Dynamical heat channels

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We consider heat conduction in a 1D dynamical channel. The channel consists of a group of noninteracting particles, which move between two heat baths according to some dynamical process. We show that the essential thermodynamic properties of the heat channel can be evaluated from the diffusion properties of the underlying particles. Emphasis is put on the conduction under anomalous diffusion conditions.

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The link between thermodynamic phenomena and microscopic dynamical chaos has been a subject of interest for a long time [1]. Examples of such a relationship is deterministic diffusion [2], where local dynamical properties, such as stability (or instability) of several fixed points can change the global diffusion transport from normal to anomalous [3]. Another question which has attracted a lot of attention recently, is the problem of heat conductivity in deterministic extended dynamical systems [4-8]. A large number of models have been proposed in order to understand the conditions under which a system obeys the Fourier heat conduction law [4]. Recently, a new class of 1D models, "billiard gas channels", has been proposed [5-8]. These channels consist of two parallel walls with a series of scatterers, distributed along walls, and noninteracting particles that move inside. The two ends of the channel are in contact with the heat baths. By changing the shapes and positions of scatterers it is possible to change the conductivity of the channel [5-8].

In this Letter we show that such billiard gas channels belong to a wider class of models, which we call dynamical heat channels. The absence of interactions between particles and the independence of the particle dynamics on kinetic energy allow a complete separation between the thermodynamic aspect, which is governed by properties of the thermostats, and the dynamics inside channel, which is governed by diffusion properties within the channel. All the essential information on heat conductivity of such a dynamical heat conductor can be obtained from the diffusion properties of channel.

Dynamical heat channel. To model dynamics within the channel we consider \( N \) particles that move along direction \( X \), following the dynamical equations of motion

\[
\dot{x} = f(x, t), \quad X \in x,
\]

where the function \( f \) can be either deterministic or random.

To consider transport of heat, two heat baths with temperatures \( T_+ \) and \( T_- \) are attached to the left and right ends of the channel. The heat bath is characterized by a velocity probability density function (pdf), \( P_T(v_{Th}) \), where \( v_{Th} \) is the thermal velocity. After colliding with the heat bath, the particle is ejected back to the channel with a velocity \( v_{Th} \) which is chosen from \( P_T(v_{Th}) \).

As particles do not interact, the dynamics of the ensemble inside the channel can be described by a long trajectory of a single particle and the flux should be rescaled by the factor \( N \). The trajectory of a particle is independent of the particle velocity \( v_{Th} \). The only difference between "hot" and "cold" particles is that the hot ones cover the same trajectories faster then the cold ones. The velocity \( v_{Th} \) does not change during the propagation through the channel and it can be interpreted as a temperature "label" of a particle. The dependence of the dynamics in Eq. (1) on \( v_{Th} \) can be taken into account by introducing a scaling factor for the time \( t \rightarrow t/v_{Th} \).

Due to the separation of the thermodynamic characteristics from the dynamical ones, the proposed approach is not limited to Hamiltonian systems only [5-8]. We only assume that the dynamics inside the channel has a diffusional character, and can be characterized by evolution of the mean square displacement (msd)

\[
\langle X^2(t) \rangle \sim t^\alpha.
\]

This diffusion can be normal (\( \alpha = 1 \)), subdiffusive (\( \alpha < 1 \)) or superdiffusive (\( \alpha > 1 \)) [9].

Following Ref. [5], heat transfer by a particle through the channel is

\[
Q(t) = \sum_{j=1}^{M(t)} \Delta E_j = \sum_{j=1}^{M(t)} q_j \cdot (E_j^{in} - E_j^{out}),
\]

where \( E_j^{in} \) and \( E_j^{out} \) are the energies before and after the \( j \)-collision with the heat bath. \( q_j \) is the direction factor, \( q_j = 1 \) if the \( (j-1) \)-collision is with the hot end, and \( q_j = -1 \) in the case of the cold end. \( M(t) \) is the total number of collision events during time \( t \). In the case of normal heat conductivity, \( Q \) grows linearly with \( t \) and the heat flux is defined by

\[
J = \lim_{t \rightarrow \infty} \frac{Q(t)}{t}.
\]

