$  be the energy exchange at  $j$ th collision. Then

$$\begin{aligned}
 K(T, t) &= \frac{1}{T^2 t} \int_0^t dt_0 \langle J(t_0) \Delta Q(t_0, t) \rangle \\
 &= \frac{1}{NT^2 t} \langle \Delta Q_1 (\frac{1}{2} \Delta Q_1 + \Delta Q_2 + \Delta Q_3 + \dots \\
 &\quad + \Delta Q_2 (\frac{1}{2} \Delta Q_2 + \Delta Q_3 + \dots) + \dots \rangle \\
 &= \frac{1}{NT^2 t} \left\langle \sum_{i=1}^{\nu(t)-1} \sum_{j=i+1}^{\nu(t)} \Delta Q_i \Delta Q_j + \frac{1}{2} \sum_{i=1}^{\nu(t)} \Delta Q_i^2 \right\rangle \\
 &= \frac{1}{2NT^2 t} \left\langle \left( \sum_{i=1}^{\nu(t)} \Delta Q_i \right)^2 \right\rangle \tag{19}
 \end{aligned}$$

$$K(T) = \lim_{t \rightarrow \infty} K(T, t). \tag{20}$$

We have used the formula for integration over the  $\delta$ -function  $\int dt \delta(t - t_c) f(t) = \frac{1}{2}(f(t_c + 0) + f(t_c - 0))$ . One can rewrite the result (19) in a more compact form

$$K(T) = \lim_{t \rightarrow \infty} \frac{\langle \Delta Q(0, t)^2 \rangle}{2NT^2 t}. \tag{21}$$

We have used the Metropolis algorithm (Press *et al* 1990) to generate initial conditions  $(q, p) = (q(t_0), p(t_0))$  and to calculate the canonical average  $\langle \rangle$  as an average over many such Metropolis iterations. At moderate temperatures of order unity typically a few thousand Metropolis iterations were needed to obtain  $K(T)$  within the given statistical error, whilst at very low temperatures below 0.1 (see table 4) we used typically a few ten thousand iterations, due to larger fluctuations. After we generate an ensemble of initial conditions we simulate the dynamics of the system until an expected time such that the average  $K(T, t)$  relaxes to the stationary value, see figure 4. The criterion of stationarity of  $K(T, t)$  is that the variation of the average value of  $K(T, t)$  is much smaller than the estimated statistical error. The only practical question which remains open is the length of the cyclic chain. The result may depend on  $N$  but the experience shows that this dependence is not drastic, for example  $K(T = \frac{1}{2}, N = 25) = 6.5 \pm 0.3$ ,  $K(T = \frac{1}{2}, N = 50) = 6.1 \pm 0.2$ . Typical values of  $N$  in our numerical experiments were between 20 and 50. Table 4 shows the results for  $K(T)$  obtained by the Green-Kubo formula. The numbers in the second half of the table should be compared with those in table 3 (the direct method). As we have already mentioned, the Green-Kubo formula is particularly suitable for investigation at very low temperatures. One can verify the asymptotic formula as derived in the appendix

$$K(T \rightarrow 0) = (0.38 \pm 0.02) \exp(-1/4T) \tag{22}$$

which holds very well for  $T < 0.1$ .

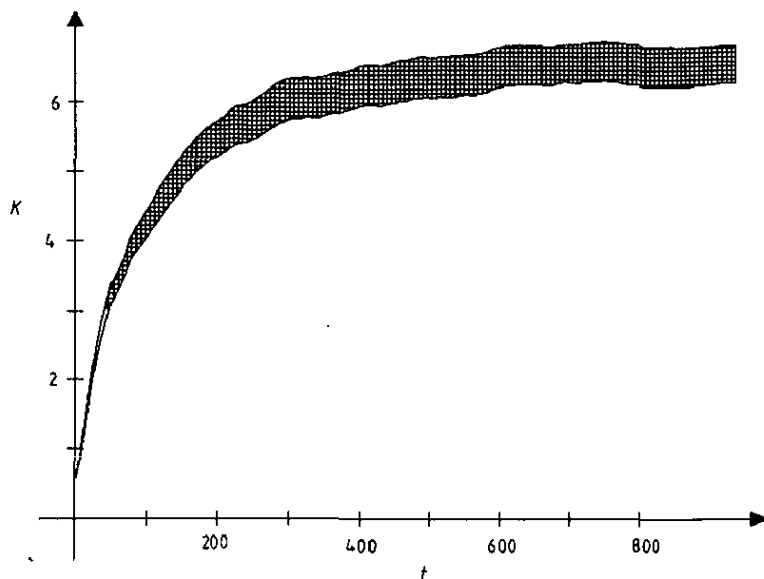


Figure 4. The convergence of  $K(T, t)$  with  $t$  as defined by the Green-Kubo formula (19) for  $T = 0.5$ . The average was taken over 3000 different initial conditions. The points in the hatch-filled area are within the statistical one-sigma error.

