Heat Transport in Quantum Spin Chains

Stochastic Baths vs Quantum Trajectories

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Abstract. We discuss the problem of heat conduction in quantum spin chain models. To investigate this problem it is necessary to consider the finite open system connected to heat baths. We describe two different procedures to couple the system with the reservoirs: a model of stochastic heat baths and the quantum trajectories solution of the quantum master equation. The stochastic heat bath procedure operates on the pure wave function of the isolated system, so that it is locally and periodically collapsed to a quantum state consistent with a boundary nonequilibrium state. In contrast, the quantum trajectories procedure evaluates ensemble averages in terms of the reduced density matrix operator of the system. We apply these procedures to different models of quantum spin chains and numerically show their applicability to study the heat flow.

1 Introduction

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\cite{1}. This problem, in spite of having a long history, is not completely settled: 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 $J = -\kappa \nabla T$, relating the macroscopic heat flux to the temperature gradient $\nabla T$\cite{2}.

At the classical level a great amount of work has focused on the relation between the chaotic character of the microscopic dynamics and the normal macroscopic transport\cite{3–18}, (see also Ref.\cite{19} for a recent review ). The general picture that emerges from these investigations is that deterministic chaos appears to be an essential ingredient required by transport theory. However, strictly speaking, the exponential instability that characterizes the chaotic dynamics is neither sufficient\cite{7} nor necessary\cite{10,16} for the validity of Fourier law. What has been shown in Ref.\cite{16} is that the diffusive behavior, which is at the root of normal heat transport, can be obtained even if the Lyapunov exponents are zero. This constitutes a strong suggestion that normal heat conduction can take place even without the strong requirement of exponential instability.

At the quantum level, the question whether normal transport may arise from the underlying quantum dynamics is a controversial issue\cite{20–26}. This is mostly because it is not clear how to describe the transport of energy or heat from a microscopic point of view. In analogy to classical systems, a quantum derivation of the Fourier’s law calls directly in question the issue

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of quantum chaos \cite{37}. However, a main feature of quantum motion is the lack of exponential dynamical instability \cite{27}. This fact may render very questionable the possibility to derive the Fourier law of heat conduction in quantum mechanics. Thus it is interesting to inquire if, and under what conditions, Fourier law emerges from the laws of quantum mechanics (for a recent review of the microscopic foundations of the quantum Fourier’s law see \cite{28}).

To investigate the problem of quantum heat transport one has to deal with a finite open system connected to heat baths. This fact renders the problem to obtain a derivation of the quantum Fourier’s law extraordinary difficult. In this paper we present two complementary methods to study the problem of heat conduction in quantum spin chain models. We consider one-dimensional quantum spin chain models like the one schematically shown in Fig. 1. Each spin in the chain interacts with its neighbours and possibly with an external field. The range and type of interaction does not limit the applicability of our methods. Furthermore, the spin chain is in contact with two heat reservoirs. The Hamiltonian of the system can be written as

\[
H = H_{\text{system}} + H_{\text{reservoirs}}(T_L, T_R) + H_{\text{int}},
\]

where \(H_{\text{int}}\) represents the coupling between the system and the heat reservoirs.

In recent years the transport of heat in quantum spin chains has been the subject of intense experimental \cite{31} and theoretical investigations \cite{20–26, 32–36}. In analogy to classical systems it has been found that non integrable quantum spin chains show normal heat transport, while integrable chains lead to ballistic transport and thus, to divergent heat conductivity. In particular, in Ref. \cite{25} the validity of the quantum Fourier’s law has been linked to the onset of quantum chaos, in the statistical sense of Random Matrix Theory. Moreover, in Ref. \cite{25} an intermediate case for which the spin chain is neither integrable nor chaotic was shown to have divergent heat conductivity. Up to our knowledge, this is the only example for which a quantum spin chain with intermediate statistics leads to an abnormal heat transport (see also \cite{26} where almost integrable models have been studied). In spite of the general evidence, in Ref. \cite{22} the Fourier’s law was numerically confirmed for a class of integrable, albeit small, quantum spin chains.