Let us start from a situation where the particle is initially located at the hot end. During diffusion it can come back and collide with the hot bath again. According to Eq.(3) this event, on average, does not lead to...
heat transfer. But when the particle reaches the opposite cold end \( Q \) increases on average as 
\[
\int_0^\infty \frac{\gamma f}{2} [P_{\gamma f}(v_{Th}) - P_{\gamma f}(v_{Th})] dv_{Th}.
\]
After that the process is reiterated starting from the cold end. Thus, the problem of heat transfer 
is reduced to the problem of diffusion in a finite interval under reflecting and absorbing boundary conditions. 
As the initial condition we assume that at \( t = 0 \) the particle is located at the reflecting end. The average time \( \tau \) needed to reach an absorbing boundary is the first moment of the pdf \( \phi(t) \) for first arrival times. To take into account the effect of thermodynamic velocity on the time \( \tau \) should be rescaled, as mentioned above, 
\[
\tau \rightarrow \frac{1}{v_y} \int_0^\infty P_{\tau f}(v_{Th}) dv_{Th}.
\]
Due to the absence of mass flux, the number of transitions from left to right and vice versa should be the same. Finally, we obtain the following equation for the one-particle heat flux through the channel of length \( L \)
\[
J(L) = \tau^{-1} \int_0^\infty \frac{\gamma f}{2} [P_{\gamma f}(v_{Th}) - P_{\gamma f}(v_{Th})] dv_{Th}. 
\tag{5}
\]
For an ensemble of particles the heat flux should be written as \( J_{ens} = N \cdot J(L) \). Here we take into account that in order to keep a density of particles in the channel fixed, \( N \) should be proportional to \( L \); namely \( N \propto L \).

Equation (5) demonstrates a complete separation between thermodynamic and dynamical aspects. Without loss of generality we consider the “delta”-heat bath with a simple pdf, \( P_T(v_{Th}) = \delta(v_{Th} - \sqrt{2T}) \) [8].

As a model for the dynamics in the channel we consider continuous time random walks (CTRW) [10] in a discrete lattice. This allows to cover the spectrum of diffusion regimes, from subdiffusion to superdiffusion, and to describe kinetics of deterministic Hamiltonian [11,12] and dissipative [3] systems.

The CTRW-model is a stochastic process which represents an alternating sequence of waiting and jumping events [10]. A particle waits at each point for a time chosen from a waiting time pdf \( \psi_w(t) \), and makes a jump (flight) to the left or right with equal probabilities. The jumps are characterized by the pdf \( \psi_f(x,t) \), the probability density to move a distance \( x \) at time \( t \) in a single flight event. We consider power laws for both pdf’s [10]
\[
\psi_w(t) \sim t^{-\gamma w - 1}, \quad \psi_f(x,t) \sim x^{-\gamma_f - 1}. \tag{6}
\]
Depending on asymptotic properties of \( \psi_w(t) \) and \( \psi_f(x,t) \), we have regimes of superdiffusion, normal diffusion or subdiffusion [10].

Superdiffusion. To achieve superdiffusion with a finite msd \( \langle x^2(t) \rangle \) there should be a correlation between the length and duration of the individual flights. Such correlation leads to the model of the \( \mathcal{L} \)evy walks with spatiotemporal pdf [10]
\[
\psi_f(x,t) = \psi_f(t) \delta(|x| - vt), \quad \psi_f(t) \sim t^{-\gamma_f - 1} \tag{7}
\]
that corresponds to flights with a constant velocity \( v \). Here we assume that \( \gamma_w > 1 \), so there is a finite mean waiting time. Depending on \( \gamma_f \) we distinguish among three regimes of diffusion [10], according to the exponent \( \alpha \) in Eq.(2),
\[
\alpha = \begin{cases} 
2, & 0 < \gamma_f < 1 \\
3 - \gamma_f, & 1 < \gamma_f < 2 \\
1, & 2 < \gamma_f 
\end{cases} \tag{8}
\]
In order to derive the dependence of the heat flux \( J \) on the length \( L \) of the channel we start from a consideration of the survival probability \( \Phi(t) \) for a particle walking on the finite interval of the length \( L \) bounded by reflecting and absorbing boundaries. We find that for \( \gamma_w = 2.6, \gamma_f = 1.6 \) for \( L = 100 \) and \( \gamma_f = 1.6 \) for \( L = 100 \).