## 5. One-sided heating of semi-infinite cold chain

### 5.1. Preparation of the numerical experiment and scaling exponents

According to the results of the direct and the Green-Kubo methods we cannot decide whether the Fourier heat law holds at high temperatures ( $T > 3$ ) or not. We need a new method which will not depend on the length of a chain. We have constructed such a method which is non-stationary and therefore depends on the time of simulation. But fortunately, the average time behaviour of the results is quite predictable and can be easily extrapolated to infinity where definite conclusions about validity of the Fourier heat law can be drawn.

Now we will present our ideas in detail. We are heating an initially cold semi-infinite chain on one side. By *cold* we mean that all oscillators are at rest. In practice we have a very long ding-dong chain of several ten thousands of particles which is coupled to the stochastic heat reservoir with temperature  $T_L$  through its first oscillator particle. The coupling is the same as in the simple direct method. Then we follow the time evolution of such a system with initial conditions  $q_k = 0, p_k = 0$ . We are especially interested in the total energy of the system as a function of time  $E(t)$  which is equal to the integral of the heat current from the heat reservoir to the system from time 0 to  $t$ . Asymptotically it should scale like a power law

$$E(t) \propto t^\nu \quad t \rightarrow \infty. \quad (23)$$

One would expect  $\nu = 1$  for non-diffusive sound-like transport of energy and  $\nu = \frac{1}{2}$  for diffusive energy transport typical of the Fourier heat law. In the first case the energy propagates in mutually independent modes which flow from the heat reservoir with constant velocity. The ability of the system to absorb energy does not change in time and therefore  $E(t)$  grows linearly. On the other hand in the second case  $E(t)$



must increase like a square root  $\sqrt{t}$  as a consequence of the symmetry property of the generalized diffusive equation as we will show in our phenomenological theory in the next subsection.

The major task is to carefully determine the exponent  $\nu$  from our numerical data. In practice we calculate the functions such as  $E(t)$  as the averages over many such heatings and we call them *macro iterations*. Fluctuations around these averages give us information about the statistical error of our results.

For the sake of completeness we have observed the behaviour of another three quantities, as functions of time  $t$ ,

$$\langle k \rangle(t) = \frac{1}{2E(t)} \sum_{k=1}^{\infty} (q_k^2 + p_k^2)k \tag{24}$$

$$\sqrt{\langle k^2 \rangle}(t) = \sqrt{\frac{1}{2E(t)} \sum_{k=1}^{\infty} (q_k^2 + p_k^2)k^2} \tag{25}$$

$$k_{\max}(t) = \max\{k | q_k^2 + p_k^2 > 0\}. \tag{26}$$

We also define the corresponding asymptotic exponents  $\mu_{1,2}, \lambda$  by  $\langle k \rangle(t) \propto t^{\mu_1}, \sqrt{\langle k^2 \rangle}(t) \propto t^{\mu_2}, k_{\max}(t) \propto t^{\lambda}$ . It will soon become clear (in the next subsection) that in a well defined regime of energy transport the exponents  $\nu, \mu_{1,2}$  must be equal  $\mu_1 = \mu_2 = \nu$ . But the exponent  $\lambda$  of the *wavefront propagation* cannot be calculated at the phenomenological level. We can explain its behaviour by means of quasi-solitons (mentioned in section 2). They represent the most effective propagation of a disturbance into a cold chain.

