Magnetically Induced Thermal Rectification

Giulio Casati\textsuperscript{1,2,3}, Carlos Mejía-Monasterio\textsuperscript{4}, and Tomaz Prosen\textsuperscript{5}

\textit{Center for Nonlinear and Complex Systems, Università degli Studi dell’Insubria, Como Italy}\textsuperscript{3}
\textit{CNR-INFM and Istituto Nazionale di Fisica Nucleare, Sezione di Milano}\textsuperscript{2}
\textit{Department of Physics, National University of Singapore, Republic of Singapore}\textsuperscript{3}
\textit{Dipartimento di Matematica, Politecnico di Torino, Italy}\textsuperscript{4} and
\textit{Physics Department, Faculty of Mathematics and Physics, University of Ljubljana, Ljubljana, Slovenia}\textsuperscript{5}

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We consider far from equilibrium heat transport in chaotic billiard chains with non-interacting charged particles in the presence of non-uniform transverse magnetic field. If half of the chain is placed in a strong magnetic field, or if the strength of the magnetic field has a large gradient along the chain, heat current is shown to be asymmetric with respect to exchange of the temperatures of the heat baths. Thermal rectification factor can be arbitrarily large for sufficiently small temperature of one of the baths.

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The problem of explaining irreversible macroscopic transport laws, such as the Fourier law of heat conduction, from the reversible microscopic equations of motion is one of the open problems in nonequilibrium statistical mechanics [1, 2]. The problem is still far from being settled, in particular in the framework of low dimensional systems, e.g. one dimensional particle chains, where different instances of anomalous transport can be identified due to various kinematic or dynamic mechanisms.

In systems of non-interacting particles, e.g. quasi 1-d chaotic billiards, the validity of Fourier law has clearly been confirmed [3], even though such non-interacting system cannot exhibit local thermal equilibrium in the non-equilibrium steady state [4, 5]. Furthermore, interesting connection between the Fourier law and particle diffusion has been established [6]. These problems are not only interesting for understanding the fundamentals of statistical mechanics, but they may also have straightforward applications, e.g. for connecting dynamics and transport in emerging nano-technology, engineering of molecular motors, understanding and control of energy flow in bio-molecules, etc.

In view of these ideas, Terraneo et al. [7] have recently proposed a mechanism for thermal rectification in an anharmonically interacting particle chain. Using an effective phonon approach, they have shown that a chain composed of three different parts may have asymmetric heat transport properties due to (non)matching of the effective phonon bands. This and related ideas have been further elaborated and improved [8, 9]. A further step to devise a thermal transistor has been discussed in [10] in terms of the negative differential thermal resistance observed in some anharmonic chains.

Since these first works, other different mechanisms leading to thermal rectification have been described. In [11] it was shown that the nonlinearity of the dynamics of an asymmetric two-level system leads to an asymmetric heat flow. More recently in [13] it was shown that thermal rectification can be observed in asymmetric billiards of interacting particles. When the billiard is subjected to an external temperature gradient the effective interaction leads to a temperature dependence of the transmission coefficient and thus, it is possible to dynamically controls the transmission probability of the billiard. For this type of billiard systems rectifications as large as $10^3$ were observed. However, the theory presented in [13] requires the knowledge of the microscopic transmission coefficients, which is, at best phenomenological. Another, simple phenomenological mechanism of thermal rectification, based on strong positional and temperature dependence of local thermal conductivity, has been proposed by Peyrard [12].

A common problem with most of these proposals is that the rectification factor has always been rather limited, i.e. it is very difficult to achieve a situation in which heat flows only in one direction and not in the opposite one. Moreover, the fact that the thermal rectification depends directly or indirectly on the microscopic particle-particle interaction, renders difficult the ability to control the power of rectification.

In this letter we propose a novel microscopic mechanism for thermal rectification which works in the absence of particle interactions. Instead, thermal rectification is controlled with an external non-uniform magnetic field, leading to an \textit{arbitrarily large} power of rectification. In our model heat is carried by charged particles and the only restriction is that the typical mean-free-paths due to dissipative mechanisms should be much larger than the Larmor radius of the charged particles in the magnetic field. In practice this means that the temperatures of the baths should be quite low, but such regimes are nowadays easily accessible for example in mesoscopic physics, quantum dots/wires, anti-dot lattices etc. The rectification mechanism is very simple, it is based on asymmetric reflection of slow and fast particles off the interface between regions with different magnetic field intensities and predicts arbitrary large rectification factors for sufficiently low temperatures.

