Normal Transport Behavior in Finite One-Dimensional Chaotic Quantum Systems

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Abstract. – We investigate the transport of energy, magnetization, etc. in several finite one-dimensional (1D) quantum systems only by solving the corresponding time-dependent Schrödinger equation. We explicitly renounce on any other transport-analysis technique. Varying model parameters we find a sharp transition from non-normal to normal transport and a transition from integrability to chaos, i.e., from Poissonian to Wigner-like level statistics. These transitions always appear in conjunction with each other. We investigate some rather abstract “design models” and a (locally perturbed) Heisenberg spin chain.

The transport behavior of one-dimensional (1D) systems has intensively been investigated for several decades, as well in the context of classical mechanics as in the context of quantum mechanics [1–16]. Nevertheless, the precise conditions under which normal transport occurs, i.e., under which there is neither ballistic transport nor localization but normal spatial diffusion, are still not known [17].

In the classical domain it seems to be largely accepted that normal transport (in any dimension) requires the chaotic dynamics of a non-integrable system whereas non-normal transport is typical for the regular dynamics of (completely) integrable systems, see [3]. However, there have also been successful attempts to observe normal transport in the absence of exponential instability, the latter being a basic feature of (deterministic) chaos [4]. In the quantum domain there are only very few examples which can be reliably shown to exhibit normal, diffusive transport at all [5–7]. But, also in this field, it has been argued that non-normal transport is related to the macroscopic number of conserved quantities which characterize integrable systems [10–13]. Moreover, recent numerical computations for spin chains have led to the assumption that normal transport might strictly depend on quantum chaos [1, 2].

Although this assumption is plausible, it has not been proved yet [15]. Moreover, almost all computations are either based on special models of reservoirs which might effect the transport

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behavior, or they rely on the Kubo formula. The latter has originally been derived for field-driven electrical conductance and its validity for diffusive transport phenomena such as, e.g., thermal conductance is still under dispute, see [7–9,18]. We refer to [19] where the rather limited validity of the Kubo formula for thermal conductance has explicitly been demonstrated. Especially considerations which are restricted to the analysis of the so-called “Drude-weight” are not sufficient to determine the transport behavior. Thus the main intent of the letter at hand is to examine the relation between transport behavior and quantum chaos without modelling, e.g., external heat baths at different temperatures or using the Kubo formula.

This letter is structured as follows: First of all we briefly comment on the theory of quantum chaos, mainly on the nearest neighbor level spacing distribution (NNLSD). Thereafter we introduce two measures for deviations: i) a measure for the deviation of a given system from the fully chaotic Wigner NNLSD ($\chi_W$), ii) a measure for the deviation of a given system from fully diffusive behavior ($D$). Different finite 1D models are considered and for each model a parameter that drives an “integrable to chaotic transition” is varied. The corresponding Schrödinger equations are solved. This allows to plot both measures ($\chi_W$, $D$) over the respective parameter in order to reveal correlations. This reveals that, at least in our models, the “integrable to chaotic” induces a “non-normal to normal transport” transition.

We investigate some “design models” featuring random interactions and a (locally perturbed) Heisenberg spin chain. We close with a summary and a conclusion.

The theory of quantum chaos is principally concerned with the level statistics of quantum systems which possess a classical limit [20–26]. A commonly used statistical measure is the nearest neighbor level spacing distribution (NNLSD), $P(s)$, where $P(s) \, ds$ is the probability that the distance, $s$, between two adjacent eigenvalues lies in the interval $[s, s + ds]$. Typically, $P(s)$ is well described by a Wigner distribution $P_W(s) = \frac{\pi s}{2} \exp(-\frac{\pi s^2}{4})$, when the classical limit is chaotic, and by a Poissonian distribution $P_P(s) = \exp(-s)$, when the classical limit is regular, i.e., (completely) integrable [20, 21]. Interestingly, $P(s)$ can differ from these distributions [26]. Two things are crucial for the computation of the NNLSD: First of all one has to select a subspace consisting of states from a single symmetry class. Thereafter one has to unfold the subspace’s spectrum, such that the local average of $s$ equals one ($\bar{s} = 1$) everywhere in the spectrum. A detailed description of the unfolding procedure can be found in [20, 21]. In order to compare the resulting NNLSD, given as a normalized histogram with $L$ bins, with the above distributions we define the measure

$$\chi^2_W = \sum_{\mu=1}^{L} \left( \frac{P_\mu - P_{W,\mu}}{P_{W,\mu}} \right)^2,$$

and $\chi^2_P$, respectively, where $P_\mu$ is the probability that $s$ lies inside the $\mu$’th bin of the histogram. $P_{W,\mu}$ and $P_{P,\mu}$ are the probabilities according to $P_W(s)$ and $P_P(s)$, respectively.