Figures 5, 6 and 7 respectively show the time behaviour of the quantities  $E(t), \langle k \rangle(t), \sqrt{\langle k^2 \rangle}(t)$  and the corresponding effective exponents  $d \log E(t)/d \log t, \dots$  which must asymptotically (as  $t \rightarrow \infty$ ) converge towards the scaling exponents  $\nu, \mu_{1,2}$ . Although this limit has not been reached in time of observation these quantities can be excellently fitted by the ansatz of the form

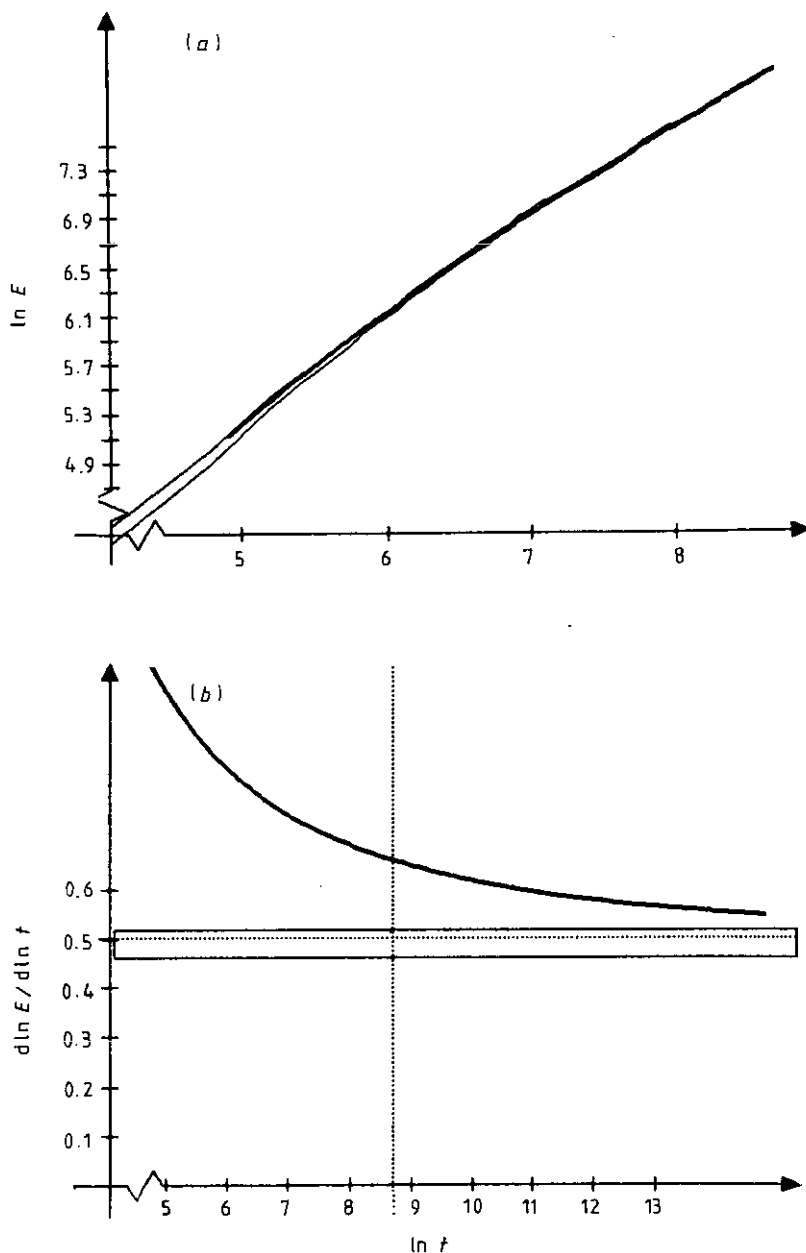
$$\log E(t) = A + B \log t + C / \log t \tag{27}$$

where  $A, B$  and  $C$  are the fitting parameters. This ansatz has the property that its derivative  $d \log E(t)/d \log t$  possesses a finite limit  $\lim_{t \rightarrow \infty} d \log E(t)/d \log t = B = \nu$  and it gives the smallest value of standard  $\chi^2$  test, which makes it unique. The value of  $\chi^2$  is so small that we could not decrease it by adding any additional parameters to (27), for example  $+ D/(\log t)^2$ .

There is another argument in support of the ansatz (27), namely the high quality of the results. All values of the parameter  $B$  (which is equal to the scaling exponent  $\nu$  or  $\mu_{1,2}$  for other two functions ((24) and (25)) are equal to  $1/2$  within the estimated error with no exceptions for all temperatures  $T = 0.25, 1, 2, 4, 6$ . See table 5. This result is really striking and it provides us with the strongest numerical proof for the validity of the Fourier heat law.

