

Fourier's law in a quantum spin chain and the onset of quantum chaos

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Abstract. – We study heat transport in a nonequilibrium steady state of a quantum interacting spin chain. We provide clear numerical evidence of the validity of Fourier law. The regime of normal conductivity is shown to set in at the transition to quantum chaos.

The derivation of Fourier's law of heat conduction from the microscopic dynamics, without any *ad hoc* statistical assumption, is one of the great challenges of nonequilibrium statistical mechanics [1]. Even in the context of classical dynamical systems, the issue of energy (heat) transport, in spite of having a long history (recently reviewed in [2]), is not completely settled. It has become clear that transport theory requires that the underlying deterministic dynamics yield a truly diffusive process. On the other hand, it is known that classical nonlinear systems of interacting particles, above a critical interaction strength, typically exhibit chaotic and diffusive behaviour which then leads to the onset of Fourier law $J = -\kappa \nabla T$, relating the macroscopic heat flux to the temperature gradient ∇T . Therefore deterministic chaos appears to be an essential ingredient required by transport theory. In this perspective, of particular interest is the problem, almost completely unexplored, of the derivation of Fourier law from quantum dynamics. So far, investigations have been mainly focused on linear-response theory [3]. The possibility instead to derive the Fourier law from quantum dynamics, by establishing the dependence of J on ∇T in a *nonequilibrium steady state*, calls directly into question the issue of quantum chaos. In this connection, a main feature of quantum motion is the lack of exponential dynamical instability [4], a property which is at the heart of classical dynamical chaos. This fact may render very questionable the possibility to derive the Fourier law of heat conduction in quantum mechanics. However, quite interestingly, it has been shown that strong, exponential unstable, classical chaos is not necessary [5] (actually, strictly speaking, is not even sufficient [6]) for normal transport. Thus it is interesting to inquire if, and

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under what conditions, Fourier law emerges from the laws of quantum mechanics. This is the purpose of the present paper.

To investigate this problem one has to deal with a finite open system connected to heat baths. Here we consider an interacting quantum spin-(1/2) chain which exhibits the transition from integrability to quantum chaos as a parameter, *e.g.* the magnetic field, is varied. The standard treatment of this problem is based on the master equation, thus limiting investigations to relatively small system sizes. By using this method, in an interesting paper [7], the decay of current correlation function in a model of non-integrable chain of quantum spins is computed. However, this results were not fully conclusive and its conclusions rely on linear-response theory. Also, in [8] Lindblad formalism was used to study the validity of Fourier's law for different type of spin-spin interaction.

Here we take a different approach, namely we follow the evolution of the system described by a *pure* state, which is *stochastically* coupled to an idealized model of heat baths. Stochastic coupling is realized in terms of a local measurement at the boundary of the system and stochastic but unitary exchange of energy between the system and the bath. By this method we have been able to perform very effective numerical simulations which allow to observe a clear energy/temperature profile and to measure the heat current J . In the nonintegrable regime where the spectral statistics is described by random matrix theory (RMT) —the regime of “quantum chaos”— we found very accurate Fourier law scaling $J/\Delta T \propto 1/L$, where L is the size of the chain. In the integrable and near-integrable regimes instead, we found that the heat transport is ballistic $J \propto L^0$.

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

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

where the operators $\vec{\sigma}_n = (\sigma_n^x, \sigma_n^y, \sigma_n^z)$ are the Pauli matrices for the n -th spin, $n=0, 1, \dots, L-1$. We set the coupling constant $Q = 2$. In this system, the only trivial symmetry is a reflection symmetry, $\vec{\sigma}_n \rightarrow \vec{\sigma}_{L-1-n}$. Moreover, the direction of the magnetic field affects the qualitative behavior of the system: If $h_z = 0$, the Hamiltonian (1) corresponds to the Ising chain in a transversal magnetic field. In this case the system is integrable as (1) 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. 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 RMT [9]. 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 $P_P(s) = \exp[-s]$. 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 $P_{WD}(s) = (\pi s/2) \exp[-\pi s^2/4]$, exhibiting the so-called “level repulsion”.

