I. INTRODUCTION

The origin of the macroscopic phenomenological “laws” of thermodynamic transport is still one of the major challenges to theoretical physics. In particular the issue of energy (heat) transport, in spite of having a long history, is not completely settled \[1, 2\]. Given a particular classical, many-body Hamiltonian system, neither phenomenological nor fundamental transport theory can predict whether or not this specific Hamiltonian system yields an energy transport governed by the Fourier law of heat conduction by nonlinearity opens the possibility to propose new devices such as a thermal rectifier.

Indeed modern ergodic theory tells us that for K-systems, a sequence of measurements with finite precision mimics a truly random sequence and therefore these systems appear precisely those deterministically random systems tacitly required by transport theory. In fact the thermal conductivity has been studied for a Lorentz channel –a quasi one dimensional billiard with circular

scatterers– and it was shown to obey Fourier law \[15\]. Yet we do not have rigorous results and in spite of several efforts, the connection between Lyapunov exponents, correlations decay, diffusive and transport properties is still not completely clear. For example, in a recent paper \[26\] a model has been presented which has zero Lyapunov exponent and yet it exhibits unbounded Gaussian diffusive behavior. Since diffusive behavior is at the root of normal heat transport then the above result \[26\] constitutes a strong suggestion that normal heat conduction can take place even without the strong requirement of exponential instability. Moreover, the models in \[15, 23\] are noninteracting and thus, the condition of Local Thermal Equilibrium (LTE) is not satisfied. Noninteracting particle systems are certainly less realistic. They are good models for gases in the Knudsen limit in which the mean free path is larger than the characteristic length of the container and their use in other physical situations is open to criticism \[24\]. Therefore, it is interesting to investigate up to what extend one can simplify the microscopic dynamics, and yet obtain a normal transport behavior.

An additional interesting problem, almost completely unexplored, is the derivation of Fourier law from quantum dynamics. Indeed at the quantum level, investigations have been mainly focused on linear response theory \[25\]. The possibility to derive the Fourier law by directly establishing the dependence of \( J \) on \( \nabla T \) in a nonequilibrium steady state calls directly in question the issue of quantum chaos. In this connection we recall that a main feature of quantum motion is the lack of exponential dynamical instability \[26\], a property which is at the heart of classical dynamical chaos.

The aim of this paper is to discuss the transport of heat in several classical and quantum microscopic models by direct numerical simulation of energy flow in the system in contact with thermal baths. At the classical level our results in section \[14\] provide convincing evidence that linear mixing systems (i.e. with zero Lyapunov exponent)
obey Fourier law. At the quantum level we study in section III an Ising chain of $L$ coupled spins 1/2 in a tilted magnetic field. We provide clear numerical evidence of the validity of Fourier law at the onset of quantum chaos. In section IV we then investigate the possibility to control the energy transport and discuss different microscopic mechanical models in which thermal rectification can be observed. The possibility to control heat conduction by nonlinearity opens the way to design a thermal rectifier, i.e. a lattice that carries heat preferentially in one direction while it behaves as an insulator in the opposite direction.

II. DYNAMICAL INSTABILITY AND FOURIER LAW

A Lorentz gas consists of noninteracting point particles that collide elastically with a set of circular scatterers on the plane. Motivated by the ergodicity and mixing properties of the Lorentz gas, in Fig. 1 a channel geometry of this model was considered to study the problem of heat conduction. By imposing and external thermal gradient it was found that in a Lorentz channel the Fourier law is satisfied. Yet this system is not described by LTE. A modification of this model in which particles and scatterers can exchange energy through their collisions appeared in [20]. This effective interaction leads to the establishment of LTE. As a consequence, this model has proven to reproduce realistically macroscopic transport in many different situations [21]. In particular, the validity of Fourier law was verified, indicating that the interaction among the different particles is not fundamental for the observation of normal transport.