### 5.2. The inverse transform and calculation of $K(T)$

Besides the average quantities such as  $E(t), \langle k \rangle(t)$  and  $\sqrt{\langle k^2 \rangle}(t)$  we can study the evolution of the entire temperature profile of the chain  $T(x = k, t) = \langle p_k^2 \rangle$ . We



**Figure 5.** The convergence of the scaling exponent  $\nu$  for one-sided heating of semi-infinite cold chain at  $T_L = 4$  is shown. Graph (a) shows the scaling exponent obtained by the simulation (the dark line is the best fit) whereas graph (b) shows its logarithmic derivative (and its extrapolation on the right side of the vertical dotted lines). The vertical position of the box on (b) is the limiting value of the corresponding scaling exponent and its height is the estimated statistical error ( $1 \sigma$ ).

can determine  $K(T)$  by measuring  $T(x, t)$ . At first sight we have too much data in the function of two variables  $T(x, t)$  to determine the function of a single variable  $K(T)$ . But due to the scaling properties in time we can relate it uniquely to the

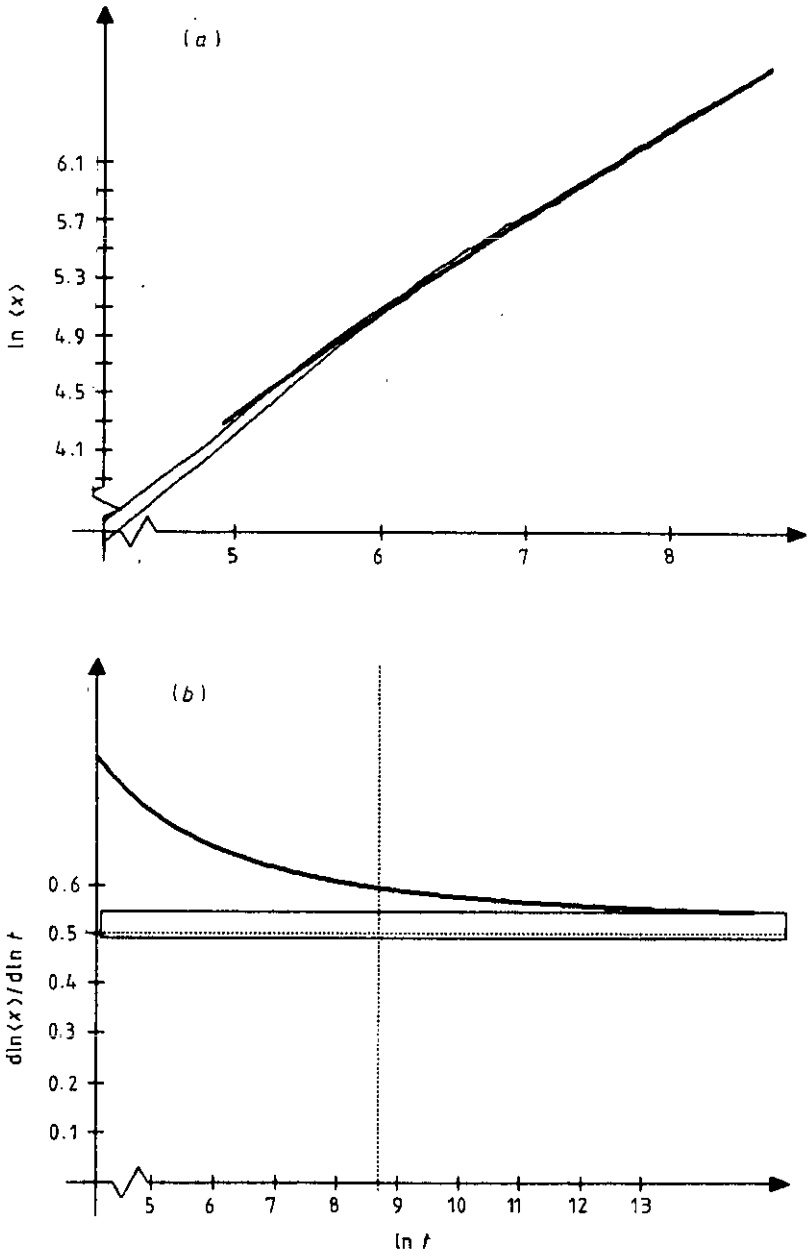


Figure 6. As figure 5, but for the scaling exponent  $\mu_1$ .

function  $K(T)$ .