In this letter we consider chain-like quantum systems which may be described by Hamiltonians of the form

$$\hat{H} = \sum_{\mu=1}^{N} \hat{h}_\mu + \sum_{\mu=1}^{N-1} \hat{v}_{\mu,\mu+1},$$

where $\hat{h}_\mu$ denotes the local Hamiltonian of some subunit $\mu$ and $\hat{v}_{\mu,\mu+1}$ the interaction between neighboring subunits, $N$ is the total number of subunits. The model is primarily intended to investigate energy transport in a chain of coupled quantum systems (like, e.g., molecules) but may also be viewed as a Hubbard-type model for particles on a lattice (see below). Furthermore, most (almost) periodic systems should allow for a description according to 2.
as will be illustrated below with the example of a spin chain and is explained in detail in [19]. Since we intend to identify the diffusion of, e.g., energy, we have to introduce a measure for the energy density or the local energy. We define the local energy operator at site $\mu$ simply as $\hat{h}_\mu$. Of course, this definition neglects the energy contained in the interaction and eventually implies a weak coupling limit.

If the transport behavior of, e.g., energy was perfectly diffusive, then the local energies $E_\mu(t) = \langle \psi(t)|\hat{h}_\mu|\psi(t) \rangle$ (where $|\psi(t)\rangle$ is the full system’s wavefunction) would obey the following set of equations for, e.g., a chain-like system

$$
\dot{E}_1 = \eta (E_2 - E_1), \\
\dot{E}_\mu = \eta [(E_{\mu+1} - E_\mu) - (E_\mu - E_{\mu-1})], \quad (3) \\
\dot{E}_N = \eta (E_{N-1} - E_N).
$$

This may be viewed as a discrete form of the diffusion equation $\dot{\rho}_E = \eta \Delta \rho_E$, $\rho_E$ being the energy density. Diffusive behavior of any other quantity may be defined by a respective set of equations.

A suitable measure for the deviation of the (numerically) exact time evolution of the local energies as obtained from the Schrödinger equation from the fully diffusive dynamics as generated by (3) is given by

$$
D^2 = \frac{1}{N} \frac{1}{5\tau} \sum_{\mu=1}^{N} \int_0^{5\tau} \left[ E_\mu^{\text{normal}}(t) - E_\mu^{\text{exact}}(t) \right]^2 dt \quad (4)
$$

with $\tau = 1/\eta$. In the letter at hand we determine $\eta$ through fitting the dynamics generated by (3) to the (numerically) exact time evolution of the local energies. For a possible analytic computation of $\eta$, see, e.g., [6].

Let us now investigate two abstract examples (“design models”) of (2). The first model consists of $N$ identical subunits: Each subunit features a nondegenerate ground state, a wide energy gap ($\Delta E$) and a comparatively narrow energy band ($\delta \epsilon$) which contains $n$, energetic equidistant, states, cf. Fig. 1. The next-neighbor interaction is defined as

$$
\hat{v}_{\mu,\mu+1} = \lambda \sum_{i,j=1}^{n} v_{ij} \hat{p}_{\mu,i}^+ \hat{p}_{\mu+1,j}^- + h.c., \quad (5)
$$

where $h.c.$ is the hermitian conjugate of the previous sum. $\hat{p}_{\mu,i}^+$ corresponds to an upwards transition of the $\mu$'th subunit from its ground state to the $i$'th state of its band and $\hat{p}_{\mu,i}^-$ corresponds to a downwards transition, respectively. $v_{ij}$ are randomly distributed complex numbers which are normalized to $\sum_{i,j=1}^{n} |v_{ij}|^2 / n^2 = 1$, such that $\lambda$ sets the total interaction

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Fig. 1 – A chain of $N$ identical subunits: Each subunit features a nondegenerate ground state, a wide energy gap ($\Delta E$) and a comparatively narrow energy band ($\delta \epsilon$) which contains $n$, energetic equidistant, states.
strength. Since \( v_{ij} \) does not change with \( \mu \), there is no disorder. Obviously, we can restrict our analysis to the one-excitation subspace (the space where one subsystem is excited and all others are in their ground state), if the initial state \( \psi(0) \) belongs to this subspace. The subspace’s dimension is \( N \cdot n \) and grows linearly rather than exponentially with \( N \).

The model may be also illustrated as a “single-particle multi-channel quantum wire”, as already mentioned above, with random hoppings but without disorder. Therefore, unlike the single-particle Hubbard models with randomness in, e.g., [27], no localization occurs. Thus all deviations from normal transport which are discussed below (see Fig. 2a) are deviations towards a ballistic-type behavior, not towards localization.