In fig. 1 we show the results of our numerical simulations of system (1) 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*

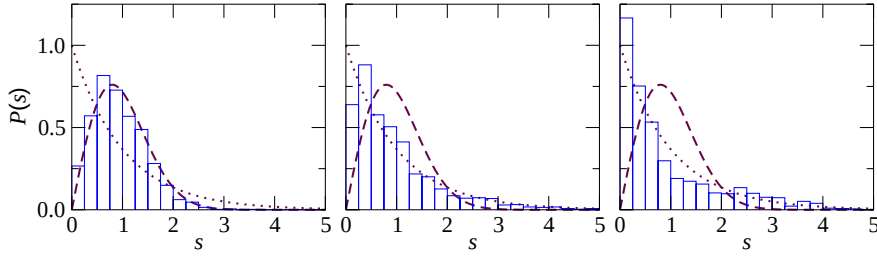


Fig. 1 – Nearest-neighbor level spacing distribution $P(s)$ for the chaotic (left), intermediate (center) and integrable (right) chains. $P(s)$ was obtained by diagonalizing the Hamiltonian (1) for a chain of length $L = 12$, averaging over even- and odd-parity sub-spectra. The curves correspond to P_{WD} (dashed line) and to P_P (dotted line).

$\vec{h} = (7.875, 0, 2)$ at which the distribution $P(s)$ shows a combination of (weak) level repulsion and an exponential tail. We have consistently observed signatures for the onset of quantum chaos also in other spectral correlations as well as in the structure of eigenfunctions. Let us now turn to study energy transport in this model system. To this end we need to couple both ends of the chain of spins to thermal reservoirs at temperature T . 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 used in classical simulations [10] and we thus call it a *quantum stochastic reservoir*. We use units in which Planck and Boltzmann constants are set to unity $\hbar = k_B = 1$.

In the representation basis of σ_n^z the wave function at time t can be written as

$$|\psi(t)\rangle = \sum_{s_0, s_1, \dots, s_{L-1}} C_{s_0, s_1, \dots, s_{L-1}}(t) |s_0, s_1 \dots s_{L-1}\rangle, \quad (2)$$

where $s_n = 0, 1$ represents the *up*, *down* state of the n -th spin, respectively. The wave function at time t is obtained from the unitary evolution operator $U(t) = \exp[-i\mathcal{H}t]$. The interaction with the reservoir is not included in the unitary evolution. Instead, we assume that the spin chain and the reservoir interact only at discrete times with period τ at which the states of the leftmost (s_0) and the rightmost (s_{L-1}) spins are stochastically reset. Thus, the evolution of the wave function from time t to time $t + \tau$ can be represented as

$$|\psi(t + \tau)\rangle = \Xi(\beta_l, \beta_r) U(\tau) |\psi(t)\rangle, \quad (3)$$

where $\Xi(\beta_l, \beta_r)$ represents the unitary stochastic action of the interaction with the left and right reservoirs at temperatures β_l^{-1} and β_r^{-1} respectively.

The action of $\Xi(\beta_l, \beta_r)$ takes place in several steps:

- i) The wave function is first rotated by the angle $\alpha = \tan^{-1}(h_x/h_z)$ to the eigenbasis of the components $\sigma_l = \vec{h} \cdot \vec{\sigma}_0/h$, $\sigma_r = \vec{h} \cdot \vec{\sigma}_{L-1}/h$ of the edge spins along the field, that is $|\psi\rangle \rightarrow e^{-i\alpha(\sigma_0^y + \sigma_{L-1}^y)/2} |\psi\rangle$. Here, $h = |\vec{h}|$ stands for the strength of the magnetic field.
- ii) A local measurement of the observables σ_l , σ_r is performed. Then the state of the spins at the borders collapses to a state (s_0^*, s_{L-1}^*) with probability

$$p(s_0^*, s_{L-1}^*) = \sum_{s_1, \dots, s_{L-2}} |C_{s_0^*, s_1, \dots, s_{L-2}, s_{L-1}^*}|^2. \quad (4)$$