We neglect the discrete microscopic structure of our system and replace the discrete index  $k$  by the smooth variable  $x$ . Let us first postulate the Fourier heat law

$$J(x, t) = -K(T(x, t)) \frac{\partial}{\partial x} T(x, t). \tag{28}$$

The current  $J$  satisfies the continuity equation  $(\partial J(x, t) / \partial x) = -(\partial E(x, t) / \partial t)$

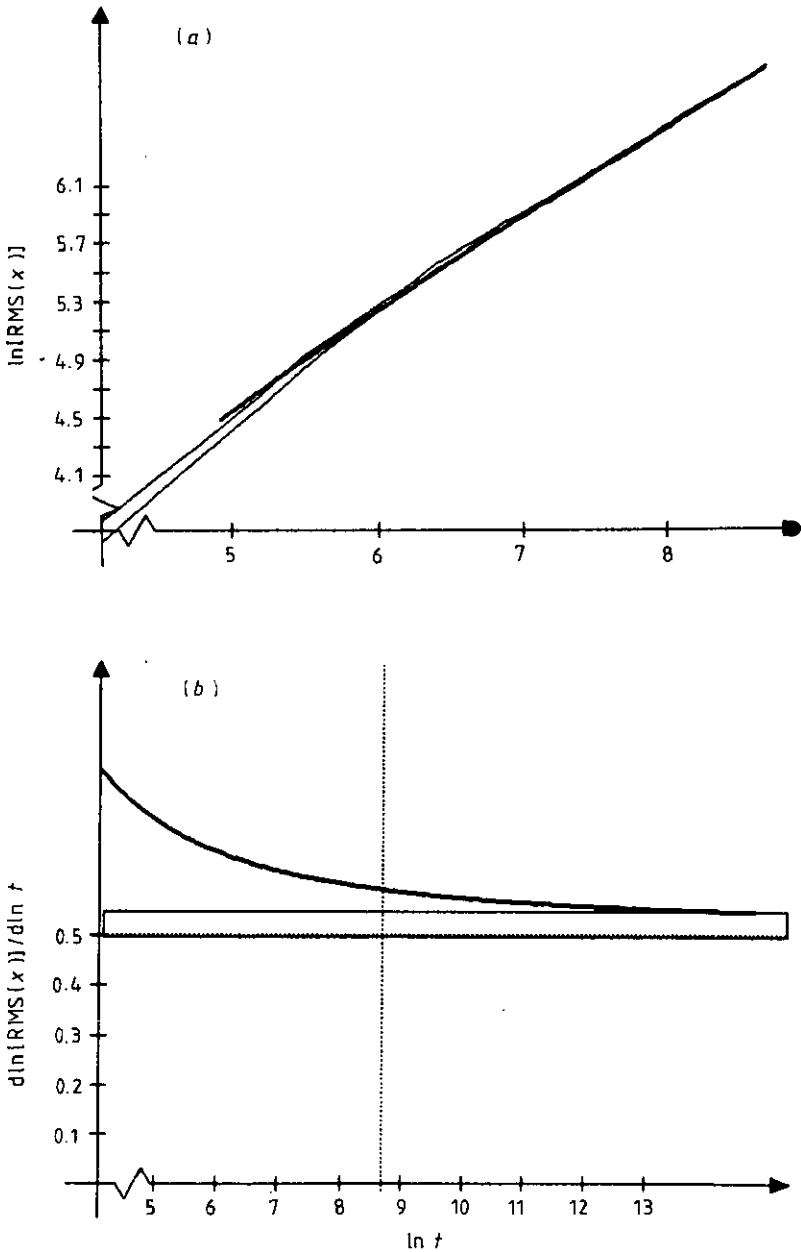


Figure 7. As figure 5, but for the scaling exponent  $\mu_2$ .

where  $E(x, t)$  is now energy per lattice site at  $x$  or energy density and is assumed to depend only on temperature  $E(x, t) = E(T(x, t))$ . When we insert equation (28) in the continuity equation we get a generalized diffusion equation in (1+1) dimensions

$$\frac{\partial}{\partial x} (K(T(x, t)) \frac{\partial}{\partial x} T(x, t)) = C(T(x, t)) \frac{\partial}{\partial t} T(x, t) \quad (29)$$

where we have introduced  $C(T)$  as the specific heat capacity  $C(T) = (\partial E(T) / \partial T)$ .

**Table 5.** The extrapolated limiting values of the scaling exponents for a wide range of temperatures. They are all close to the predicted limiting value  $\frac{1}{2}$  within the standard deviation which is about 0.02 for most of them.

