Equivalence of transport coefficients in bath-induced and dynamical scenarios

R. Steinigeweg(a), M. Ogiewa and J. Gemmer

Fachbereich Physik, Universität Osnabrück - Barbarastrasse 7, D-49069 Osnabrück, Germany, EU

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Abstract – We investigate the transport of a single excitation through a chain of weakly coupled subunits. At both ends the chain is exposed to baths which are incorporated by means of a master equation in Lindblad form. This master equation is solved by the use of stochastic unraveling in order to obtain excitation profile and current in the steady state. Completely diffusive transport is found for a range of model parameters, whereas signatures of ballistic behavior are observed outside this range. In the diffusive regime the conductivity is rather independent of the strength of the bath coupling and quantitatively agrees with the diffusion coefficient which has been derived from an investigation of the same model without baths. Also the ballistic behavior in the non-diffusive regime is in accord with results from this alternative approach.

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There essentially exist two direct approaches to the investigation of gradient-driven transport phenomena such as, e.g., heat conduction: i) A closed scenario is considered, where transport is driven by an internal gradient, i.e., transport is somehow analyzed for the relaxation of a spatially non-uniform energy distribution (this relaxation is in accord with a diffusion equation in the case of normal transport) [1–5]. ii) An open scenario is considered, where transport is induced by an external gradient, i.e., baths with different temperatures are locally coupled to both ends of a system such that a stationary non-equilibrium state results (with a finite current and a spatially linear energy profile in the normal transport case) [3–12].

Furthermore, there are two indirect approaches to gradient-driven transport: iii) The Green-Kubo approach [13] which essentially gives a diffusion coefficient as an integral over the current auto-correlation function corresponding to the spatially uniform equilibrium state. iv) The Einstein-Herzfeld approach [14] which relates the diffusion coefficient to the mean square displacement in the equilibrium state. (For a comprehensive fundamental review of iii) and iv) in the context gradient-driven transport see ref. [15] and references therein.) However, even though all those approaches are commonly expected to yield equivalent results on transport, direct, say, qualitative comparisons for concrete quantum models appear to be rare in the literature [5–7,11]. Quantitative ones are even more rare. For the model addressed below the equivalence of i) and iii) has been investigated and partially confirmed (in the diffusive regime) in ref. [1]. Thus, in this letter we focus exclusively on the equivalence of i) and ii), leaving the comparison of, say, i) and iv) as a relevant subject of future work in that direction.

The letter at hand provides such a comparison for a quantum model which describes the transport of a single excitation through a finite chain of weakly interacting subunits. This chain has already been treated as a closed system and is known to exhibit both purely diffusive and completely ballistic dynamics, depending on the model parameters [1,2]. At both ends the chain is now exposed to baths which are incorporated by means of a master equation in Lindblad form [16,17] such that the efficient numerical method of stochastic unraveling is applicable [18,19]. For this open system we also find the above regimes of diffusive and ballistic transport.

In the normal transport case we particularly show the following: i) The steady state of the open system has a constant current and a linear excitation profile; ii) the resulting conductivity is almost independent of
the strength of the bath coupling; iii) this conductivity coincides with the theoretical diffusion coefficient of the closed system, too. The latter two points deserve closer attention, since it generally is difficult to ensure that the extracted conductivity is a pure bulk property, especially for a finite system [3,4,7].

In the ballistic transport case we finally demonstrate the sensitive dependence of the conductivity on the bath coupling strength. In particular we illustrate that huge, say, infinite conductivities can be observed solely in the limit of weak bath couplings, e.g., where the resistance due to the bath contact is large.

Concretely, we investigate an open quantum system according to fig. 1: It is a one-dimensional structure which is connected to baths at both ends. Before the realization of these baths is discussed below, we specify the chain itself, i.e., we introduce the closed quantum system at first. It consists of $N$ identical subunits which feature a non-degenerate ground state, a wide energy gap $\Delta E$, and a narrow energy band $\delta \epsilon$ with $n$ equidistant levels $\epsilon_i = \Delta E + i \delta \epsilon / (n-1)$.

