Quantum transport properties of low dimensional materials are currently an object of intensive theoretical (see Ref. [1] for a recent review) and experimental research. Particularly interesting is the case of quasi-1d strongly interacting particle systems, where an important link between conductivity and integrability has been recently established [2]. However, most of theoretical studies focused on the close to equilibrium situation by using the linear response formalism, and almost nothing is known about the physics of such systems far from equilibrium (FFE). In order to drive a small interacting quantum system FFE one has to couple it strongly to some macroscopic reservoirs. Theoretical description of this situation usually goes via master equation for the density matrix where the non-unitary (dissipative) term depends on the coupling of the model to the reservoirs. Numerical simulations of such situations in non-trivial models have only recently became computationally feasible [3].

In this paper we propose conceptually simple and perhaps experimentally realizable form of coupling of a small 1d interacting quantum system to a pair of macroscopic baths of spins (or spinless fermions, or any other quantum two level systems – qubits). Our setting can also be viewed as a simple model of the qubit transport which may be of relevance in quantum information. In addition it allows for a very efficient (stochastic) numerical simulation of the non-equilibrium steady state (NESS) in terms of a pure state which only after averaging over stochastic bath interactions statistically converges to the proper density-matrix of NESS. We believe that, for a generic, non-pathological quantum interacting system, the bulk properties of NESS in the thermodynamic limit should not depend on the model of the baths. And now we come to the main point. We apply our model to simulate FFE spin transport in the well known Heisenberg XXZ spin 1/2 chain. While in the regime, known as ideally conducting [3, 4], we find expected results, namely that the spin current increases monotonically (and almost linearly) with the increasing driving field, we find a very different result in the other regime, which is for zero magnetization and close to equilibrium known as an ideal insulator. Namely there the spin (or qubit) current appears to have a clear maximum as a function of the driving field, hence for sufficiently strong field we find that the current decreases upon the increase of driving, and practically vanishes for a maximal field. This result can be reproduced analytically for a small chain of \(N = 4\) spins, while numerical simulations up to \(N = 16\) indicate that it becomes even shaper by increasing \(N\). Negative differential conductivity has been theoretically predicted and observed before, mainly in semiconductors (see e.g. Ref. [4]), as a consequence of various dynamical current instabilities. However, we believe that our result provides a new paradigm for such a behavior in strongly interacting quantum many-body systems with possible applications in the transport of quantum information.

We begin by describing our general setting of system-bath coupling. Let our systems consist of \(N\) spins 1/2, or qubits, described by Pauli variables \(\vec{\sigma}_n, n = 1, \ldots, N\). The first and the last spin, \(\sigma_1\) and \(\sigma_N\), shall be coupled to the baths, so let us decompose the total \(2^N\) dimensional Hilbert space to \(2^{N-2}\) dimensional Hilbert space of interior chain and 4 dimensional space of border qubits, \(\mathcal{H} = \mathcal{H}_{in} \otimes \mathcal{H}_{bo}\). Let the left and the right bath be characterized by some chemical potentials \(\mu_L, \mu_R \in [0, 1]\), and let \(U(t)\) denote \(2^N\) dimensional unitary evolution matrix of an autonomous spin chain for duration \(t\). Usually we can write \(U(t) = \text{exp}(-i t \mathcal{H})\) in terms of some Hamiltonian matrix \(\mathcal{H}\), but working with a unitary map \(U(t)\) may be more general, e.g. representing also periodically kicked (or driven) systems (such as in Ref. [4]). Concerning the evolution \(U(t)\) we shall only assume that it conserves the total magnetization \(M = \sum_{n=1}^N \sigma_n^z\), i.e. the qubit number \((M + N)/2\) if spin up represents a qubit state, namely \([U(t), M] = 0\). Let the canonical (qubit) basis \(|c\rangle\) of \(\mathcal{H}\), i.e. eigenbasis of \(\sigma_n^z\), be labelled by \(N\)-digit binary decompositions \(c = \sum_{n=1}^N c_n 2^{n-1}\), \(c_n \in \{0, 1\}\), where \(2c_n - 1\) is an eigenvalue of \(\sigma_n^z\). Any \(|c\rangle\) can be written as a direct product \(|c\rangle = |a\rangle_{in} \otimes |b\rangle_{bo}\) where \(a = \sum_{n=2}^{N-1} c_n 2^{n-2}\) and \(b = c_1 + 2c_N\). Conversely, we define \(\gamma(a, b) := c\).