$T$	$\nu$	$\mu_1$	$\mu_2$
0.25	0.46	0.54	0.54
1.0	0.47	0.49	0.51
2.0	0.44	0.50	0.51
4.0	0.49	0.52	0.52
6.0	0.52	0.49	0.49

We note that equation (29) is invariant on one-parameter group of transformations  $(x, t) \rightarrow (\alpha x, \alpha^2 t)$  for arbitrary real positive  $\alpha$ , and so are the boundary and the initial conditions  $T(0, t) = T_L$ ,  $T(x > 0, 0) = 0$ . The solution  $T(x, t)$  must have the same symmetries, i.e. we can write it as a function of a single variable  $s = x/\sqrt{t}$ ,  $T(x, t) = \tau(x/\sqrt{t}) = \tau(s)$ . This is also the reason why all scaling exponents  $\nu, \mu_1, \mu_2$  must be equal to  $\frac{1}{2}$ . When performing this substitution in equation (29) it becomes an ordinary second-order differential equation for function  $\tau(s)$

$$\frac{d}{ds} \left( K(\tau) \frac{d\tau}{ds} \right) = -\frac{1}{2} s C(\tau) \frac{d\tau}{ds}. \quad (30)$$

But we are seeking the function  $K(\tau)$ , which is obtained by direct integration of (30)

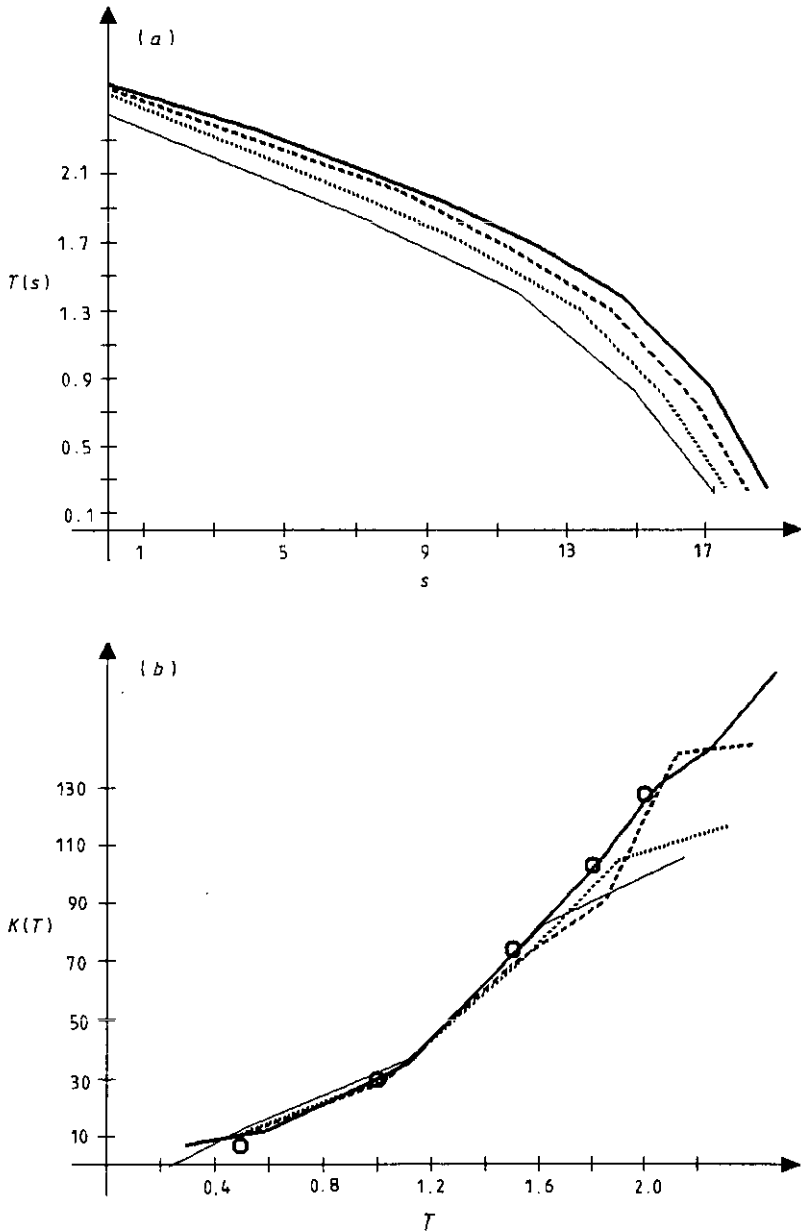
$$K(\tau) = \frac{1}{2} \frac{ds}{d\tau} \int_{s(\tau)}^{\infty} ds' s' C(\tau(s')) \frac{d\tau(s')}{ds}. \quad (31)$$