In the following the consideration will be focused on the invariant zero- and one-excitation subspace which is spanned by the basis \{0\}, $\{|\mu, i\rangle\}$. In the single state $|0\rangle$ all subunits are in their ground state. In the $N$ states $|\mu, i\rangle$ only the $i$th subunit is excited to the $i$-th level of its band, while all other subunits are still in their ground state. By the use of this notation the local Hamiltonian of the $\mu$-th subunit may be written as $\hat{h}_\mu = \sum_{i=1}^n \epsilon_i \hat{c}_{\mu, i}|\mu, i\rangle\langle\mu, i|$. The next-neighbor interaction between two adjacent subunits $\mu$ and $\mu + 1$ is supposed to be

$$\hat{v}_{\mu} = \lambda \sum_{i,j=1}^n c_{i,j} |\mu, i\rangle \langle \mu + 1, j| + \text{H.c.}$$

with the overall coupling strength $\lambda$. The $\mu$-independent coefficients $c_{i,j}$ are complex, independent, and random numbers: their real and imaginary parts are both chosen corresponding to a Gaussian distribution with mean 0 and variance $1/2$. Note that only a single realization of the $c_{i,j}$ (and not some ensemble average over different realizations) is considered throughout this letter. The total Hamiltonian may be written as $\hat{H} = \hat{H}_0 + \hat{V}$, where $\hat{H}_0$ is the sum of the local Hamiltonians $h_\mu$ and $\hat{V}$ is the sum of the next-neighbor interactions $\hat{v}_\mu$, respectively.

Of particular interest are the local probabilities $p_\mu(t)$ for finding an excitation of the $\mu$th subunit somewhere to its band. These quantities are conveniently expressed as the expectation values $p_\mu(t) = \text{Tr}[\rho(t) \hat{p}_\mu]$ of respective operators $\hat{p}_\mu = \sum_{i=1}^n |\mu, i\rangle\langle\mu, i|$, where $\rho(t)$ denotes the density matrix of the whole chain. The associated local currents $\hat{j}_\mu(t)$ may be defined as the expectation values of the operators $\hat{j}_\mu = i [\hat{p}_\mu - \hat{p}_{\mu+1}] / 2$, cf. ref. [1].

Even though this system is not meant to represent a concrete physical situation, it may be illustrated as a simplified model for a chain of, say, coupled atoms, molecules, or quantum dots. In this case the hopping of the excitation from one subunit to another corresponds to energy transport, especially if $\lambda \ll \Delta E$. It may also be viewed as a model for non-interacting particles on a lattice with many orbitals per site. The hopping of the excitation corresponds to transport of particles in this case. A more detailed discussion of physical realizations can be found in refs. [1,2].

However, for the closed system it has reliably been shown that the dynamical behavior of the $p_\mu(t)$ is well described by a diffusion equation of the form $\rho_\mu(t) = D [p_{\mu-1}(t) - 2 p_\mu(t) + p_{\mu+1}(t)]$, if only the two conditions

$$8 \pi n \lambda^2 / \delta \epsilon^2 \ll 1, \quad \left(4 \pi^2 n^2 \lambda^2 / N \delta \epsilon\right)^2 \gg 1$$

are fulfilled, see ref. [2]. The pertinent diffusion constant is given by $D = 2 \pi n \lambda^2 / \delta \epsilon$. Thus, the relaxation time of the excitation profile’s Fourier component with wavelength $s$, i.e., the characteristic time for transport on this length scale, is $\tau_R = 1 / [2 D (1 - \cos 2 \pi/s)]$.

The first condition (2) guarantees that the dynamics on the shortest length scale ($s = 1$) is much slower than a generic correlation time as generated by the local parts of the Hamiltonian: $\tau_C \sim 1 / \delta \epsilon$.

The second condition (2) ensures that the dynamics on the longest length scale ($s = N$) is much faster than the period of any correlation function as generated by the local parts of the Hamiltonian: $T = 2 \pi n / \delta \epsilon$. When this criterion is broken, e.g., by $\lambda \rightarrow 0$ or $N \rightarrow \infty$, a transition towards ballistic transport is caused in the large $s$-limit. In that case the dynamics is still found to be governed by the above diffusion-type equation but now with a time-dependent rate, i.e., $D = 2 D(t)/T$, cf. ref. [2].