In these investigations, particularly those that are numerical, the thermodynamical limit at which the heat conductivity is formally defined is difficult, if not impossible to address. This limitation is emphasized when one deals with non integrable systems for which a theoretical perturbative analysis is not possible. So far the most popular theoretical framework to study heat transport is the Green-Kubo formula \cite{29}, derived on the basis of linear response theory. However, the use of GK formula for heat transport requires \textit{ad-hoc} statistical assumptions that lack of a microscopic justification of its applicability (see \textit{e.g.}, \cite{28} and also \cite{30} for a plausible derivation of a Green-Kubo formula for heat transport). A second standard treatment is based on the Quantum Master Equation (QME). However, this method involves the calculation of the reduced density matrix of the system, thus limiting numerical investigations to relatively small system sizes.

Given this state of affairs, the development of numerical methods that can deal with both integrable and non integrable spin models and that are amenable to study large system sizes is very desirable. In the present paper we present two methods recently introduced to study the transport of heat in quantum systems. In section 2, we discuss a model of stochastic quantum heat baths where \(H_{\text{int}}\) consists of a stochastic time-periodic local perturbation \cite{25}. This perturbative term acts on the, otherwise, pure state of the system. We show that this procedure leads to a well defined local temperature and discuss the validity of Fourier’s law in a Quantum spin-1/2 Ising chain in a tilted external magnetic field. This method allows to study finite but
large spin chains as its implementation only requires the knowledge of the pure vector state of
the system. In Section 3 we present a QME in Lindblad form that can appropriately describe
nonequilibrium steady states [36]. Furthermore, we use the Monte Carlo wave function formal-
ism to study the heat transport in the spin-1/2 Heisenberg chain. In Section 4 a discussion of
the results and applicability of our integration methods is presented, followed in Section 5 by
our final remarks.

2 Stochastic Quantum Heat Baths

In this Section we describe the implementation of a stochastic model of quantum heat baths.
We consider a one-dimensional quantum spin-1/2 chain of length N. The Hamiltonian of
the system can be written in general as in Eq. (1) Each spin in the chain is coupled to its
neighbours and possibly to an external field. Furthermore, let us consider that the leftmost
(s₀) and rightmost (s₁₋₁) spins are coupled via the Hᵢₙₜ term, with external ideal heat baths
at temperatures T_L and T_R respectively. A schematic representation of this general model is
shown in Fig. (1). The aim of this procedure is to focus on the evolution of the state of the spin chain,
avoiding to introduce any particular model for the heat reservoirs. Therefore, we only assume that the
heat baths act locally on the state of the respective spin so that the state of s₀ and of s₁₋₁ are
thermal states at the respective temperatures. This model for the reservoirs is analogous to the
thermal states at the respective temperatures. This model for the reservoirs is analogous to the
stochastic thermal reservoirs used in classical simulations [15] and we thus call it a
stochastic quantum heat baths.

To be precise, we work in the representation basis of σ^z. Furthermore, we use units in which
Planck and Boltzmann constants are set to unity $\hbar = k_b = 1$ In this the wave function at time $t$
can be written as

$$|\psi(t)\rangle = \sum_{s_0, s_1, \ldots, s_{N-1}} C_{s_0, s_1, \ldots, s_{N-1}}(t) |s_0, s_1, \ldots, s_{N-1}\rangle,$$

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 $\tau$ at which the states of the
spins $s_0$ and $s_{N-1}$ are stochastically reset. The evolution of the wave function from time $t$ to
time $t + \tau$ can be represented as

$$|\psi(t + \tau)\rangle = \Xi(T_L, T_R) U(\tau) |\psi(t)\rangle,$$

where $\Xi(T_L, T_R)$ represents the unitary stochastic action of the interaction with the left and
right reservoirs at temperatures $T_L$ and $T_R$ respectively.

The action of $\Xi(T_L, T_R)$ takes place in two steps:

(i) A local measurement of the state of the spins coupled to the heat baths is performed. Then
then state collapses to a state $(s_0^*, s_{N-1}^*)$ with probability

$$p(s_0^*, s_{N-1}^*) = \sum_{s_1, \ldots, s_{N-2}} |C_{s_0^*, s_1, \ldots, s_{N-2}, s_{N-1}^*}|^2.$$

Numerically this means that we put all coefficients $C_{s_0, s_1, \ldots, s_{N-1}}$ with $(s_0, s_{N-1}) \neq (s_0^*, s_{N-1}^*)$
to zero. Afterwards, the wave function is renormalized.