To clarify the role of dynamical instability on the validity of Fourier law, let us consider a two dimensional billiard model which consists of two parallel lines of length $L$ at distance $d$ and a series of triangular scatterers (Fig. 1). In this geometry, no particle can move between the two reservoirs without suffering elastic collisions with the triangles. Therefore this model is analogous to the one studied in [17] with triangles instead of discs and the essential difference is that in the triangular model discussed here the dynamical instability is linear and therefore the Lyapunov exponent is zero. Strong numerical evidence has been recently given [18] that the motion inside a triangular billiard, with all angles irrational with $\pi$ is mixing, without any time scale, (see also [14]). Moreover, an area preserving map, which was derived as an approximation of the boundary map for the irrational triangle, when considered on the cylinder shows a nice Gaussian diffusive behavior even though the Lyapunov exponent of the map is zero [23]. It is therefore reasonable to expect that the motion inside the irrational polygonal area of Fig. 1 is diffusive thus leading to normal conductivity.

We consider a channel of total length $L = NL$ where $N$ and $l$ are the number and the length of the fundamental cells. For the irrational angles we take $\theta = (\sqrt{2} - 1)\pi/2$ and $\phi = 1$. By increasing $L$, the number of particles per cell must be kept constant. However, since the particles do not interact one may consider the motion of a single particle over long times and then rescale the flux.

Heat conductivity of this model has been numerically studied in [22]. Heat baths have been simulated with stochastic kernels of Gaussian type, namely, the probability distribution of velocities for particles coming out from the baths is

$$P(v_x) = \frac{v_x}{T} \exp\left(-\frac{v_x^2}{2T}\right), P(v_y) = \frac{1}{\sqrt{2\pi}T} \exp\left(-\frac{v_y^2}{2T}\right)$$

for $v_x$ and $v_y$, respectively.

Since the energy changes only at collisions with the heat baths, the heat flux is given by

$$j(t_c) = \frac{1}{t_c} \sum_{k=1}^{N_c} \Delta E_k,$$

where $(\Delta E)_k = E_{in} - E_{out}$ is the change of energy at the $k$-th collision with the heat bath and $N_c$ is the total number of such collisions which occur during time $t_c$. We have checked that for sufficiently long integration times ($> 10^{10}$ time unit) the system reach a stationary value.

In Fig. 2, we plot the heat flux $J$ as a function of the system size $N$. For the case of irrational angles, the best fit gives $J \propto N^{-\gamma}$, with $\gamma = 0.99 \pm 0.01$. The coefficient of thermal conductivity is therefore independent on $N$, which means that the Fourier law is obeyed.

As a consistency check we have also performed an independent check of the above results via a Green-Kubo type formalism [25] from which consistent results with those presented above have been obtained.

A completely different behavior is obtained when the angles $\theta$ and $\phi$ are rational multiples of $\pi$. The case with $\theta = \pi/5$ and $\phi = \pi/3$, is shown in Fig. 2 (triangles), from which a divergent behavior of the coefficient of thermal conductivity $\kappa \propto N^{-0.22}$ is observed, indicating the absence of Fourier law.

![Fig. 1: The geometry of the model. Particles move in the region outside the triangular scatterers. The $x$ coordinate goes along the channel and $y$ is perpendicular to it. The two heat reservoirs at temperatures $T_L$ and $T_R$ are indicated. The length of each cell is $l = 3$, the base of the triangles is $a = 2.19$ and the distance between the two parallel lines is $d = 1.8$. The geometry is then uniquely specified by assigning the internal angles $\theta$ and $\phi$.](image-url)
In conclusion, when all angles are irrational multiples of $\pi$ the model shown in Fig. 1 exhibits Fourier law of heat conduction together with nice diffusive properties. However, when all angles are rational multiple of $\pi$, the model shows abnormal diffusion and the heat conduction does not follow the Fourier law.

One may argue that the model considered here is somehow artificial and far from realistic physical models. Indeed, noninteracting particle systems are certainly less realistic as in general, LTE is not established. However the problem under discussion is quite delicate and controversial and our main purpose is to understand which dynamical properties are necessary and sufficient to derive Fourier law.

In this respect we mention two different billiards like models that are genuinely interacting many-particle models and that share some of the properties of the model discussed here. The first one is the 1d hard-point particles with alternating masses that consists of a one-dimensional chain of elastically colliding free particles with alternate masses $m$ and $M$ [12, 13]. For this model all Lyapunov exponents are zero like the irrational triangle channel. In [27] the problem of heat conduction in this model was considered. It was found that in the alternating mass model the heat current follows a power-law behavior $J \propto N^{-a}$ with $a \approx 0.745$. In contrast with the irrational triangle channel, the alternating mass model does not obey Fourier law.