For simplicity, we start with \( N = 2 \), i.e., only two subunits. Figure 2a shows \( D^2 \) versus \( \lambda \), averaged for 200 adequately restricted random pure initial states \( \psi(0) \), cf. (4). The model parameters \( \Delta E = 10 \) and \( \delta \epsilon = 0.5 \) are fixed, but \( n \) runs from 125 (+) over 250 (×) and 500 (+) till 1000 (□). Evidently, Wigner-like level statistics and normal transport are correlated.

We have additionally checked chains up to \( N = 15 \) and \( n = 500 \). Furthermore, we have varied details of the model, e.g., the band’s level distribution. We shortly summarize that the results do not significantly differ from the results of the case \( N = 2 \). The interested reader is referred to [6, 19] where, e.g., the finite size scaling is discussed in detail.

However, since real physical systems do not typically feature the gapped local spectra of the above model, we consider another example of (2). The model is pictured in Fig. 3 and consists of \( N \) identical subunits: Each subunit features \( n \) eigenstates which are randomly, but uniformly distributed within an energy interval \( \Delta E \). As before \( \hat{v}_{\mu,\mu+1} \) is a randomly chosen complex matrix, but now without restriction to any subspace (no “particle-number conservation”). Nevertheless, \( \hat{v}_{\mu,\mu+1} \) is supposed to be given by \( \hat{v}_{\mu,\mu+1} = \lambda \hat{v} \) with \( \text{Tr} (\hat{v}^2) / n^2 = 1 \). Again, for each \( \lambda \) we average over an adequate set of 200 random pure initial states. For the case \( N = 2 \)
the results do not qualitatively differ from the results in Fig. 2a and 2b, e.g., for the model parameters \( n = 60 \) and \( \Delta E = 10 \) the minimum of \( D^2 \) and \( \chi^2_W \) lies at \( \lambda = 0.0005 \).

What about larger \( N \)? Since for this system class the dimension of the relevant Hilbert space is \( n^N \), we are forced to decrease \( n \). But for smaller \( n \) deviations from the fully diffusive behavior typically increase, cf. Fig. 2a. Nevertheless, in principle we find the above result also confirmed for \( N = 3 \) and \( n = 20 \). Remarkably, even for \( N = 6 \) and \( n = 4 \) the time evolution of the local energies is in tolerably good agreement with (3), again for a parameter regime where the NNLSD is Wigner-like. (We do not display all those data here, since they essentially look like Fig. 2.)

However, for a chain of two level subunits, that is, for a chain of “spins” relaxation and local fluctuations are indistinguishable on the scale of a single subunit, i.e., on this scale (6) does not apply. This changes if the scale is changed, i.e., if various neighboring spins (including their mutual interactions) are grouped together to form a subunit as addressed by (2). However, since a spin chain with random next neighbor interaction may always be viewed as a “mixture” of different wellknown spin models, it is more meaningful to consider directly a single spin model, e.g., the Heisenberg model. Furthermore, other than our “design models”, those spin models possess a classical counterpart which is unambiguously either integrable or not [21, 28]. Thus, in the following we consider a Heisenberg spin chain in an external magnetic field \( B \). Concretely, the Hamiltonian reads

\[
\hat{H} = \frac{1}{2} \sum_{\mu=1}^{N} (B + B_\mu) \hat{\sigma}_\mu^z + \lambda \sum_{\mu=1}^{N-1} \hat{\sigma}_\mu \cdot \hat{\sigma}_{\mu+1}, \ N \text{ even},
\]

where \( \hat{\sigma}_\mu \) are the standard Pauli operators and \( B_\mu \) are local variations from \( B \). Furthermore, \( B_\mu \) are chosen as Gaussian distributed random numbers with \( \langle B_\mu \rangle = 0 \) and \( \langle B_\mu B_\nu \rangle = \delta_{\mu\nu} \epsilon^2 \).

The parameter \( \lambda \) sets the coupling strength, but the Heisenberg interaction is not normalized to 1, unlike (5). As mentioned above we operationally divide the chain into only two subunits, namely the first and second half. Note that due to the local fields \( B_\mu \) the spectra of those halves may not be identical.