(ii) The new state of the edge spins is stochastically chosen: $s_0$ and $s_{N-1}$ are 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:

$$\mu(\beta) = \frac{e^{-\beta E_{down}}}{e^{-\beta E_{down}} + e^{-\beta E_{up}}},$$

where $E_{down}$ and $E_{up}$ are the energy levels of the down and up states, respectively.
where $\beta = 1/T$ is the inverse temperature. This simulates the thermal interaction with the reservoirs.

This interaction thus (periodically) resets the value of the local energy 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 $\tau$ controls the strength of the coupling to the bath. We have found that, in our units, $\tau = 1$ provides an optimal choice. On one hand, large values of $\tau$ correspond to a “microcanonical” situation: if $\tau$ is much larger than the relaxation time of the system then the spin chain behave as an isolated system, leading to an equidistributed mean energy. On the other hand, a strong coupling with the reservoirs, i.e., $\tau \ll 1$, the state of the system freezes due to the quasi-continuous monitoring, a situation similar to the Zeno effect. We have checked that intermediate values of $\tau$ lead to qualitatively similar results.

Also, note that our method does not correspond to a stochastic unraveling of a QME. Here the evolution of the system between two consecutive interactions with the baths is purely unitary and not dissipative as for the QME in Section 3.

The use of stochastic quantum heat baths has the advantage that it only requires the calculation of the vector state of the system [4]. This allows to compute time averages for spin chains longer than the sizes that can be studied with other methods.

Finally, we remark that the stochastic quantum heat baths method does not depend on the range and type of the interaction.

### 2.1 Fourier’s law in the Ising chain in a tilted magnetic field

In this Section we discuss the heat transport in an Ising chain of $N$ spins 1/2 with coupling constant $Q$ subject to a uniform magnetic field $\mathbf{h} = (h_x, 0, h_z)$, with open boundaries. The Hamiltonian reads

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

(6)

where $H_n$ are local energy density operators

$$H_n = -Q\sigma_n^x \sigma_{n+1}^x + \frac{\hbar}{2}(\sigma_n + \sigma_{n+1}) ,$$

(7)

and $\sigma_1 = \mathbf{h} \cdot \sigma_0 / h$, $\sigma_l = \mathbf{h} \cdot \sigma_{N-l} / h$ are the spin operators along the direction of the magnetic field of $s_0$ and $s_{N-1}$ respectively. The operators $\sigma_0 = (\sigma_0^x, \sigma_0^y, \sigma_0^z)$ are the Pauli matrices for the $n$-th spin, $n = 0, 1, \ldots, N - 1$. The direction of the magnetic field affects the qualitative behavior of the system: it is integrable for $h_z = 0$ and not integrable otherwise. When $h_z$ is of the same order of $h_x$ quantum chaos sets in [25]. Using the stochastic quantum heat bath formalism, in Ref. [25] it was shown that the validity of the Fourier’s law is related to the onset of quantum chaos. In what follows, we consider a chaotic chain (with parameters $Q = 2$, $h_x = 3.375$, $h_y = 0$ and $h_z = 2$) and discuss the establishment of local thermal equilibrium in terms of the density matrix operator. Furthermore, we also recall some of the results presented in Ref. [25] concerning the validity of the Fourier’s law.

In order to apply the stochastic formalism to this model one needs first to rotate the state of the edge spins to the direction of the external field $\mathbf{h}$, so that the local measurement described above (i) is meaningful. This is done by rotating the wave function by the angle $\alpha = \tan^{-1}(h_x/h_z)$ to the eigenbasis of the components $\sigma_1$ and $\sigma_z$, that is $|\psi\rangle \rightarrow e^{-i\alpha(\sigma_0^y + \sigma_{N-1}^y)/2}|\psi\rangle$. After the stochastic reset of the edge spins the wave function is rotated back to the $\sigma^z$ basis, $|\psi\rangle \rightarrow e^{i\alpha(\sigma_0^y + \sigma_{N-1}^y)/2}|\psi\rangle$.