In other words, this means that we put all coefficients $C_{s_0, s_1, \dots, s_{L-1}}$ with $(s_0, s_{L-1}) \neq (s_0^*, s_{L-1}^*)$ to zero.

iii) The new state of the edge spins is stochastically chosen. After this, which simulates the thermal interaction with the reservoirs, each of the edge spins is set to *down*, (*up*) state with probability $\mu, (1 - \mu)$. The probability $\mu(\beta)$ depends on the canonical temperature of each of the thermal reservoirs:

$$\mu(\beta_j) = \frac{e^{\beta_j h}}{e^{-\beta_j h} + e^{\beta_j h}}, \quad j \in \{l, r\}. \quad (5)$$

iv) Finally, the wave function is rotated back to the σ_n^z basis, $|\psi\rangle \rightarrow e^{i\alpha(\sigma_0^y + \sigma_{L-1}^y)/2}|\psi\rangle$.

This completes the description of the interaction with the quantum stochastic bath. This interaction thus (periodically) resets the value of the local energy $h\sigma_{l,r}$ of the spins in contact with the reservoirs. This information is then transmitted to the rest of the system during its dynamical evolution and relaxation towards equilibrium. Therefore, the value of τ controls the strength of the coupling to the bath. We have found that, in our units, $\tau = 1$ provides an optimal choice. We have nevertheless performed simulations for other values of τ with qualitatively similar results. In particular, for weak couplings ($\tau \gtrsim 1$) the heat conductivity does not depend on the coupling strength. Note that our method does not correspond to a stochastic unraveling of a master equation (ME) for the density operator (*e.g.*, in the Lindblad form) [11]. Here the evolution of the system between two consecutive interactions with the baths is purely unitary and not diffusive as in the ME. However, we have tested that, using our prescription, 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.

The unitary evolution $U(t)|\psi\rangle$ of the system has been computed by an accurate high-order split-step factorization of the unitary evolution operator [12]. For each run the initial wave function $|\psi(0)\rangle$ of the system is chosen at random. The system is then evolved for some relaxation time τ_{rel} after which it is assumed to fluctuate around a unique steady state. Measurements are then performed as time averages of the expectation value of suitable observables. We further average these quantities over different random realizations of “quantum trajectories”. In order to compute the energy profile we write Hamiltonian (1) in terms of local energy density operators H_n :

$$H_n = -Q\sigma_n^z\sigma_{n+1}^z + \frac{\hbar}{2} \cdot (\vec{\sigma}_n + \vec{\sigma}_{n+1}) . \quad (6)$$

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. (6) the Hamiltonian of the system can be rewritten as

$$\mathcal{H} = \sum_{n=0}^{L-2} H_n + \frac{\hbar}{2}(\sigma_1 + \sigma_r) . \quad (7)$$

First, we have performed equilibrium simulations in order to show that time-averaged expectation values of the local energy density can be used as a consistent canonical local temperature. To this end we set the left and right reservoirs to the same temperature T . In fig. 2 we plot the mean local energy $E = \langle H_n \rangle$ where the average is taken over time and over the $L - 5$ central values of the profile, for the chaotic and for the integrable chain (inset). For low T , E saturates to a constant which, together with the energy profile $\langle H_n \rangle$, is determined by the ground state. However, for larger $T > 1$, the energy profile is constant within numerical accuracy, and numerical simulations give $E \sim -1/T$, all results being almost independent of L for $L \geq 6$. The numerical data for $E(T)$ can be well approximated with a simple calculation of energy density for a two-spin chain ($L = 2$) in a canonical state at temperature T (smooth