We shall now describe the system’s evolution when it is coupled to the baths. Consider an ordered sequence of times \(t_k, k \in \mathbb{Z}, t_k < t_j\) for \(k < l\), such that \(\lim_{k \to \pm \infty} t_k = \pm \infty\). Between two subsequent times, say \(t_{k-1}\) and \(t_k\), the evolution is described by a unitary prop-
agator $U(t_k - t_{k-1})$. Then, at time $t_k$ we perform a measurement of the $z$-component of the first and the last spin, $\sigma_z^j, \sigma_z^N$. If $|\psi\rangle = \sum_c \psi_c |c\rangle$ is a pure state drawn from a statistical ensemble describing a state just before the measurement then, after the measurement, the state collapses with probability $p_b = \sum_a |\psi_{\gamma(a)}(b)\rangle^2$ to one of the four pure states $|\psi_b\rangle = (\sum_a \psi_{\gamma(a)}(a)|a\rangle_{in}) \otimes |b\rangle_{bo}$. After the measurement, since the states of the two border spins are known, we can adjust their expectation value to the ones of the reservoirs. This is simply achieved by applying, conditionally, spin-flips, i.e. one-qubit gates $\sigma_x^j$ (or $\sigma_x^N$), such that after the flips the probability that the left (right) spin points up is exactly $\mu_L$ ($\mu_R$). In a practical Monte-Carlo simulation, this means that we generate two uniform random numbers $\zeta_L, \zeta_R \in [0,1]$. If $\zeta_L > \mu_L$, we require that $c_{1,N} = 1$ so we apply $\sigma_x^N$ only if $b_{1,2} = 0$, where $b = b_1 + 2b_2$. On the contrary, if $\zeta_R > \mu_R$ we require that $c_{1,N} = 0$ so we apply $\sigma_x^j$ only if $b_{1,2} = 1$. Since conditional spin flips only affect the states of the border spins $|b\rangle_{bo} \rightarrow |b\rangle'_{bo}$, the state at time $t_k + 0$ is still a direct product $|\psi'\rangle = (\sum_B \psi_{\gamma(a)}(a)|a\rangle_{in}) \otimes |b\rangle'_{bo}$. Then we continue with autonomous evolution $U(t_{k+1} - t_k)$ to the next instant $t_{k+1}$ and repeat the probabilistic procedure of measurement and conditional spin flips. Provided that the distribution of time lags $\tau_k := t_{k+1} - t_k$ has stationary statistical properties we conjecture that a well defined NESS is approached as $t_k \rightarrow \infty$. This is evident in case $\tau_k = \tau = \text{const}$ which shall mostly be studied below. During such a simulation, an average spin (or qubit) current $j_L$ is calculated by looking at the left bath and summing up all down-up spin flips minus all up-down flips and dividing by the time of simulation. Due to conservation of $M$ this current should be after long time precisely equal to the analogous quantity $j_R$ at the right bath.

The procedure described above is very suitable for efficient numerical method which is by far superior to any density matrix simulations since one has to deal only with $2^N$ dimensional vector $\psi_{\text{c}}$ whereas in solving master equations we have to treat the full $2^N \times 2^N$ density matrices. However, for analytical treatment, the above procedure can be written by means of probabilistic ensembles and density matrices, i.e. in terms of a effective master equation. Statistical state averaged over an ensemble of bath interactions $\langle |\psi'\rangle\langle \psi'\rangle\rangle_{\text{bath}}$ at time $t_k + 0$ can always be written as a direct product $\rho_b \otimes \omega$ where $\omega = \sum_{\zeta} \omega_{\zeta} |b\rangle_{bo} \langle b|_{bo}$, $\omega_{\zeta} = \frac{1}{2}(1 + (-1)^{\mu_L})\frac{1}{2}(1 + (-1)^{\mu_R})$ is the density matrix of the border spins controlled by the baths. Writing the dynamical equation for the interior part $\rho_b$ is straightforward. If $P_b : \mathcal{H}_{\text{in}} \rightarrow \mathcal{H}$ denotes the lift $P_b|\psi_{\text{in}}\rangle := |\psi_{\text{in}}\rangle \otimes |b\rangle_{bo}$ and $P_b^{\dagger} : \mathcal{H} \rightarrow \mathcal{H}_{\text{in}}$ the corresponding projection, then

$$\rho_{k+1} = \sum_b P_b^{\dagger} U(\tau_k) (\rho_b \otimes \omega) U^{\dagger}(\tau_k) P_b.$$  

(1)

Assuming the simple case $\tau_k = \text{const}$, and writing $U = U(\tau)$, NESS $\rho_\infty$ is an eigenvalue 1 eigenvector of a completely positive master operator

$$\hat{\mathcal{L}}\rho := \sum_b P_b^{\dagger} U(\rho \otimes \omega) U^{\dagger}(\tau_k) P_b,$$  