To integrate the unitary evolution $U(t)|\psi\rangle$ of the system we have used an accurate high order split-step factorization of the unitary evolution operator described in Ref. [38]. We then consider different random quantum trajectories of the randomly chosen initial wave function $|\psi(0)\rangle$ of the system. The state is then evolved for some relaxation time $\tau_{rel}$ 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 the ensemble of “quantum trajectories”.

In order to test the effectiveness of the coupling between the stochastic quantum baths and the system, we have computed the time averaged density matrix of the system

$$\bar{\rho} = \lim_{t \to \infty} \int_0^t |\psi(s)\rangle \langle \psi(s)| ds ,$$  

Eq. (8)

where $\psi(s)$ is the state of the system at time $s$. Quantum statistical mechanics postulates that if a system, described by a Hamiltonian $H$, is in a thermal equilibrium state at temperature $\beta^{-1}$ then in the energy basis ($H|\phi_n\rangle = E_n|\phi_n\rangle$), the density matrix operator is

$$\langle \phi_n|\rho|\phi_m\rangle = \frac{e^{-\beta E_n}}{Z} \delta_{m,n} ,$$  

Eq. (9)

where $Z = \sum_n e^{-\beta E_n}$ is the canonical partition function.

We have performed equilibrium simulations, i.e., $T_L = T_R = T$ and computed the time averaged density matrix. We have found that $\bar{\rho}$ is diagonal in within numerical accuracy. Moreover, $\rho_n \equiv \langle \phi_n|\rho|\phi_n\rangle$ is an exponential function of $E_n$ inside each symmetry band. This verifies Eq. (9) and thus, that the system reach a canonical equilibrium. Furthermore, from a best fit to a exponential of $\rho_n(E_n)$ one can extract a value for the effective temperature at the bulk of the system. In Fig. 2 we show the obtained effective bulk temperature $\beta^{-1}$ as a function of the nominal value of the bath’s temperature $T$. At low temperatures the effective temperature at the bulk saturates to a constant which, together with the energy profile $E_n$, is in principle determined by the ground state. However, we have found that the saturation value does not correspond to neither the ground state of the two-body energy density operator $H_n$ nor to the ground state of the many-body operator $\mathcal{H}$. At high temperatures ($T > 5$), the spin chain thermalizes to exactly the same temperature as that set by the stochastic heat baths. This strongly supports the effectiveness of our bath model. Moreover, this also suggests the validity
of the ergodic property, namely the averages over the canonical ensemble are equivalent to time averages.

Out of equilibrium, we have verified that at high temperatures, the local temperature obtained from time average of the reduced density matrix of subsets of few spins centered around the $n$-th spin coincide with time averages of the expectation value of the energy density operator $E_n = \langle H_n \rangle$. However, we have observed that out of equilibrium the local temperature of the edge spins may not coincide with the nominal value of the temperature of the corresponding bath. This energy jumps are commonly observed in quantum and classical systems. They can be understood as the result of an thermal resistance of the particular contact model.

Following Ref. [25], one can define a local energy current operator for the spin model of Eq. (6) as

$$J_n = h_x Q \left( \sigma^z_{n-1} - \sigma^z_{n+1} \right) \sigma^y_n, \quad 1 \leq n \leq N - 2,$$

that is consistent with the conservation of energy at the bulk. In Fig. 3 we show the heat conductivity $\kappa = J / \nabla T$ as a function of the size $N$ of the chaotic chain for sizes up to $N = 20$. The mean current $J$ was calculated as an average of $\langle J_n \rangle$ over time and over the $N - 8$ central spins. Three spins near each bath have been discarded in order to be in the bulk regime. For the particular choice of the energy density operator (7), its averaged expectation value is related to the local temperature as $\langle H_n \rangle \propto -1/T$ [25]. The temperature difference was thus obtained as $\Delta T = -1/\langle H_{N-5} \rangle + 1/\langle H_3 \rangle$. For large $N$ the heat conductivity of the chaotic chain converges to a constant value, thus confirming the validity of the Fourier's law. In [25] it was also shown that for the integrable and an intermediate chains the Fourier's law does not hold as $\kappa$ diverges. The results of Ref. [25] supports the relation between a normal transport and the onset of quantum chaos.