Finally, for the one-particle heat flux, following Eqs. (5) and (8), we arrive at the following equation for \( J(L) \) in term of the msd exponent \( \alpha \),
\[
J(L) \propto L^{-\beta}, \quad \beta = \begin{cases} 
1, & \gamma_f = 3 - \alpha, \quad 1 < \alpha < 2 \\
2, & \alpha = 1 
\end{cases} \tag{9}
\]
In Fig3.b we show the numerical results for \( J(L) \) obtained for \( \gamma_f = 1.6 \) (stars) and \( \gamma_f = 2.4 \) (squares). The results
are in good agreement with the scaling law suggested by Eq. (9) (straight lines in Fig. 3b).

Then taking Eq. (9) into consideration the thermal conductivity $k = -J_{ns}(N)/\nabla T$, shows the following behavior for $1 < \alpha < 2$,

$$k \propto L^{2-\gamma_f} \propto L^{\alpha^{-1}}. \quad (10)$$

This diverges as one goes to the thermodynamic limit $L \to \infty$. For the ballistic case $\alpha = 2$, $k \propto L$ and for $\alpha = 1$ $k \propto const$ as expected.

The Lévy walk model is an adequate approach for modeling of Hamiltonian kinetic in a mixed phase space [12]. Previous numerical results which have been obtained for Hamiltonian billiard channels, show that $\alpha = 1.3$ corresponds to the flux exponent $\beta = 1.72$ [7], and $\alpha = 1.8$ to $\beta = 1.178$ [8], which are in good agreement with the relation in Eq. (9).

In the case of Lévy flights [10], unlike the Lévy walks, the velocity is not introduced explicitly. Here we assume that all flights have the same duration $t_f$ and use the following decoupled representation for flights pdf,

$$\psi_f(x,t) = \psi_f(x)\delta(t - t_f), \quad \psi_f(x) \sim x^{-\gamma_f^{-1}}. \quad (11)$$

In this case the msd diverges and one is tempted to use $\langle |x(t)|^2 \rangle$ to characterize the dynamics. In the asymptotic regime this quantity scales as $\langle |x(t)|^2 \rangle \sim t^{2/\gamma_f}[10]$. As in the previous case, here the exponent $\gamma_f$ determines the dynamics in the channel and the dependence of flux $J(L)$ on $L$. The scaling of the mean arrival time, $\tau \propto L^{\gamma_f}$, is consistent with the result obtained from a direct solution of a fractional Fokker-Planck equation [14]. We note that using of $\langle |x(t)|^2 \rangle$ instead of msd gives a different, yet unphysical scaling, $J(L) \propto L^{-3}$, with an exponent which is close to that in the scaling in Eq. (9) and coincides with it at the points $\gamma_f = 2$ (normal diffusion) and $\gamma_f = 2$ (ballistic diffusion).

Subdiffusion. In the case of subdiffusion $\gamma_w < 1$ and $\gamma_f > 2$ in Eq. (6) and the mean waiting time $\tau_w$ diverges [10]. The motion is characterized by long localized events and the msd grows sublinearly, $\langle x^2(t) \rangle \sim t^{\gamma_w}$. The pdf of the first arrival time, $\phi(t)$, has a power-law asymptotics $\phi(t) \propto t^{-\gamma_w^{-1}}$ (Fig. 1b). This finding is in line with a result for subdiffusion under a bias in a seminfinite interval with an absorbing boundary [15]. The anomalous character of the pdf $\phi(t)$ leads to a divergence of $\tau$. Thus, in the case of subdiffusion the heat $Q(t)$ carried through the channel grows sublinearly with time (see line (1) in Fig. 2),

$$Q(t) \sim t^{\gamma_w}. \quad (12)$$

Within a traditional definition of the flux, Eq. (4), the subdiffusive anomalous heat conductivity can not be distinguished from a heat isolator. We note that subdiffusion regimes can not be achieved in the case of channels with Hamiltonian dynamics due to a finiteness of recurrence time [9].