Our aim is to compare these findings with the results which are obtained in the following treatment of the same model as an open system which is exposed to baths. In order to incorporate these baths we now postulate that a quantum master equation (QME) in Lindblad form holds, namely

$$\dot{\rho}(t) = \mathcal{L}[\rho(t)] + \mathcal{D}[\rho(t)]$$

The first part on the r.h.s. of this equation describes the coherent time evolution of $\rho(t)$ w.r.t. $\hat{H}$. The second part

$$\mathcal{D}[\rho(t)] = \sum_{\mu} \sum_{\mu' \neq \mu} \frac{\delta \epsilon}{2} \left(\hat{p}_\mu - \hat{p}_{\mu+1}\right) \rho(t) \left(\hat{p}_{\mu+1} - \hat{p}_\mu\right)$$

represents the dissipation into the baths of the $\mu$-th level. The Lindblad operators are determined by the density matrix $\rho(t)$ and the local properties of the $\mu$-th subunit. The specific choice of the Lindblad operators is based on the assumption that the baths are Markovian and that the interaction with the $\mu$-th subunit is described by a linear and instantaneous perturbation $\hat{V}_\mu$. The Lindblad operators are chosen such that the dissipative terms in the master equation are second order in $\delta \epsilon$ and such that the dissipative rates are exponential in $\delta \epsilon$. The dissipative terms are linear in the density matrix $\rho(t)$ and quadratic in the Lindblad operators.

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is an incoherent damping term and given by
\[ D \rho(t) = \sum_i a_i \left( \hat{A}_i \rho(t) \hat{A}_i^\dagger - \frac{1}{2} [\rho(t), \hat{A}_i \hat{A}_i^\dagger] \right) \]
(4)

with non-negative rates \( a_i \), Lindblad operators \( \hat{A}_i \), and the anti-commutator \([ , , ]_+\). Equations (3), (4) are the most general form of a linear and time-local QME which defines a trace- and hermiticity-perserving, completely positive dynamical map. This particularly means that any density matrix is mapped to a density matrix \([16,17]\).

It is well known that a strict derivation of a physically reasonable Lindblad form from a microscopic bath model is somewhat subtle for conduction scenarios \([8]\). However, since numerics eventually turns out to be rather involved in that case, here we primarily choose the computationally least costly bath implementation (within the established framework of open quantum systems) which yields a physically acceptable result. Lindblad forms are computationally preferable, since those allow for the efficient numerical method of stochastic unravelling \([18,19]\). But for our below choice of Lindblad operators the underlying microscopic formulation can in principle be found by following the ideas in ref. \([8]\).

Thus, we choose only two left-bath operators
\[ \hat{A}_0 \equiv \hat{L}^+ = \frac{1}{\sqrt{n}} \sum_{i=1}^{n} |0,i\rangle \langle 0|, \quad \hat{A}_1 \equiv \hat{L}^- = (\hat{L}^+)^\dagger \]
(5)

with rates \( a_0 \equiv l^+ \), \( a_1 \equiv l^- \) but \( 2n \) right-bath operators
\[ \hat{A}_{2i} \equiv \hat{R}_i^+ = |N-1,i\rangle \langle 0|, \quad \hat{A}_{2i+1} \equiv \hat{R}_i^- = (\hat{R}_i^+)^\dagger, \]
(6)
i = 1, \ldots, n with rates \( a_{2i} \equiv r^+ \), \( a_{2i+1} \equiv r^- \). \( \hat{L}^+ \) and \( \hat{L}^- \) describe transitions between the ground state \( |0\rangle \) and a state where the excitation is equally distributed over all band levels of the leftmost subunit. \( \hat{R}_i^+ \) and \( \hat{R}_i^- \) are responsible for transitions between the ground state and the band state \( N-1,i \) of the rightmost subunit. (Note that this contact modelling goes beyond the secular approximation and is not in principle conflict with some microscopic picture \([8]\)). We further choose \( r^+ = 0 \), i.e., we suppose that the right bath is at zero temperature. The temperature of the left bath is finite, cf. fig. 1.