Obviously, (6) is invariant under rotations around the \( z \)-axis. In order to compute the NNLSD we choose the subspace with \( \hat{S}_z = 0 \), where \( \hat{S}_z \) is the quantum number with respect to \( \hat{S}_z = \sum_{\mu=1}^{N} \hat{\sigma}_\mu^z / 2 \), the generator of these rotations. For a model as given by (6) with \( N = 12 \) the dimension of this subspace is \( d = 924 \). Figure 4a shows \( \chi^2_W \) versus \( \epsilon \), averaged for 100 sequences \( B_\mu \), that is, the average deviation of the NNLSD from the Wigner distribution, and \( \chi^2_P \), respectively, cf. 11. Since the system is integrable for \( \epsilon = 0 \), a Poisson-like NNLSD is obtained. When \( \epsilon \) increases from zero, the system undergoes a transition to chaos and consequently the NNLSD becomes Wigner-like. The minimum of \( \chi^2_W \) (the maximum of \( \chi^2_P \)) is reached at \( \epsilon \approx \lambda / 4 \). When \( \epsilon \) further increases and becomes larger than \( \lambda \), the system becomes localized and accordingly a Poisson-like NNLSD reappears, see [22–24], too.
Fig. 4 – (a) Average deviation of the level statistics from the Wigner distribution (+) and the Poisson distribution (×) for the spin model corresponding to (6). (b) Time evolution of the first half’s local magnetization for \(\epsilon/\lambda = 0\) (dashed curve), 0.25 (dotted curve) and 1 (solid curve). Evidently, exponential decay indicating normal transport occurs only for \(\epsilon/\lambda = 0.25\), the parameter for which the level statistics are most Wigner-like.

Since neither the level statistics nor the dynamics within the mentioned subspace depend on the constant field \(B\), we set \(B = 0\). Here we analyze the transport of magnetization which is, just like energy, a conserved quantity in this model. According to our above partition scheme we define two local magnetizations:

\[
M_1 := \frac{1}{2} \langle \psi(t) | \sum_{\mu=1}^{6} \hat{\sigma}_z^\mu | \psi(t) \rangle \quad \text{and} \quad M_2 := \frac{1}{2} \langle \psi(t) | \sum_{\mu=7}^{12} \hat{\sigma}_z^\mu | \psi(t) \rangle .
\]

(7)

If the transport behavior of magnetization was diffusive on this scale, the \(M\)’s should exhibit a dynamics as generated by a direct analogue to (3), i.e., they should simply relax exponentially to equilibrium. In Fig. 4b, \(M_1\) is displayed for the cases \(\epsilon/\lambda = 0\) (dashed), 0.25 (dotted) and 1 (solid). The chosen initial state \(\psi(0)\) is the only state with \(M_1 = 3\) and \(M_2 = -3\). Obviously, for the case \(\epsilon/\lambda = 0\) the transport is non-normal, the “bouncing” behavior of the magnetization could rather be interpreted as a hint for ballistic transport. This issue has been discussed very controversially in the literature [12–16]. So far, we also have no definite conclusion. For \(\epsilon/\lambda = 1\) almost no transport is observable, the magnetization seems to be stuck, i.e., localized. But at the minimum of \(\chi^2_W\) (the maximum of \(\chi^2_P\)), \(\epsilon/\lambda = 0.25\), there is a tolerably good agreement with (6): the first half’s local magnetization decays almost exponentially from the initial value \(M_1 = 3\) to the equilibrium value \(M_1 = 0\), as expected for normal transport.

What is to be expected for longer chains? Regular transport and localization scenarios should be unaffected in the thermodynamic limit as the investigations of the first system class and theories in [6,19,29] suggest. The ballistic-like transport may possibly become normal on a larger scale.

Of course, our Heisenberg model can be mapped on a 1D twelve-site Hubbard model of interacting spinless fermions with disorder. Such systems have recently been studied in [30] with the result that the interaction may lead to finite conductivity (above some critical temperature) for systems that would be localized (in real space) otherwise. Although our states are far from being thermal, our results are in accord with those findings: If we remove the interactions (the \(\hat{\sigma}_z^\mu \hat{\sigma}_z^{\mu+1}\)-term) for the normal transport case (\(\epsilon/\lambda = 0.25\)) we find that magnetization essentially stays in the first half, i.e., localization occurs. Consistently, the NNLSD becomes Poissonian again.
Let us finally summarize and conclude: We investigated several finite one-dimensional quantum systems. We introduced definitions for perfectly diffusive, normal transport behavior and for the level statistics expected from a perfectly chaotic system (Wigner statistics). By numerically solving the corresponding Schrödinger equations we got the exact energy spectra as well as the exact dynamics of our systems. With those data we computed the deviation of our model’s level statistics from a perfectly chaotic system’s level statistics and the deviation of our model’s exact transport dynamics from a perfectly diffusive transport dynamics. From comparing those deviations we found that models featuring nearly perfect diffusive transport always feature nearly perfect chaotic level statistics, while the inverse is not true. This result is eye-catching and eventually leads to our conclusion that a Wigner-like NNLSD might be a necessary, but not sufficient condition for normal transport.

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