(2)

namely

$$\hat{\mathcal{L}}\rho_\infty = \rho_\infty,$$  

(3)

and is unique provided 1 is a non-degenerate eigenvalue. The next largest eigenvalue of $\hat{\mathcal{L}}$ would determine the rate of relaxation of an arbitrary initial state to NESS $\rho_\infty$. To determine the spin current $\langle j \rangle_\infty$ in the steady state we have to compute the probabilities of measurements

$$p_b = \text{tr} P_b^{\dagger} U(\rho_\infty \otimes \omega) U^{\dagger} P_b$$  

(4)

and then, considering either left or right bath,

$$\langle j \rangle_\infty = \frac{p_0 + p_2 - \omega_0 - \omega_2}{\tau} = \frac{\omega_0 + \omega_1 - p_0 - p_1}{\tau}.$$  

(5)

In the following we concentrate on analytical calculations and numerical simulations in a specific important model, namely the anisotropic Heisenberg XXZ spin chain with the Hamiltonian

$$H = \sum_{n=1}^{N-1}[J_x(\sigma^x_n \sigma^x_{n+1} + \sigma^y_n \sigma^y_{n+1}) + J_z \sigma^z_n \sigma^z_{n+1}].$$  

(6)

The autonomous model is completely solvable (either with open or periodic boundary conditions) in terms of Bethe Ansatz (see e.g. [8]), and its thermodynamic ($N \rightarrow \infty$) transport properties are determined [3] by $\Delta = J_z/J_x$, and $s = M/N$. The model is ideal conductor, i.e. d.c. conductivity diverges for $s \neq 0$, whereas for $s = 0$, also corresponding to thermodynamical grand canonical state, the model shows a transition from ideal conductor for $|\Delta| < 1$ to ideal insulator for $|\Delta| > 1$. All the classical results about this model are based on linear response calculation and thus refer to the close to equilibrium situation. In this paper we analyze its FFE properties with the model of spin baths described above.

First we perform numerical Monte-Carlo simulations of quantum NESS exactly as described above. We choose a symmetric driving, $\mu_{L,R} = \frac{1}{2}(1 \mp \mu)$ so $\mu = \mu_R - \mu_L \in [0,1]$ is a parameter controlling the ‘field strength’. $\mu = 1$ corresponds to the maximum driving, where after the bath-interaction left/right-most spin is always pointing down/up. We always started from an initial random state, where coefficients $\psi_{\text{c}}$ were chosen as complex random Gaussian numbers of equal variance. Then we performed $10^6$ steps of integration, while first $10^4$ steps were omitted to ensure convergence to steady state. Time averages of all the quantities have been carefully checked for convergence. Three different choices for the distribution of time-lags $\tau$ have been chosen: (A) constant time-lag $\tau_k = \tau = 1$, (B) uniform distribution of time-lags $dP/d\tau = 1/2$ in the interval $[0,2]$, (C) exponential distribution of time-lags $dP/d\tau = \exp(-\tau)$ meaning that instants $t_k$ are independent Poissonian events.
In Fig. 1, we show steady state current $\langle j \rangle = j_L = j_R$ as a function of the field strength $\mu$ for $N=12$. For $\Delta = 1/2$ ($J_x = 1$, $J_z = 1/2$), we find almost perfectly linear behavior $\langle j \rangle \propto \mu$ meaning that linear response results can be extended to arbitrary field strength. Repeating the simulation for other values of $N = 8, 16$ and fixed $\mu = 0.3$, we find also that the current is almost independent of $N$, namely $\langle j \rangle |_{N=8} = 0.2198, \langle j \rangle |_{N=12} = 0.2182, \langle j \rangle |_{N=16} = 0.2187$, which is consistent with ideal conductivity.

The we turn into the insulating regime and put $\Delta = 2$ while keeping $J_z = 1/2$. Here we find a very strange behavior of $\langle j \rangle$ as a function of $\mu$ as seen in Fig. 1b. The current has a maximum around $\mu \approx 1/2$ and then for further increasing $\mu$ it decreases, so that it essentially vanishes at $\mu = 1$. This seems extremely surprising phenomenon for which we have no intuitive explanation. In order to exclude possible interference effects due to periodic bath-interactions we repeat the same simulation for randomized time lags, (B) and (C), and find qualitatively exactly the same behavior (fig. 1b).