The function  $s(\tau)$  is the inverse of  $\tau(s)$ , and exists uniquely because  $\tau(s)$  falls monotonically. The limits in the definite integral are chosen to give  $K(0) = 0$ . Formula (31) can be put into a nicer form by changing the parameter of integration

$$K(\tau) = -\frac{1}{2} \frac{ds}{d\tau} \int_0^{\tau} d\tau' s(\tau') C(\tau'). \quad (32)$$

This is a very useful formula, because it connects a function  $s(\tau)$  which is a result of a single simulation with  $K(T)$  for  $T < T_L$ . Thus a single computer run yields the whole function  $K(T)$  at once whilst in other methods a number of simulations at all the different temperatures are needed. Now, notice that  $C(T)$  is not yet specified and indeed we know it only approximately. But fortunately  $K(T)$  depends much more sensitively on  $s(\tau)$  than on  $C(T)$ . In our case,  $C(T)$  is almost a constant function. It equals one if  $T$  approaches 0 and it becomes  $\frac{1}{2}$  when  $T$  tends to infinity (which is the result for the hard-point gas). On the other hand, the numerical determination of  $C(T)$  is an easy problem. We found out that  $C(T)$  can be approximated almost perfectly with a rational approximation

$$C(T) = \frac{1}{2}(1 + (1 + T)^{-2}). \quad (33)$$



**Figure 8.** The temperature profiles  $T(s\sqrt{t}, t)$  for four successive times  $t = 1200, 1200\sqrt{2}, 2400, 2400\sqrt{2}$  (a) (from the left to the right) as the result of one-sided heating of the semi-infinite cold chain for  $T_L = 3$ . (b) The corresponding inverse transforms  $K(T)$  are in excellent agreement with the direct method (the circles) although the convergence of temperature profiles is not yet established.

In figure 8 we present the results of the numerical simulation for  $T_L = 3$ . The dependence  $K(T)$  is in excellent agreement with the results of the direct method (considering the numerical efforts) although the temperature profiles  $T(s\sqrt{t}, t)$  have

not yet converged to its asymptotic function  $\tau(s) = \lim_{t \rightarrow \infty} T(s\sqrt{t}, t)$  too well†. Note that  $\tau(s)$  is calculated as the average over many macro iterations. In practice we have used equation (31) rather than (32), so that there is no problem with inversion of  $\tau(s)$  and its monotonicity. We have also performed such simulations for several other temperatures  $T_L = 0.25, 1, 4$  and we have always found the same function  $K(T)$  for  $T < T_L$ .

## 6. Discussion and conclusions

The present work is a numerical demonstration of the diffusive energy transport in a very simple dynamical system. As explained in the introduction the importance of such studies lies in the attempt to understand and demonstrate the (irreversible) Fourier heat law in a simple Hamiltonian system having deterministic dynamics, rather than an ensemble of statistically similar systems with infinitely complicated internal structure such as the important case of the Lorentz gas in the Boltzmann–Grad limit discussed by Lebowitz and Spohn (1978).

We have improved the statistical significance of the results (for the heat conductivity) as compared with the results of Casati *et al* (1984). Our system is even simpler than Casati's which is decisive for a considerable improvement of the computational speed, and this in turn enables us to study larger systems thereby diminishing the statistical fluctuations. Moreover, we have checked the validity of the Fourier heat law for a large temperature interval, including in particular high temperatures (in appropriately chosen dimensionless units defined in section 2) at which the system approaches the integrable regime of (almost) free particles. Here for the said range of temperatures we have definitely excluded the possibility of an abrupt breakdown in the Fourier heat law. Finally, we have devised and used a new method (observation of the one-sided heating of the cold semi-infinite chain discussed in section 5) to confirm the results of the direct simulation method and of the Green–Kubo formalism. For the purpose of verifying the validity of the Fourier heat law we found that this new method is superior to the previous ones. It will be useful also in analysing other systems particularly when one is interested in the temperature dependence of the heat conductivity. The new method is quite robust in the sense that the extrapolated values of the scaling exponents and inferred  $K(T)$  converge rapidly in relation to the convergence of the temperature profiles. This convergence might become somewhat slower at higher temperatures.

We believe that we have convincingly demonstrated the validity of the Fourier heat law in our simple Hamiltonian system. As discussed in the introduction there is no doubt that the non-integrability of classical dynamics is a necessary condition for the Fourier heat law to manifest itself. However, it remains an open theoretical question as to whether the positivity of  $K$ -entropy is also a necessary condition. Thereby we succeeded in relating the chaoticity of a simple deterministic Hamiltonian system to an irreversible macroscopic law.