Therefore we have two models which are both mixing and without exponential instability: (i) the triangular billiard channel [28] (see also [24]), which exhibits Fourier law and (ii) the alternate mass hard point gas model [27] in which the coefficient of thermal conductivity diverges with the system size. The difference between the two models is that in case (ii) the total momentum is conserved while in case (i) it is not. We recall that in several recent papers [12, 30, 31] it has been suggested that total momentum conservation does not allow Fourier law and this may explain the lack of Fourier law for the one dimensional alternating mass model.

To clarify the role of total momentum conservation, in [32] a model which is identical to the alternate mass hardpoint gas but without total momentum conservation was considered. Numerical results clearly indicate that this model, contrary to the translationally invariant model, obeys the Fourier law.

In perspective, these results demonstrate that diffusive energy transport and Fourier law can take place in marginally stable (non-chaotic) interacting many-particle systems. As a consequence exponential instability (Lyapunov chaos) is not necessary for the establishment of the Fourier law. Furthermore, they show that breaking the total momentum conservation is crucial for the validity of Fourier law while, somehow surprisingly, a less important role seems to be played by the degree of dynamical chaos.

III. FOURIER LAW AND THE ONSET OF QUANTUM CHAOS

In section II we have shown that strong, exponential unstable, classical chaos is not necessary (actually, strictly speaking, is not even sufficient) for normal transport. In this connection, a main feature of quantum motion is the lack of exponential dynamical instability [15]. Thus it is interesting to inquire if, and under what conditions, Fourier law emerges from the laws of quantum mechanics.

We consider an Ising chain of $L$ spins $1/2$ with coupling constant $Q$ subject to a uniform magnetic field $\vec{h} = (h_x, 0, h_z)$, with open boundaries. The Hamiltonian reads

$$\mathcal{H} = -Q \sum_{n=0}^{L-2} \sigma_n^x \sigma_{n+1}^x + \vec{h} \cdot \sum_{n=0}^{L-1} \vec{\sigma}_n,$$

where the operators $\vec{\sigma}_n = (\sigma_n^x, \sigma_n^y, \sigma_n^z)$ are the Pauli matrices for the $n$-th spin, $n = 0, 1, \ldots, L - 1$. We set the coupling constant $Q = 2$. In this system, the only trivial symmetry is a reflection symmetry, $\sigma_n \rightarrow -\sigma_{L-1-n}$. Moreover the direction of the magnetic field affects the qualitative behavior of the system: If $h_z = 0$, the Hamiltonian [3] corresponds to the Ising chain in a transversal magnetic field. In this case the system is integrable as [3] can be mapped into a model of free fermions through standard Wigner-Jordan transformations. When $h_z$ is increased from zero, the system is no longer integrable and when $h_z$ is of the same order of $h_x$ quantum chaos sets in leading to a very complex structure of quantum states as well as to fluctuations in the spectrum that are statistically described by Random Matrix Theory (RMT).
The system becomes again (nearly) integrable when $h_z \gg h_x$. Therefore, by choosing the direction of the external field we can explore different regimes of quantum dynamics.

The onset of quantum chaos is commonly studied in terms of the nearest neighbor level spacing distribution $P(s)$ that gives the probability density to find two adjacent levels at a distance $s$. For an integrable system the distribution $P(s)$ has typically a Poisson distribution $P_{\text{P}}(s) = \exp(-s)$. In contrast, in the quantum chaos regime (for Hamiltonians obeying time-reversal invariance), $P(s)$ is given by the Gaussian Orthogonal Ensemble of random matrices (GOE). In this case, $P(s)$ is well-approximated by the Wigner surmise $P_{\text{WD}}(s) = (\pi s/2) \exp(-\pi s^2/4)$, exhibiting the so-called “level repulsion”.

In Fig. 3 we show the results of our numerical simulations of system 4 for three different values of the magnetic field: (i) chaotic case $\vec{h} = (3.375, 0, 2)$ at which the distribution $P(s)$ agrees with GOE and thus corresponds to the regime of quantum chaos, (ii) integrable case $\vec{h} = (3.375, 0, 0)$, at which $P(s)$ is close to the Poisson distribution, and (iii) intermediate case $\vec{h} = (7.875, 0, 2)$ at which the distribution $P(s)$ shows a combination of (weak) level repulsion and an exponential tail.