**Fig. 3.** Size dependence of the energy current for the chaotic chain with $T_L = 5$ and $T_R = 50$. The dashed line corresponds to a $1/N$ scaling. In the inset, energy profile computed from the time average of the expectation value of the energy density operator $E_n = \langle H_n \rangle$. 
3 Quantum Master Equation for Nonequilibrium States

In this Section we present an alternative way of modeling a nonequilibrium transport scenario. We consider a spin-$\frac{1}{2}$ chain of length $N$ with homogeneous and isotropic nearest-neighbor Heisenberg interaction $V$ and a contribution $H_{\text{ext}}$ due to the interaction with an external uniform magnetic field in $z$-direction. The Hamiltonian of the spin chain reads

$$H = H_{\text{ext}} + V,$$

$$H_{\text{ext}} = \sum_{n=0}^{N-1} H_n = \sum_{n=0}^{N-1} \frac{\Omega}{2} \sigma_n^z,$$

$$V = \sum_{n=0}^{N-2} V_{n,n+1} = \lambda \sum_{n=0}^{N-2} \sigma_n \cdot \sigma_{n+1}.$$

The energy contribution due to the external field of strength $\Omega$ is assumed to be an approximately conserved quantity. This is well justified if $\Omega$ is large compared to the coupling strength $\lambda$. By making use of a discretized version of the continuity equation, the following form of the energy current operator is found

$$J_{n,n+1} = i [V_{n,n+1}, H_n].$$

The central ideas of the following considerations stem from the theory of open quantum system, commonly used to study the properties of systems in thermal equilibrium, or to account for environmental effects in otherwise perfectly coherent quantum dynamics. Our aim is to describe the nonequilibrium steady state, that arises when the chain of spins is in contact with two thermal baths at different temperatures, leading to a steady energy current that will flow from the hotter towards the colder heat bath through the chain of spins.

Our method is based on a Markovian quantum master equation for the reduced density operator $\rho_S$ of the spin chain, which is designed to model energy transport under a thermal gradient. In addition to the usual assumption of weak system-bath interactions, and to neglect all memory effects (Born/Markov approximation), we require the internal interactions between spins to be weak. By further assuming not too low temperatures of the baths the following QME is well justified (see [36], and references therein):

$$\frac{d}{dt} \rho_S(t) = -i[H, \rho_S(t)] + D_L(\rho_S(t)) + D_R(\rho_S(t))$$

$$D_L(\rho_S(t)) = \sum_{k,l=1}^{2} (\gamma_L)_{kl} \left( F_k \rho_S F_l^\dagger - \frac{1}{2} [F_l^\dagger F_k, \rho_S] \right)$$

$$F_1 \equiv \sigma_0^+, \quad F_2 \equiv \sigma_0^- .$$

The dissipator of the right heat bath $D_R$ is defined correspondingly. The coefficient matrices $\gamma_{L/R}$ read

$$\gamma_{L/R} \equiv \pi \lambda_B I(\Omega) \left( \frac{N(\Omega)}{\sqrt{N(\Omega)^2 + N(\Omega)}} \sqrt{\frac{N(\Omega)^2 + N(\Omega)}{N(\Omega) + 1}} \right), \quad N(\Omega) = \frac{1}{e^{\beta_{L/R}} - 1} ,$$

where $\beta_{L/R}$ refers to the reciprocal temperature of left/right bath respectively, $\lambda_B$ controls the system-bath coupling strength and $I(\Omega)$ denotes the spectral density of the bath, that we choose Ohmic. A remarkable property of Equation (15) is that it can be brought into Lindblad form [40, 41]

$$\frac{d}{dt} \rho_S(t) = -i[H, \rho_S(t)] + \sum_k \alpha_k \left( L_k \rho_S L_k^\dagger - \frac{1}{2} [L_k^\dagger L_k, \rho_S] \right)$$

by diagonalizing the coefficient matrices $\gamma_{L/R}$. Therefore Equation (15) can be treated with the Monte Carlo wave function technique that will be briefly described in the following Section.
3.1 Monte Carlo wave function method

As the solution of QME’s is rarely available analytically one is most likely confronted with the numerical time propagation of the reduced density operator. Standard methods for the numerical solution of linear differential equations like Runge Kutta solvers can readily be applied for small systems, but fail if the dimension of the Hilbert space $d$ becomes large in view of computer memory limitations.