† According to our phenomenological theory in which the temperature is a continuous function of the position the exact scaling exponents should be  $\frac{1}{2}$  and a unique rescaled temperature profile  $\tau(s)$  should exist for all times. This is not so due to the discreteness of our model but asymptotically for large times the system approaches this regime.

**Appendix. Asymptotic behaviour of  $K(T)$  at low temperatures**

We derive the asymptotic behaviour (22) analytically. We use a few approximations.

In a cold ding-dong chain there are very few collisions per unit time. We shall therefore consider oscillators as independent and interaction as an effectively small perturbation. For the sake of assumed independence we may consider only two oscillators, we call them 1 and 2, at inverse temperatures  $1/T_1 = \beta_1 = \beta - \frac{1}{2}\Delta\beta$ ,  $1/T_2 = \beta_2 = \beta + \frac{1}{2}\Delta\beta$  and study the average heat current

$$\langle j \rangle = \frac{1}{2} \langle (p_2 - p_1)(p_2^2 - p_1^2) \delta(q_2 - q_1 + 1) \rangle. \tag{A.1}$$

We are interested in the quasi-equilibrium case  $|\Delta\beta/\beta| \ll 1$ , so we will always keep only the lowest-order terms in  $\Delta\beta$ . Now we must find an adequate approximation for the statistical distribution in calculating the average (A.1). One might use locally canonical distribution  $\rho_0$  (10) but we have already seen that this distribution gives  $\langle j \rangle_0 = 0$  although it might be a very good approximation in most of the phase space. But we need a distribution which should be accurate at collision plane  $q_2 - q_1 + 1 = 0$  where the current (A.1) differs from zero. So, let us study the collision in detail. Before the collision the oscillators 1 and 2 have temperatures  $T_1$  and  $T_2$  respectively and  $p_1 > p_2$  holds. After the collision the momenta are exchanged,  $p_2^f = p_1^i > p_1^f = p_2^i$ , which can also be interpreted as an *effective exchange of temperatures*. We must notice that this holds only near the collision plane which is the only segment of phase space which is important at the moment. So, in the lowest allowed order our *effective distribution* would be

$$\begin{aligned} \rho_{\text{eff}}(q_{1,2}, p_{1,2}) &= \rho_{\text{eff}}^{(p)}(p_1, p_2) \rho_{\text{eff}}^{(q)}(q_1, q_2) \\ &= \frac{\beta^2}{4\pi^2} \left\{ \theta(p_1 - p_2) \exp\left(-\frac{1}{2}(\beta_1 p_1^2 + \beta_2 p_2^2)\right) \right. \\ &\quad \left. + \theta(p_2 - p_1) \exp\left(-\frac{1}{2}(\beta_2 p_1^2 + \beta_1 p_2^2)\right) \right\} \exp\left(-\frac{1}{2}\beta(q_1^2 + q_2^2)\right). \end{aligned} \tag{A.2}$$

We can separate the averaging (A.1) into two parts. The first is averaging over the momenta and gives

$$\langle j^{(p)} \rangle_{\text{eff}}^{(p)} = \int dp_1 dp_2 \frac{1}{2} (p_1 - p_2) (p_1^2 - p_2^2) \rho_{\text{eff}}^{(p)}(p_1, p_2) = -4 \sqrt{\frac{T}{\pi}} \Delta T \tag{A.3}$$

and the second is over the positions

$$\langle j^{(q)} \rangle_{\text{eff}}^{(q)} = \int dq_1 dq_2 \delta(q_2 - q_1 + 1) \rho_{\text{eff}}^{(q)}(q_1, q_2) = \frac{1}{2\sqrt{\pi T}} \exp\left(-\frac{1}{4T}\right). \tag{A.4}$$

The integrals are all Gaussian. We have used  $\Delta\beta = -\Delta T/T^2$ . Now we get the result by multiplying both factors

$$\langle j \rangle_{\text{eff}} = \langle j^{(p)} \rangle_{\text{eff}}^{(p)} \langle j^{(q)} \rangle_{\text{eff}}^{(q)} = -\frac{2}{\pi} \exp\left(-\frac{1}{4T}\right) \Delta T. \tag{A.5}$$



$\Delta T$  is equal to the gradient of temperature because lattice spacing is unity. This result confirms the asymptotic formula (22) with a slightly inaccurate leading constant  $2/\pi = 0.637$  which is a consequence of the approximations we made.

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