We consider a gas of noninteracting point particles of mass $m$ and electric charge $e$ that move freely inside a two-dimensional billiard region. The billiard is shaped as a chain of equal cells as depicted in Fig. 1. Let the circular obstacles have radius $R$ and centers of the discs be arranged in a hexagonal array with lattice distance $4/\sqrt{3}$, such that the billiard...
motion has a closed horizon for \( R \geq 1 \). Then we cut out a quasi one-dimensional billiard channel of width \( \delta y = 2/\sqrt{3} \) through the centers of two nearby rows of discs, so that one rectangular \( \delta x \times \delta y \) cell of the channel, containing one half disk and two quarter disk obstacles, has length \( \delta x = 4 \). Negative curvature of the billiard boundary ensures that the motion in the absence of the magnetic field is completely chaotic - hyperbolic.

The simplest model that we consider is composed of two cells (Fig. 1). The left cell contains no magnetic field, whereas the right cell is subjected to a uniform magnetic field of strength \( B \). In what follows we will refer to a channel of \( N \) cells for which the \( N/2 \) left cells contain no magnetic field and the \( N/2 \) right cells contain a magnetic field of density \( B \). Let \( \lambda \) denote the smallest length scale in the problem, namely the width of the opening between the neighboring cells in our model,

\[
\lambda = \frac{2}{\sqrt{3}} - R. \tag{1}
\]

The transmission probability of the billiard is controlled by the strength of the magnetic field. Consider the particles that cross the junction between the two cells from left to right. There exist a critical velocity \( v_c \): fast particles of velocity \( v > v_c \) always enter the right cell, and thus contribute to the left to right energy flow provided they reach the right end of the system which is coupled to a heat bath as explained below. Instead, slow particles of velocity \( v < v_c \), such that the gyromagnetic radius \( g(v) = mv/(eB) \) is less than \( \lambda/2 \) will be reflected or transmitted depending on the position at which they reach the interface.

Using a statistical ensemble of trajectories, the condition for the critical velocity \( g(v_c) = \lambda/2 \) can be rewritten as the condition giving a critical temperature

\[
T_c = \frac{(eB\lambda)^2}{8\pi m k_B} . \tag{2}
\]

such that particles which are colder than \( T_c \) will be reflected in their majority.

However, for the particles that cross the junction from right to left there is no condition on their velocity and they always enter the left cell. The above qualitative argument makes it clear that the transport of heat will be strongly asymmetric with respect to exchange of effective temperatures of particles on different sides of magnetic field boundary, provided the temperatures are strongly different, one being larger and the other smaller than \( T_c \). In the rest of the letter we measure the temperature in units of \( T_c \), and denote it as \( \tau = T/T_c = 2\pi eB/\delta x \).

We couple the left cell with a stochastic heat bath [3] of dimensionless temperature \( \tau_L \) and the right cell with a heat bath of temperature \( \tau_R \), namely if a particle reaches the end boundary of the billiard that is in contact with a heat bath it is reflected with a velocity chosen from a distribution with probability densities

\[
P_n(v_x) = \frac{1}{\tau} |v_x| \exp \left( -\frac{v_x^2}{2\tau} \right),
\]

\[
P_l(v_y) = \frac{1}{\sqrt{2\pi\tau}} \exp \left( -\frac{v_y^2}{2\tau} \right),
\]

where \( \tau \) is the temperature of the respective heat bath in dimensionless units.

If the left bath is cold, i.e. \( \tau_L \ll 1 \), then the particles will most of the time remain in the left cell and there will be no heat current between the baths, irrespective of the temperature of the right bath, which we assume is larger than 1. If we exchange the temperatures of the baths, then we will in general have some non-small heat current flowing, since cold particles have no problem in leaving the region with a magnetic field.
we have

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\(v\) spend long time before being able to cross the

magnetic field). This is mainly because the cold particles in

the left cell spend long time before being able to cross the

interface: \(\tau_L = \tau_{\text{max}}\) (triangles) and \(\tau_R = \tau_{\text{min}}\) (circles) respectively.