In order to study energy transport we need to couple both ends of the chain of spins to thermal reservoirs at different temperatures. In 3 we have devised a simple way to simulate this coupling, namely the state of the spin in contact with the bath is statistically determined by a Boltzmann distribution with parameter $T$. Our model for the reservoirs is analogous to the stochastic thermal reservoirs defined by Eqs. 1 and we thus call it a quantum stochastic reservoir. In what follows we use units in which Planck and Boltzmann constants are set to unity $\hbar = k_B = 1$.

The dynamics of the spins is obtained from the unitary evolution operator $U(t) = \exp(-i\vec{H}t)$. Additionally the leftmost and rightmost spins of the chain are coupled to quantum stochastic reservoirs at temperatures $\beta^{-1}$ and $\beta^{-1}$ respectively.

The action of the quantum reservoirs is as follows: at times $t = nr$ with $n$ integer the boundary spins couple to the quantum reservoirs. A local measurement of the boundary spins is performed and their new state is set to the state down (up) with probability $\mu$ ($1-\mu$) where the probability $\mu(\beta)$ depends on the canonical temperature of each of the thermal reservoirs as

$$\mu(\beta_j) = \frac{e^{\beta_j} \hbar}{e^{\beta_j} \hbar + e^{\beta_j} \hbar}; \quad j \in \{1, r\}. \quad (4)$$

The value of $\tau$ controls the strength of the coupling to the bath. In it was shown that averages over the ensemble of quantum trajectories or time averages over a quantum trajectory are sufficient to reconstruct a thermal density matrix operator that correctly describes the internal thermal state of the system in and out of equilibrium. Moreover, the time averaged expectation values of the local energy density can be used as a consistent canonical local temperature. In order to compute the energy profile we write the Hamiltonian 3 in terms of local energy density operators $H_n$:

$$H_n = -Q\sigma_n^z\sigma_{n+1}^z + \frac{\hbar}{2}(\overline{\sigma}_n + \overline{\sigma}_{n+1}) \quad (5)$$

The local Hamiltonian $H_n$ (defined for $0 < n < L - 2$), gives the energy density between the $n$-th and $(n+1)$-th spins. In terms of eq. 5 the Hamiltonian of the system can be rewritten as

$$H = \sum_{n=0}^{L-2} H_n + \frac{\hbar}{2}(\sigma_1 + \sigma_r) \quad (6)$$

In Fig. 4 we show the energy profile $\langle H_n \rangle$ for an out of equilibrium simulation of the chaotic chain. In all nonequilibrium simulations, the temperatures of the baths were set to $T_1 = 5$ and $T_r = 50$. After an appropriate scaling the profiles for different sizes collapse to the same curve. More interesting, in the bulk of the chain the energy profile is in very good approximation linear. In contrast, we show that in the case of the integrable (inset I) and intermediate (inset II) chains, no energy gradient is created.

We now define the local current operators through the equation of continuity: $\partial_t H_n = i[H, H_n] = -(J_{n+1} - J_n)$, requiring that $J_n = [H_n, H_{n-1}]$. Using eqs. 5 and 6 the local current operators are explicitly given by

$$J_n = \hbar x Q (\sigma_n^{z-1} - \sigma_{n+1}^{z+1}) \sigma_n^{y}, \quad 1 \leq n \leq L - 2. \quad (7)$$

In Fig. 5 we plot $J/\Delta T$ as a function of the size $L$ of the system for sizes up to $L = 20$. The mean current $J$ is calculated as an average of $\langle J_n \rangle$ over time and the $L - 8$ central values of $n$. Since $\Delta L = L - 8$ is an effective size of the truncated system, the observed $1/\Delta L$ dependence confirms that the transport is normal. On the other hand, in integrable and intermediate chains we have observed that the average heat current does not depend on the size $J \propto L^0$, clearly indicating a ballistic transport.
FIG. 4: Out of equilibrium energy profile $\langle H_n \rangle$ for the chaotic chain. The temperatures of the baths were set to $T_L = 5$ and $T_R = 50$. Results for chains of size $L = 8$ (crosses), $L = 14$ (open circles) and $L = 20$ (solid circles) are shown. The dashed line was obtained from a linear fit of the data for $L = 20$ for the $L - 4$ central spins. Insets (I) and (II) show the energy profile for the integrable and intermediate cases respectively, for $L = 15$.