Since the early 1990’s the Monte Carlo Wave Function (MCWF) technique (also known as the quantum jump approach), has become increasingly popular. Introduced in the context of quantum optics [44, 45] the MCWF technique has also been used in quantum state diffusion unraveling of the QME [46] and in the study of the stability of quantum algorithms [47, 48]. The basic idea is to depart from a statistical treatment by means of density operators and turn to a description in terms of stochastic wave functions. One might be tempted to think of single systems being continuously monitored, but this analogy is sometimes criticized. Nevertheless, the MCWF technique has proved to be a powerful method for the numerical solution of Lindblad-type QME’s.

The Lindblad QME (19) can equivalently be formulated in terms of a stochastic Schrödinger equation (SSE)

$$|d\psi\rangle = \left( H_{\text{eff}} + \frac{p}{2} \right) |\psi\rangle \, dt + \sum_k \left( \frac{J_k}{\sqrt{p_k}} - 1 \right) |\psi\rangle \, dn_k, \quad (20)$$

describing a piecewise deterministic process in Hilbert space [39], a solution of which is is called a realization. The first term in Eq. (20) corresponds to a deterministic time-evolution due to an effective non-Hermitian Hamiltonian given by

$$H_{\text{eff}} \equiv -iH - \frac{\alpha}{2} \sum_{k=1} L_k^\dagger L_k. \quad (21)$$

whereas the second term in Eq. (20) refers to jump-like, stochastic evolution induced by the jump operators

$$J_k \equiv \sqrt{\alpha_k} L_k. \quad (22)$$

The Poisson increments $dn_k \in \{0,1\}$ obey the following statistical properties

$$\mathbb{E}(dn_k) = p_k \, dt, \quad (23)$$

$$dn_k \, dn_l = \delta_{kl} \, dn_k. \quad (24)$$

$\mathbb{E}(\cdot)$ stands for the expectation value, whereas $p_k$ denotes a jump rate given by

$$p_k = \| J_k |\psi\| \|^2, \quad (25)$$

and is therefore time-dependent. $\rho = \sum_k p_k$ refers to the total jump rate. The SSE (20) is an equivalent formulation of the Lindblad QME (19) insofar as

$$\mathbb{E}(\langle \psi(t) | \psi(t) \rangle) = \rho_S(t), \quad (26)$$

given that $\mathbb{E}(\langle \psi(t_0) | \psi(t_0) \rangle) = \rho_S(t_0)$. Thus the expectation value of an observable $A$ at time $t$ can be estimated through

$$\langle A \rangle(t) = \text{Tr}\{A \rho_S(t)\} \simeq \frac{1}{m} \sum_{k=1}^m \langle \psi_k(t) | A | \psi_k(t) \rangle \quad (27)$$
in a finite ensemble of $m$ realizations of (20) to arbitrary precision. This is of huge practical importance, as one deals with wave functions with $O(d)$ elements instead of density operators.

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having $O(d^2)$ elements, where $d$ is the dimension of the Hilbert space under consideration. Furthermore, if one is interested in the stationary state, ensemble averages can be replaced by time averages and one single realization suffices to determine stationary expectation values [42, 43]

$$\langle A \rangle_{\text{stat}} = \text{Tr} \{ A \rho_{\text{stat}} \} \approx \frac{1}{(T+1)} \sum_{k=0}^{T} \langle \psi(t_k) | A | \psi(t_k) \rangle , \quad t_k \equiv t_0 + k \Delta t .$$

The MCWF approximation to the exact solution depends on the number of quantum trajectories that are considered, as well as the integration time of each trajectory. We have found that one single trajectory, integrated during a sufficiently long time, results in a very good approximation. Nevertheless, following [43], we consider $i = 1 \ldots m$ different realizations, so that, an estimate of $\text{Tr} \{ A \rho_{\text{stat}} \}$ can be obtained as the sample mean of the $\langle A \rangle_{\text{stat}}$'s. Moreover, considering several quantum trajectories enables us to get a measure for the statistical error $\delta \langle A \rangle_{\text{stat}} / \sqrt{m}$, where $\delta \langle A \rangle_{\text{stat}}$ is the standard deviation of the $\langle A \rangle_{\text{stat}}$'s. The results presented below were obtained from $m = 4$ different realizations, integrated for long times of the order of $10^5$ to $10^7$.