In Fig. 2, we plot the current-field characteristics for different system sizes up to $N = 16$. We find that for small $\mu$, current is in fact proportional to the field gradient $\mu/N$, like for a normal conductor obeying some diffusion law. However, this cannot hold in the thermodynamics limit, since we know that for $N = \infty$ the system should behave as an insulator. Indeed, we observe that the maxima of the curves $\langle j \rangle (\mu)$ decrease towards smaller $\mu$ as we increase $N$. Yet, the behavior of current-field characteristic for a finite value of $N$ is highly intriguing and requires further analysis and explanations.

During the simulations we have also computed the spin-density profile, namely the time-averages of expectation value $\langle \sigma^x_n \rangle$ as a function of the lattice index. For ideal conductor we expect that no density-gradient can be build and indeed we find very flat spin-density profile for the case $\Delta = 1/2$ shown in Fig. 2. Further we show in the same figure two density profiles for the insulating case $\Delta = 2$, one in the regime left to the maximum of current-field characteristic, namely for $\mu = 0.3$, and one for the extreme field $\mu = 1$ where the current is practically zero. We observe that for $\mu = 0.3$ the density-profile is very nicely scaling with $(n - 1)/(N - 1)$ indicating that the system can support a linear density-gradient like one observes in normal conductor. Indeed in this regime the system is indistinguishable from a normal conductor. Still, for strong filed $\mu = 1$, different density-profile is observed with spin-density changing much slower near the baths than in the bulk. In this regime it seems difficult to define a thermodynamic density gradient.

Finally, we suggest to use the current at maximum field
θ = N ⟨j⟩|µ=1 as an order parameter signaling a transition form a normal behavior θ > 0 for |Δ| < 1 to anomalous behavior θ = 0 found for |Δ| > 1. In Fig. 3 we show the dependence θ(Δ) for fixed Jz = 1/2, and for different values of N, and indeed we find that for increasing N, the transition becomes increasingly abrupt at the critical parameter Δ = 1.

We note that, for other values of parameters Jz and Jx, (τk), qualitatively similar numerical results were obtained, essentially depending only on the ratio Δ apart from trivial scaling factors.

Does this phenomenon allow for a simple analytical description, at least for a small system? From Fig. 1, we learn that the phenomenon exist already for N = 4 (and still not for N = 3), for which we might hope to solve analytically the fixed point equation (3). Indeed it turns out that N = 4 is the maximal dimension which allows for explicit solution of eq. (3), however only asymptotically for small τ. This is due to the fact that the propagator 𝑈 cannot be written in a closed form so exp(−𝑖τ𝐻) has to be expanded to second order in τ. Then it turns that the 16 × 16 matrix of 𝐿 indeed has a unique right eigenvector ρ∞ of maximum eigenvalue 1. It is interesting to note that within first order in τ the matrix of ρ∞ is real and the lowest order contribution to the steady state current is only in O(τ²).

Lengthy but straightforward calculations have been performed by means of Mathematica. The final solution for the current reads

$$\langle j \rangle_\infty = \frac{2τ J_z^2 (μ_R - μ_L) (1 + 2 (μ_L + μ_R - μ_L^2 - μ_R^2) Δ^2)}{1 + (μ_L + μ_R) (2μ_L - μ_R - μ_RΔ^2}$$

with the correction O(τ³). Note that vanishing of ⟨j⟩∞ as τ → 0 is just a manifestation of quantum Zeno effect when we approach the limit of continuous measurement. For the symmetric case, μ_L + μ_R = 1, μ_R - μ_L = μ, this formula is plotted in Fig. 1, with a maximum at μ = √((1 + Δ²)/3), and is not far from numerical simulation for τ = 1. While the spin density at the border is fixed by the baths, its interior gradient can be directly computed

$$\langle \nabla σ^z \rangle_\infty = \text{tr}[(σ_3^z - σ_2^z) ρ_∞],$$

and is always monotonic, though cubic, function of the field strength μ_R - μ_L. This means that not only the external field strength is increasing, but also the interior magnetization gradient is increasing while the current is decreasing, for large μ.

In conclusion, we have studied qubit (or spin) quantum transport in finite interacting systems far from equilibrium, for which a special efficient model of macroscopic baths has been designed. The interpretation of this model is very simple: at periodic, or randomly chosen, instants of time we “look at” (measure) the border 2-level states of the system, whether they are occupied or not. Then we conditionally flip this border state (i.e. exchange the qubit with the bath) so that after this process the density of qubits (or spin magnetization) at the borders is prescribed. Applying this model to study FFE transport in finite Heisenberg XXZ chain, we find negative differential conductivity for Δ > 1 provided the spatially varying magnetization of NESS crosses the insulating point s = 0. In this regime, the optimal quantum strategy to transport qubits from left to right is not simply filling them from one end and taking out from the other, but it is better to sometimes insert 0-qubit state from the left and not taking 1-qubit state from the right.

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