Coexistence of long localized events and flights. In the case of competition between flights and localization events the msd exponent $\alpha$ is given by a relation [10]

$$\alpha = 2 + \gamma_w - \gamma_f, \quad 0 < \gamma_w < 1, \quad 1 < \gamma_f < 2. \quad (13)$$

The pdf for the arrival time, $\phi(t)$, is governed, like in the case of simple subdiffusion, by the pdf for waiting times, $\psi_w(t)$. The divergence of mean arrival time $\tau$ can
The values of the flux exponents $\beta$ obtained for the map in Eq. (14) are in agreement with the prediction in Eq.(9) for superdiffusion (see inset in Fig.4). In Fig4. we show the time evolution of $Q(t)$ for the case of subdiffusion, $\gamma_w = 0.5, \gamma_f = 1.5$. The steps in the $Q(t)$ dependence correspond to anomalously long waiting events when particle is trapped near marginal stable fixed points $x = j + \frac{1}{2}, j = 0, \ldots, L$ [3].

In summary we have introduced a class of dynamical heat conductors. This class includes as particular cases recently proposed Hamiltonian billiard channels [5-8]. In the absence of interactions between the particles and the independence of the dynamics on particle energy, the proposed aproach goes beyond Hamiltonian dynamics and allows to express heat conductivity in terms of channel diffusion properties. The Hamiltonian character of dynamics becomes essential when interactions between particles are introduced (like in the case of dynamical lattices [4]) or a dependence of dynamics on particle energy is included.

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lead to anomalous heat conductivity, Eq. (12), even in the case of superdiffusion spreading, $(x^2(t)) \sim t^\alpha, \alpha > 1$, Eq. (13). Fig1 (line (4)) shows the dependence $Q(t)$, for the ensemble of $N = 100$ particles $(\gamma_w = 0.4, \gamma_f = 1.2, \alpha = 1.2)$, rescaled for one particle.

One can go continuously among the various diffusional behaviors by tuning parameters in an iterated map. As an example of deterministic channel we consider a combined map [3]. This one-dimensional map generates intermittent chaotic motion with coexisting localized and ballistic motion events. The map is defined for one unit cell by the iterative rules,

$$X_{n+1} = f(X_n),$$

$$f(x) = \begin{cases} 
X + ax^2 - 1, & 0 < X < \frac{1}{2}, \\
X - \bar{a}(\frac{1}{2} - X)^z, & \frac{1}{2} < X < \frac{5}{2}.
\end{cases} \quad (14)$$

The thermodynamic velocity, $v_{Th}$, can be included into the map description. We fix a time step $dt$ and after one iteration of the map, Eq.(14), stretch the system time following $t = t + dt/v_{Th}$. The length of channel is determined by a number of unit cells, $0 > |X| > L$. When the particle reaches the boundary cells, $|X| = 0$ or $|X| = L$, it is randomly placed into the interval $0 < X < 1/2$ or $L - 1/2 < X < L$ respectively. This corresponds to a diffusive reflection of particle back to the channel.

FIG. 4: Evolution $Q(t)$ vs $t$ for the map in Eq. (14) with $\gamma_w = 0.5, \gamma_f = 1.5 (L = 1000, dt = 10^{-4}, T_+ = 2$ and $T_- = 1$). Straight lines correspond to power law dependence in Eq. (12). Inset shown numerically obtained relation between scaling exponent $\beta$ for one-particle flux and exponent $\alpha (\gamma_w = 1.6$ for all cases). Straight lines correspond to $\beta = 3 - \alpha$.