We now describe the procedure to obtain a realization of the SSE (20). Starting from an initial state $\langle \psi(t_0) \rangle$ we proceed as follows:

1. Draw a uniformly distributed random number $r \in [0,1]$.
2. Perform the deterministic time evolution $| \tilde{\psi}(t) \rangle = e^{(t-t_0)H_{\text{eff}}} | \psi(t_0) \rangle$ until $t = t_j$, which is determined by $\| \tilde{\psi}(t_j) \|^2 = r$, for some $r < 1$.
3. Normalize the wave function $| \psi \rangle \rightarrow | \tilde{\psi} \rangle / \| \tilde{\psi} \|$.
4. Choose randomly a particular jump $k$ with respective weight $p_k$.
5. Carry out the map $| \psi \rangle \rightarrow J_k | \psi \rangle / \sqrt{p_k}$.
6. Set $t_0 \rightarrow t$ and return to step 1.

This procedure terminates when $t = t_{\text{fin}}$, where $t_{\text{fin}}$ is the desired final time.

The jumps occur at random instants of time $t_j$, which are determined through $\| \tilde{\psi}(t_j) \|^2 = r$, by virtue of the second step of the simulation procedure. Assuming a uniform time discretization $\Delta t$ in a simulation, jumps happen only at multiples of $\Delta t$, which causes an error of order $O(\Delta t)$. Therefore $\Delta t$ has to be chosen with care. For a more detailed account on the MCWF method, the reader is referred to [39].

### 3.2 Fourier’s Law in the Heisenberg chain

We consider the Heisenberg chain of spin-$\frac{1}{2}$ with Zeeman contribution, described by the Hamiltonian \( \text{H}_{\text{eff}} \), as an example of an integrable chain. As we have mentioned, integrability is commonly associated with diverging transport coefficients and hence ballistic transport behavior. However, in Ref. [22], normal transport was observed for an integrable, albeit small, spin chain. In Fig. 4 we show the energy profile along the Heisenberg chain in the stationary state. A clean finite temperature gradient is observed.

We explicitly compute transport coefficients here for Heisenberg chains of up to 12 spins, by making use of the MCWF technique, taking time averages over single trajectories. We focus on the scaling behavior of the heat conductivity $\kappa$ with the size of the chain $N$. We define $\kappa$ as the ratio of two measures, namely the stationary energy current within the chain, in terms of the current operator given in Eq. (14) and the stationary difference in the local energy of the innermost pair of spins

$$\kappa \equiv \frac{\langle J_{1,2} \rangle_{\text{stat}}}{\Delta T_{\nu-1,\nu}} ,$$

$$\Delta T_{\nu-1,\nu} \equiv \langle H_{\nu-1} - H_{\nu} \rangle_{\text{stat}}, \quad \nu \equiv \frac{N}{2} - \text{mod}(N,2) .$$

In the upper panel of Fig. 4 it is shown that the stationary current depends linearly on the reciprocal chain length $N^{-1}$. The same result has been observed earlier in Ref. [22] on the
Fig. 4. Energy profile in a Heisenberg chain of $N = 10$ spins. A finite gradient is associated with diffusive transport behaviour. The data points refer to time averages of single stochastic realizations up to a final time $t_{\text{fin}} = 10^5$ in units of $\Omega^{-1}$. System parameters: $(\beta_L = 0.41, \beta_R = 1.39, \lambda = \lambda_B = 0.01, \Omega = 1)$.

basis of a similar QME, but for chain lengths of $N \lesssim 6$. Extrapolation of a linear best fit of the data points in the upper panel of Fig. strongly suggests that, in the limit of infinite $N$ the stationary energy current remains finite. In contrast to the diffusive behaviour observed for small systems, this is expected to wane at the thermodynamic limit $N \to \infty$.

In a real material the heat conductivity $\kappa$ is a bulk property. When transport is normal, $\kappa$ converges towards a constant value with an increasing size of the system, once finite size effects are negligible. However, our results show no sign of a convergence for $\kappa$ in the range of our computational abilities. Linear extrapolation of $\langle J_{1,2} \rangle_{\text{stat}}$ and $\Delta T_{\nu-1,\nu}$ rather predicts a divergence of the so defined heat conductivity with $N$. This agrees with a ballistic transport in the integrable systems.