The method of stochastic unraveling relies on the fact that any Lindblad QME for a density matrix \( \rho(t) \) can equivalently be formulated in terms of a stochastic Schrödinger equation (SSE) for a wave function \( |\psi(t)\rangle \), see refs. \([18,19]\). This fact advantageously allows to deal with the same problem in the lower-dimensional Hilbert space. In order to simulate the process which is defined by the SSE we apply the procedure in. e.g., ref. \([7]\): It consists of deterministic evolutions (w.r.t. an effective Hamiltonian \( \hat{H}_{\text{eff}} = \hat{H} - i/2 \sum_i a_i \hat{A}_i \hat{A}_i^\dagger \) and stochastic jumps (corresponding to one of the Lindblad operators \( \hat{A}_i \)). Each application of this procedure leads to a single realization of a so-called “trajectory” \( |\psi(t)\rangle \). The expectation value of some observable \( \hat{M} \) in the steady state \( \rho \) can be evaluated from such a trajectory by the time average \( \text{Tr} (\rho \hat{M}) \approx 1/t \int_0^t dt_1 \langle \psi(t_1) | \hat{M} | \psi(t_1) \rangle \) for a sufficiently large time interval \( t \) \([19]\). We are primarily interested in \( \hat{M} = p_0 \) and \( \hat{M} = j_\mu \), of course.

Due to our choice of Lindblad operators (and \( r^+ = 0 \), the procedure drastically simplifies, because exclusively jumps into the ground state \( |0\rangle \) or into the state \( \hat{L} |0\rangle \) can occur, cf. eqs. (5) and (6). Furthermore, since \( |0\rangle \) is an eigenstate of \( \hat{H}_{\text{eff}} \), its deterministic evolutions become trivial and feature probabilities \( p_0(t) = 0 \) and currents \( j_\mu(t) = 0 \). Consequently, to the above time average only those parts of \( |\psi(t)\rangle \) contribute, where the deterministic propagations of \( \hat{L} |0\rangle \) take place, i.e., the whole problem reduces to the evaluation of \( \langle \psi(\tau) | = \exp(-\tau \hat{H}_{\text{eff}}) \tau \hat{L} |0\rangle \) solely. Note that propagations with the length of time \( \tau \) appear in \( |\psi(\tau)\rangle \) with a frequency of occurrence which is given by \( W(\tau) = -d/d\tau \langle \psi(\tau) | \psi(\tau) \rangle \), cf. ref. \([7]\). It is therefore possible to derive an exact analytical formula for the infinite time average, namely,
\[ \text{Tr} (\rho \hat{M}) = \frac{1}{C} \int_0^\infty d\tau W(\tau) \int_0^\tau d\tau_1 \langle \psi(\tau_1) | \hat{M} | \psi(\tau_1) \rangle \]
(7)
with the constant \( C = 1/l^+ + \int_0^\infty d\tau W(\tau) \tau \). Note that the dependence on the bath rate \( l^+ \) appears as the scaling factor \( C \) solely. Thus, the remaining crucial parameters are \( l^- \) and \( r^- \). For simplicity, however, we consider the special case of a negligibly small \( l^- \) (within \( \hat{H}_{\text{eff}} \)), i.e., the case of a sufficiently weak coupling of left bath and system. (In that case also \( l^+ \) becomes small but only affects the above constant \( C \). No restriction is made for the ratio \( l^-/l^+ \), e.g., the temperature of the left bath is still finite.) Only a single bath parameter remains: \( r^- \equiv r \).

In practice the above integral (7) is approximated by a sum over discrete time steps \( \Delta \tau \) and with a finite upper limit \( \tau_{\text{max}} \). The use of not too large, i.e., numerically still accessible \( \tau_{\text{max}} \) is possible, because the function \( W(\tau) \) usually decreases rapidly with \( \tau \), e.g., it decays exponentially fast. In our numerical simulations we use \( \Delta \tau D \leq 0.01 \) and \( \tau_{\text{max}} D \geq 1000 \). This choice typically is minimum required for a good convergence in terms of \( j_\mu \) which are independent of \( \mu \), i.e., with a deviation from their average on the order of less than 1%, at least for figs. 2 and 3.