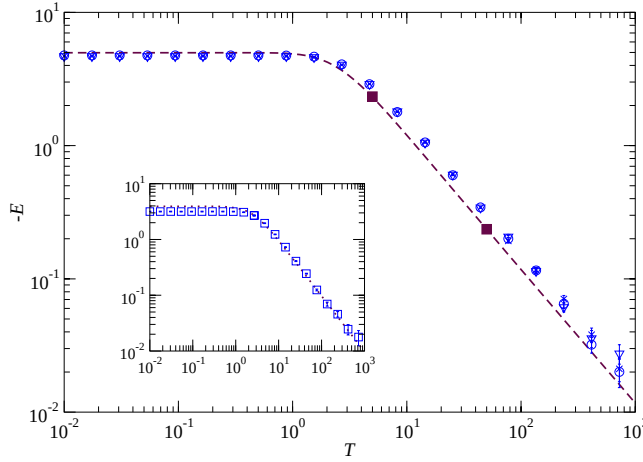


Fig. 2 – Mean local energy E as a function of the temperature T for the chaotic chain, for $L = 6$ (crosses), 8 (triangles) and 10 (circles). Each point corresponds to the equilibrium simulation ($T_l = T_r = T$). E was obtained as the average of the $L - 4$ central sites. The dashed line corresponds to the canonical average $E_{\text{can}}(T)$ of the local 2-body energy operator H_n . The two solid squares indicate the values of the temperature that were later used in the out-of-equilibrium simulations. In the inset the same data are shown for the integrable chain (squares) for $L = 8$.

curves), namely $E_{\text{can}}(T) = \text{tr} H_0 e^{-H_0/T} / \text{tr} e^{-H_0/T}$. Therefore, if the temperatures of both reservoirs are in high- T regime, then we can define the local temperature via the relation $T \propto -1/E$. We stress that equilibrium numerical data shown are insensitive to the nature of dynamics (consistent with results of ref. [13]), whether being chaotic, regular or intermediate.

In fig. 3 we show the energy profile $\langle H_n \rangle$ for an out-of-equilibrium simulation of the chaotic chain. In all non-equilibrium simulations, the temperatures of the baths were set to $T_l = 5$ and

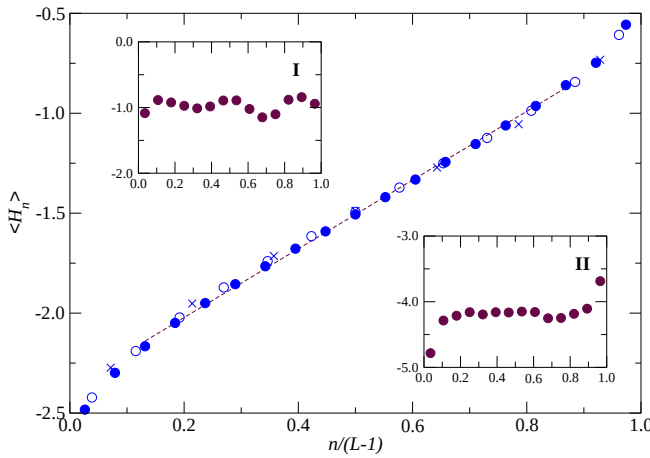


Fig. 3 – Out-of-equilibrium energy profile $\langle H_n \rangle$ for the chaotic chain. The temperatures of the baths $T_l = 5$ and $T_r = 50$, are both in the high-temperature regime (see the solid squares in fig. 2). Results for chains of size $L = 8$ (crosses), $L = 14$ (open circles) and $L = 20$ (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 $L = 15$.