Let us measure the heat currents per particle in the steady
state, and denote them as \(J^+\) if \(\tau_L < \tau_R\) and \(J^-\) if the temper-
atures are exchanged, i.e. \(\tau_L > \tau_R\). Comparing the magnitude
of these two currents we quantify the thermal rectification as

\[
\Delta = \frac{\max\{|J^+|, |J^-|\}}{\min\{|J^+|, |J^-|\}}. \tag{4}
\]

From our argument it is clear that rectification will be effec-
tive if one of the temperatures is very small, say \(\tau_L \ll 1\) and
the other is simply above the critical, \(\tau_R > 1\). It is possible to
make a quantitative prediction on the scaling of rectification
factor \(\Delta\) with temperatures. When the energy current through
the magnetic field interface is very weak, namely if \(\tau_L < \tau_R\),
the current is proportional to the transmission coefficient at
the interface, i.e. one minus the probability of reflection.

From our previous discussion it is clear that if \(\tau_L < 1 < \tau_R\)
the particle density will be larger at the left cell (with zero magnetic field). This is mainly because the cold particles in
the left cell spend long time before being able to cross the
interface. A particle of velocity \(v\) is transmitted (not reflected)
to the right cell if it crosses the interface at a distance from the
upper boundary shorter than \(2\rho(v)\) [14]. Therefore, invoking
the ergodicity of the dynamics in the left cell, we can simply
estimate the transmission coefficient \(t^+\) as

\[
t^+ \sim \frac{2\rho(v)}{\lambda}, \tag{5}
\]

where \(\rho(v(\tau)) = \sqrt{2mk_BT_{\text{min}}/eB}\) and we denote by \(\tau_{\text{min}} = \min\{\tau_L, \tau_R\}\).

However, in the reverse situation (exchanging \(\tau_L\) and \(\tau_R\))
we have \(t^- \sim 1\), so we can estimate the rectification

\[
\Delta = t^-/t^+ \propto \frac{1}{\sqrt{\tau_{\text{min}}}}. \tag{6}
\]

In Fig. 2 we show the rectification index \(\Delta\) as a function
of \(\tau_{\text{min}}\) for fixed value of the maximal temperature \(\tau_{\text{max}}\). We
clearly confirm the scaling (6), indicating also that the recti-
fication index is only very weakly depending on the maximal
temperature (as long as \(\tau_{\text{max}} > 1\). This can be seen in the
inset of Fig. 2) where the rectification index \(\Delta\) is shown as a
function of the two temperatures of the heat baths \(\tau_L\) and \(\tau_R\).

The correctness of the scaling (6) shows that the magnetically
induced rectification power is arbitrarily large for sufficiently
small temperature \(\tau_{\text{min}}\).

Even though a non-interacting system cannot reach local
thermal equilibrium, and therefore the concept of (local) tem-
perature is not well defined, it is instructive to compute tem-
perature and density profiles, as long-time averages of kinetic
energy density and particle density as a function of the hori-
zontal coordinate along the chain. In Fig. 3 we plot the kinetic
energy density and the particle density measured in each cell
of a channel of 10 cells, the right half of 5 cells being in a
uniform magnetic field. We plot the profiles for the positive
gradient, \(\tau_L < \tau_R\) (triangles), and the inverted negative gradi-
et (circles). The positive gradient for which \(\tau_L = \tau_{\text{min}}\) corre-
sponds to the insulating case, i.e. to the situation in which the
heat current is very small. In Fig. 3 we see that the insulating
case corresponds to a large gap in the kinetic energy profile. In
contrast, for the negative gradient the gap in the kinetic energy
profile is much smaller and this coincides with the observation
of a larger heat current. However, note that the energy profile
for the negative gradient is not a monotonous function due to
the lack of local thermal equilibrium. Moreover, the density
profile confirms our prediction that the low current situation is
characterized by a very small density of particles on the side of
the magnetic field.

We discuss now a slightly different situation in which the
magnetic field does not change abruptly from one half of the
system to the other, but instead changes gradually, forming a
uniform gradient of the magnetic field. We refer to this situa-

FIG. 3: Energy density (a) and particle density (b) profiles for a
10-cell channel in a \textit{step} configuration. The bath temperatures are
\(\tau_{\text{min}} = 3.34277 \times 10^{-2}, \tau_{\text{max}} = 33.4277\). In both panels
profiles are shown for the positive and negative gradient for which
\(\tau_R = \tau_{\text{max}}\) (triangles) and \(\tau_R = \tau_{\text{min}}\) (circles) respectively.