Figure 2(a) shows first numerical results for a system with \( N = 5 \), where the remaining model parameters are set to well satisfy the both conditions (2) for purely diffusive transport in the closed scenario. In the open scenario at hand, as expected for normal behavior, we indeed observe a strictly linear excitation profile \( p_0 \) over the whole chain without significant effects at the boundaries \( \mu = 0 \) and \( N = 1 \). Moreover, the conductivity \( \kappa = j_\mu/(p_0 - p_{n+1}) \) turns out to agree almost perfectly with the theoretical diffusion coefficient \( D \) from ref. \([2]\), \( \kappa/D \approx 0.98 \). This is one of the main results of this work. It already indicates that \( \kappa \) may be viewed as a bulk property and not as some
to the inverse relaxation time $1/\tau$ here. This decrease begins at those rates which are close to the inverse correlation time $1/\tau C \sim \delta \epsilon$ of the closed system. (Note that the underlying exciting profile $p_\mu$ is still linear except for an abrupt decline to zero at $\mu = N - 1$.)

The decrease of $\kappa$ in the small $r$-limit may be understood as an effect which is due to the onset of the breakdown of the weak-coupling approximation that underlies the Lindblad form in general, since it starts at those rates which are close to the inverse relaxation time $1/\tau R \sim D \lambda^2$ of the closed system (see fig. 3). This parameter regime is, however, numerically very costly and can with our resources only be explored to the extent displayed in fig. 3. It is numerically even more costly to drive the violation of the second condition (2) by increasing the length $N$ rather than decreasing $\lambda$, which prevents us from exploring this regime directly. Nevertheless, based on the above interpretation, we expect that the length scale-dependent transition to ballistic behavior discussed in ref. [2] should become visible in the present bath scenario, too.

But the further reduction of $\lambda$ eventually leads to the violation of the second condition (2), i.e., in the closed system diffusive transport is finally expected to break down towards ballistic behavior. As displayed in fig. 2(b), such a behavior is found for the open system at hand, too. The probability profile $p_\mu$ is highly non-linear and the conductivity $\kappa$, now extracted in the middle of the chain, is also much larger than the theoretical diffusion coefficient $D$, $\kappa/D \approx 4$. (Note that the integration of (7) becomes very costly, since the function $W(\tau)$ exhibits a slowly decaying long-time tail.)

Contrary to the above diffusive case, $\kappa$ turns out to be extremely $r$-dependent in the ballistic case, see the squares in fig. 3. (Note that these squares are evaluated for the maximum $r$-interval which is still accessible to our numerics). $\kappa(r)$ features a distinct peak below the inverse correlation period $1/T = \delta \epsilon / (2 \pi n)$ of the closed system. The decrease of $\kappa$ on the l.h.s. of the peak may be understood as the decline to zero which has already been observed for $r \ll 1/\tau R$. On the r.h.s. of the peak the decrease of $\kappa$ reaches rather fast a value which is close to $D$ and eventually seems to reach this value but to stagnate at it. Surprisingly, the ballistic nature of transport does not have a significant impact on $\kappa$ here.

This observation, and all other findings in fig. 3, allow for the following interpretation: Assume that the external bath resolves the internal dynamics on a corresponding time scale $t = 1/r$. Then a deviation from the transport behavior of the isolated system is to be expected, if the bath-induced dynamics is either faster than internal correlation times ($r > 1/\tau C$) or slower than internal relaxation times ($r < 1/\tau R$). (This deviation results in a decrease of $\kappa$.) If the bath-induced dynamics proceeds in the possibly huge regime in between those time scales, diffusive behavior becomes visible. However, a ballistic closed system typically features a time scale on which the non-decaying character of the correlation functions becomes crucial but relaxation has not been completed yet. As already explained, for our model such a time scale exists, if $\tau R < T$ (i.e., if the second condition (2) is violated), precisely in between those two times. Now, if the bath-induced dynamics is tuned by $r$ to the latter time scale, signatures of ballistic transport, i.e., a sharply increasing $\kappa$ appear. The larger the latter time regime becomes, the more pronounced is the maximum of $\kappa$ and its height may probably rise without bound according to the degree to which the second condition (2) is violated, see fig. 3. This parameter regime is, however, numerically very costly and can with our resources only be explored to the extend displayed in fig. 3. It is numerically even more costly to drive the violation of the second condition (2) by increasing the length $N$ rather than decreasing $\lambda$, which prevents us from exploring this regime directly.
To conclude, we investigated a transport scenario based on bath coupling for a model with quantitatively well-known transport properties. We found that a bath scenario may produce the correct bulk conductivity but this requires a careful implementation of the bath contacts.

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