In conclusion we have shown that Fourier law of heat conduction can be derived from the pure quantum dynamical evolution without any additional statistical assumption. Our results suggest that onset of quantum chaos is required for the validity of Fourier law.

FIG. 5: Size dependence of the energy current in the chaotic chain with $T_L = 5$ and $T_R = 50$. The dashed line corresponds to $1/\Delta L$ scaling. In the inset, the size dependence of the energy current is shown for the integrable (circles) and the intermediate (squares).

IV. THERMAL RECTIFICATION

We now turn our attention to the possibility to control heat flow. To this end we start with the model introduced in Ref. [38] and consider the Hamiltonian

$$H = \sum_{n=1,N} \frac{p_n^2}{2m} + V_n(y_n) + \frac{1}{2}K(y_n - y_{n-1})^2$$  \hspace{1cm} (8)$$

which describes a chain of $N$ particles with harmonic coupling of constant $K$ and a Morse on-site potential $V_n(y_n) = D_n(e^{-\alpha y_n} - 1)^2$. This model was introduced for DNA chains where $m$ is the reduced mass of a base pair, $y_n$ denotes the stretching from equilibrium position of the hydrogen bonds connecting the two bases of the $n$-th pair and $p_n$ is its momentum [38]. In the context of the present study, model (8) can simply be viewed as a generic system of anharmonic coupled oscillators, the on-site potential arising from interactions with other parts of the system, not included in the model. The Morse potential is simply an example of a highly anharmonic soft potential, which has a frequency that decreases drastically when the amplitude of the motion increases.

We consider the out-of-equilibrium properties of model (8) by numerically simulating the dynamics of the $N$ particle chain, coupled at the two ends, with thermal baths at different temperatures. We thermalize at $T_L$ and $T_R$ the first and the last $L$ particles by using Nosé-Hoover thermostats chains [37], or a Langevin description when we investigate cases very far from equilibrium. The baths temperatures $T_L, T_R$ are never large enough to drive the system beyond the thermal denaturation temperature $T_c$ above which the mean value of $y_n$ diverges [37].

We compute the temperature profile inside the system, i.e. the local temperature at site $n$ defined as
$T_n = m \langle y_n^2 \rangle$, where $\langle \rangle$ stands for temporal average, and the local heat flux $J_n = K(y_n(y_n - y_{n-1}))$. The simulations are performed long enough to allow the system to reach a non-equilibrium steady state where the local heat flux is constant along the chain.

As a preliminary step we have considered the homogeneous case in which $D_n = D$, $\alpha_n = \alpha$, $n = 1, \ldots, N$. Here, as expected, we have detected a temperature gradient inside the chain, and we have verified that the system obeys the Fourier law of heat conduction [38].

For the heterogeneous case we divide the chain between the thermostats in three regions in which $D_n$ takes different values. In the left and right regions, $D_n = D_L$ for $n = 1, \ldots, (N - M)/2$ and $D_n = D_R$ for $n = (N + M)/2 + 1, \ldots, N$, respectively. For the $M$ sites of the central region we set $D_n = D_0$. For the whole chain $\alpha_n = \alpha$.

In Fig. 6, we show the temperature profiles for three different values of $D_0$. Clearly a conductor–insulator transition occurs in the heterogeneous system as a function of the inhomogeneity measured by $D_0$. We have obtained that the averaged heat flux $\bar{J}$, which is uniform along the whole chain in the steady state, decreases by two orders of magnitude when $D_0 - D (D = D_L = D_R)$ increases from 0 to 0.7. This transition is explained in terms of a linearized version of the nonlinear Hamiltonian Eq. 3 effective phonon bands can be defined whose size and position depend on the microscopic properties of the interaction (in particular of coefficient $D$) and on the temperature. Using this dependence in a smart way one can design a thermal rectifier by choosing appropriate parameters $D_L$, $D_R$, $D_0$ and $\alpha$, depending on the range of temperatures in question. We intend for a thermal rectifier a device in which, for a fixed external temperature gradient, the magnitude of the heat current depends on the sign of the gradient.