FIG. 4: 10-cell channel in a \textit{gradient} configuration: (a) Rectifica-
tion index \(\Delta\) as a function of the minimal temperature \(\tau_{\text{min}}\) with
\(\tau_{\text{max}} = 33.4275\). The temperatures are given in units of \(T_c(B)\),
where \(B = 100\) is the strength of the magnetic field at the right-
most cell. The dashed line is for the no rectification value \(\Delta = 1\).
The solid line corresponds to \(\tau_{\text{min}}^{-1/2}\). In the panels at the right the
profiles of kinetic energy (b) and particle density (c) for the positive
(triangles) and negative (circles) gradient are shown.
applied, then the critical temperature is \( T_c \). As expected the profiles for the positive and negative gradients are also shown.

In the thermodynamic limit, a vanishingly small temperature gradient is established across the system. In Fig. 5 we show the profiles of the kinetic energy and particle density, namely one particle per cell. The dashed line corresponds to \( L^{-1} \). Inset: heat current \( J \) as a function of the size of the chain \( L \) for the positive (triangles) and negative (circles) gradient.

FIG. 5: Dependence of the thermal rectification index \( \Delta \) as a function of the size of the chain \( L \) for a chain in a step-configuration with fixed \( \tau_{\text{min}} = 3.34275 \times 10^{-5} \), \( \tau_{\text{max}} = 3.34275 \times 10^{2} \) and fixed particle density, namely one particle per cell. The dashed line corresponds to \( L^{-1} \). Inset: heat current \( J \) as a function of the size of the chain \( L \) for the positive (triangles) and negative (circles) gradient.

We have performed numerical simulations for the gradient configuration, and we found no qualitative differences with respect to the step configuration. In Fig. 4 we show the dependence of the rectification index on the minimal temperature (panel a). As for the step configuration we have found that for sufficiently low temperature \( \tau_{\text{min}} \), the rectification index again grows as \( \Delta \sim 1/\sqrt{\tau_{\text{min}}} \). In the panels (b) and (c) we show the profiles of the kinetic energy and particle density respectively. As expected the profiles for the gradient configuration are more smooth than for the step configuration.

From our analysis it follows that our rectification effect is a phenomenon which exists only in far from equilibrium situations. In the thermodynamic limit, a vanishingly small temperature gradient is established across the system. In Fig. 5 we show the results of numerical simulations which indicate that, for fixed bath temperatures, the rectification index scales as \( \Delta \sim 1/L \). In the inset of Fig. 5 the time averaged heat currents for the positive and negative gradients are also shown.

Finally, it is interesting to give a quantitative estimate of the critical temperature in Eq. (2) in physical units. Let us suppose that the gas of particles inside the billiard of Fig. 1 consists of electrons. Assuming that the dimension of the opening is \( \lambda = 100 \text{nm} \) and a magnetic field of \( B = 1 \text{T} \) is applied, then the critical temperature is \( T_c \sim 0.5 \text{K} \). Thus, a rectification power of \( \Delta \sim 10 \) would be measurable for thermal gradient given by \( T_{\text{min}} \sim 10^{-3} \text{K} \) and \( T_{\text{max}} \sim 10 \text{K} \) that appears accessible to nowadays experiments.

In this letter we have presented a novel mechanism for thermal rectification. This mechanism is fairly simple. It results from the asymmetric behavior of the dynamics at the magnetic interface, that leads to a simple temperature dependence of the transmission coefficient. Moreover, this mechanism for thermal rectification is not based on the, macroscopically unaccessible, microscopic particle interaction, but on the interaction with an external field, making possible an easy control of the power of rectification. We have shown that the thermal rectification power is arbitrarily large for sufficiently small temperature of one of the heat baths.

Furthermore, the physical scales needed for optimal implementation of our theoretical model are realizable in present nano-scale experiments with meso-scale devices. We believe that it is precisely at these scales of meso-scale physics where such a thermal rectifier would find interesting applications. This fact makes an experimental verification of the mechanism presented here very desirable.

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[14] The particles that are transmitted to the right cell bounce repeatedly with either the upper or the lower boundary of the billiard and this depends on the sign of the magnetic field.