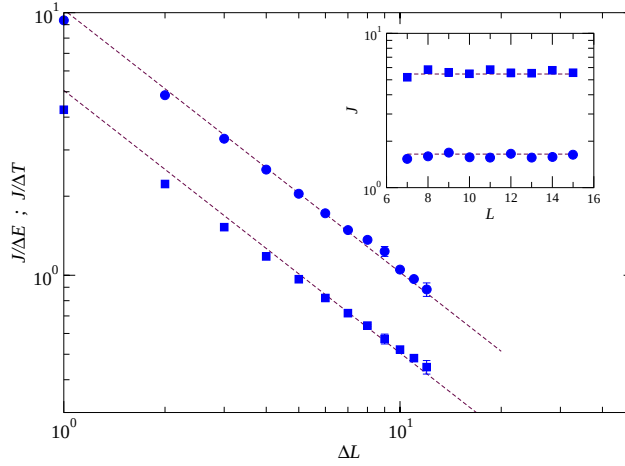


Fig. 4 – Size dependence of the energy current in the chaotic chain with $T_l = 5$ and $T_r = 50$. We show $J/\Delta E$ (circles) and $J/\Delta T$ (squares). The dashed lines corresponds to $1/\Delta L$ scaling. In the inset, the size dependence of the energy current is shown for the integrable (circles) and the intermediate (squares) chains.

$T_r = 50$. 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: $\partial_t H_n = i[\mathcal{H}, H_n] = -(J_{n+1} - J_n)$, requiring that $J_n = [H_n, H_{n-1}]$. Using eqs. (6) and (7) the local current operators are explicitly given by

$$J_n = h_x Q (\sigma_{n-1}^z - \sigma_{n+1}^z) \sigma_n^y, \quad 1 \leq n \leq L-2. \quad (8)$$

In fig. 4 we plot $J/\Delta E$ 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 $L-8$ central values of n .

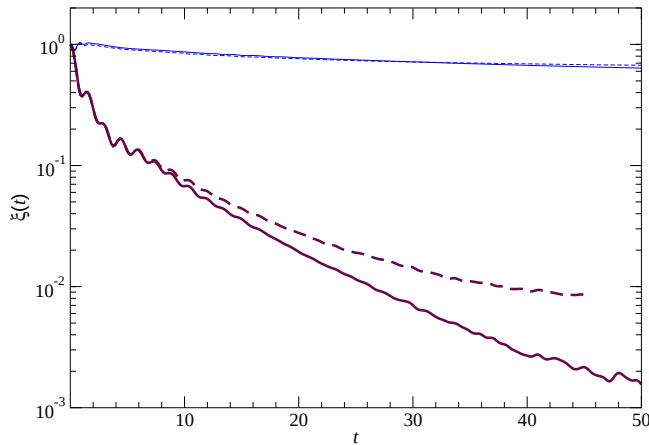


Fig. 5 – Infinite temperature current-current time correlation function $\xi(t)$, for two chaotic chains of size $L = 18$ (tick dashed line) and $L = 24$ (thick solid line) and for two integrable chains of size $L = 18$ (dashed line) and $L = 24$ (solid line).

The energy difference was obtained from the energy profile as $\Delta E = \langle H_{L-5} \rangle - \langle H_3 \rangle$. Three spins near each bath have been discarded in order to be in the bulk regime. 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. Moreover, also the quantity $J/\Delta T$, where $\Delta T = -1/\langle H_{L-5} \rangle + 1/\langle H_3 \rangle$, shows the correct scaling with the size L . 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.

As a consistency check, we have also studied the energy current-current time correlation $\xi(t) = \langle J(t)J \rangle$ of the isolated system for $\beta \rightarrow 0$ which, for high temperature, gives the conductivity as $\kappa = \beta L \int_0^\infty \xi(t) dt$. In fig. 5 we show that for the chaotic chain $\xi(t)$ exhibits fast, possibly exponential decay while for the intermediate case we observe slow decay, possibly to a finite plateau, giving rise to ballistic transport. In the integrable case $\xi(t)$ is constant since $J(t)$ is a conserved quantity.

In this paper we have shown that Fourier law of heat conduction can be derived from the pure quantum-dynamical evolution without any additional statistical assumption. This possibility is strictly related to the onset of quantum chaotic behavior.

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