4 Discussion

In the previous sections we have described two formalisms to study the dynamics of quantum spin chain models in thermal nonequilibrium states. In this section we discuss their limitations and applicability.

Both methods successfully generate a nonequilibrium state in the bulk of spin chain models. In the stochastic baths method the information of the model enters in the precise definition of the local measurement periodically performed on the spins in contact with the baths. For the QME, the particulars of the system are defined in the decay rates of Eq. [18].

However, the two methods have a very different character. The derivation presented in Section obtains a QME of Lindblad type, appropriate to describe a quantum state for which the temperature field is not uniform. The fact that Eq. [15] can be written in Lindblad form makes possible to compute averages of thermodynamical observables using the Monte Carlo wave function formalism, in which each quantum trajectory corresponds to a stochastic unraveling of the QME [15].

The model of Section positively neglects any particular model for the heat baths and defines a procedure by which the system stochastically dissipates at its boundaries. As so, this
Fig. 5. Scaling behavior of heat conductivity. The different panels show the energy current (top), the temperature gradient (middle) and heat conductivity $\kappa$ (bottom) in the stationary state as a function of the reciprocal chain length $N^{-1}$. The results where obtained by the MCWF method. In the upper and middle panels the dashed line corresponds to a linear best fit. In the middle panel only data points with $N \geq 8$ were considered. The error bars in $\kappa$ where obtained from error propagation in linear approximation. System parameters: $\beta_L = 0.25$, $\beta_R = 0.5$, $\lambda = \lambda_B = 0.01$, $\Omega = 1$. Simulation parameters: $\Delta t = 1$, $t_{\text{fin}} = 10^7 (N \geq 9)$, $t_{\text{fin}} = 10^8 (N \leq 8)$.

The formalism does not correspond to a stochastic unraveling of a master equation for the density matrix operator. The evolution of the system between two consecutive interactions with the baths is purely unitary and not continuously dissipative as in the QME. The stochastic method is an approximation of the QME.

The use of the MCWF technique to obtain averaged expectation values makes possible to numerically study larger systems than with other methods. Without this, the solution of Eq. (15) involves the integration in full Liouville space of dimension $2^{2N}$, limiting numerical investigations to small system sizes (typically of $N \leq 6$). The price to pay is that the Lindblad QME (15), is valid only for weakly coupled spins. This limitation is particularly relevant for chaotic systems as typically, chaotic behaviour is exhibited above a critical interaction strength. Despite its limitations, Eq. (15) is, up to our knowledge, the only rigorous QME of Lindblad form that is adapted to study systems in a nonequilibrium state.

The stochastic baths method does not present this limitation. The strength of the spin interaction determines the internal relaxation time of the system. Since the frequency $\tau^{-1}$ at which the system dissipates in the heat baths is a free parameter, one can always find an appropriate value of $\tau$ for which, the stationary nonequilibrium state is established. Moreover, the stochastic baths can be generalized to consider more general situations, like e.g. the coupling with thermo-magnetic baths, for which thermodynamic cross effects can be studied. Nevertheless, the lack of a model for the baths limits a precise interpretation of the physical dissipation.

5 Conclusions

We have presented two complementary methods to study heat transport in quantum spin chains. The first is based on a stochastic procedure by which, the state of the subsystems that are coupled to ideal heat baths is consistent with a global nonequilibrium state. The second is based on a QME in Lindblad form.
The stochastic baths method does only require the integration of the pure wave function of the system. The Lindblad QME \([15]\) can be integrated by means of Monte Carlo wave function techniques. Therefore, the use of any of these methods allows us to study longer spin chains than with other methods. This is particularly relevant to the study of nonequilibrium states as the quantities that determine the transport properties are formally defined in the limit of infinite volume.

We have shown the application of these two methods to study the validity of the quantum Fourier’s law in a chaotic and an integrable quantum spin chain. As generally observed, we have obtained that the Fourier’s law holds for the chaotic chain, while for the integrable chain, the heat conductivity diverges with the size of the chain.

It would be interesting to compare the nonequilibrium state generated by the two methods presented here. An investigation in this direction will appear elsewhere \([49]\).

C.M.-M. acknowledge a Lagrange fellowship from the Institute for Scientific Interchange Foundation.

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