For instance, for the heterogeneous model one can design a thermal rectifier by setting a strongly nonlinear region sandwiched between two weakly anharmonic left and right domains. In the presence of a thermal gradient in the central part, the effective phonon frequencies evolve in space in a way that depends on the orientation of the gradient. This can provide either a good matching of the bands at the interfaces, leading to a thermal conduction across the system, or a complete mismatch leading to poor conduction [38]. We exemplify this situation in Fig. 7 where the temperature profiles for the two orientations of the thermal gradient are shown. For the parameters values of Fig. 7 the heat current changes by a factor of about 2 when the direction of the thermal gradient is reversed.

Recently we have shown that using different microscopic models for the interaction like e.g. a Frenkel-Kontorova on-site potential, it is possible to strongly improve the efficiency of the rectifier [39]. Even though the underlying microscopic mechanism discussed in [38] is different from the one in [39] it is based on the same general idea: the temperature dependence of the phonon band. This dependence is due to the nonlinearity of the potential and therefore it should be possible to observe the rectifying effect in any nonlinear lattice.

But thermal rectification is not exclusive to nonlinear lattices. Recently we also have shown that this phenomenon can also be observed in billiard systems of interacting particles [40]. This model is based on the effective interaction of a gas of particles with the scatterers of a Lorentz channel [20, 21]. We have shown that the interacting character of the particles gives rise to dynamical memory effects that depend on the local thermodynamical fields, in particular on the local temperature gradients. These memory effects have been described in detail in [22, 41]. We have used this dependence to set up a particular geometry for which large thermal rectifications (the heat currents for both orientations of the thermal gradient differ by several orders of magnitude) are obtained [40]. The possibility to obtain large rectification of the heat flow in billiard systems has raised a great interest because they are more easily realizable experimentally in the rapidly expanding field of nanophysics.

![FIG. 7: Temperature profiles in a “thermal rectifier” for two opposite orientations of the thermal gradient. The dash-dotted lines show the borders of the different regions in the lattice. The thermostats have a size $L = 8$, the central region a size $M = 128$, and the left and right regions contain 64 particles. The coupling constant is $\kappa = 0.18$, and the parameters of the Morse potential are $D_L = 4.5$, $\alpha_L = 0.5$, $D_R = 0.7$, $\alpha_R = 1.4$, $D_0 = 2.8$, $\alpha_0 = 0.5$ in the left, central and right regions respectively. The temperatures of the thermostats are $T_L = 0.1$ and $0.45$. When the high temperature is on the right side of the lattice, the average flux is $\langle J \rangle = 0.146 \times 10^{-3}$ while, when the thermal gradient is reversed the flux drops to $J = 0.755 \times 10^{-4}$. Note in this case the discontinuities at the interfaces between region which attest of the bad energy transfer at these points.]

V. CONCLUSIONS

We have discussed the problem of heat conduction in classical and quantum low dimensional systems in rela-
tion to the dynamical properties of the system. At the classical level we have provided convincing numerical evidence for the validity of Fourier law of heat conduction in linear mixing systems, i.e. in systems without exponential instability. As a consequence exponential instability (Lyapunov chaos) is not necessary for the establishment of the Fourier law. Moreover, we have shown that breaking the total momentum conservation is crucial for the validity of Fourier law while, somehow surprisingly, a less important role seems to be played by the degree of dynamical chaos.

At the quantum level, where the motion is characterized by the lack of exponential dynamical instability, we have shown that Fourier law of heat conduction can be derived from the pure quantum dynamical evolution without any additional statistical assumption. Similarly to our observations in classical models, our results for a chain of interacting spins suggest that in quantum mechanics, which is characterized by the lack of exponential dynamical instability, the onset of quantum chaos is required for the validity of Fourier law.

We have also discussed the phenomenon of thermal rectification in different classical models and discussed different types of microscopic classical mechanisms that lead to the rectification of heat flow. Even though all these mechanisms are rooted in one way or another in the nonlinearity of the microscopic dynamics, we believe that, as for the case of Fourier law, thermal rectification is also possible at the quantum level. Some steps in this direction have already be taken [42, 43, 44].

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