Nonequilibrium steady-state Kubo formula: equality of transport coefficients

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We address the question of whether transport coefficients obtained from unitary closed system setting, i.e., standard equilibrium Green-Kubo formulas, are the same as the ones obtained from a weak driving nonequilibrium steady-state calculation. We first derive a Kubo-like expression for the nonequilibrium steady-state diffusion constant that is handy for the comparison. Then we show that if the unitary dynamics is diffusive the nonequilibrium steady-state calculation gives exactly the same transport coefficient. The form of finite-size correction is also predicted. Theoretical results are verified by an explicit calculation of quantum transport in several microscopic models.

Introduction.— Transport of conserved quantities is one of the simplest manifestations of nonequilibrium physics. Depending on the dynamics the transport may range from ballistic (zero bulk resistance) to diffusive (finite resistance per length), over to localization (infinite resistance), or, in principle, anything in-between these extremes, usually dubbed the anomalous transport. Our experience tells us that in general transport is diffusive and described by a phenomenological Fourier law [1], however, starting from a microscopic Hamiltonian showing that is anything but simple. In particular, in one-dimensional systems transport is often not diffusive – there can be strong effects due to dimensionality as well as integrability that typically causes ballistic transport. Understanding transport in one-dimensional systems of interacting particles has a long history, going back to the celebrated Fermi-Pasta-Ulam-Tsingou numerical experiment [2,3], and even today it is still very much an open problem [4,5].

On a theoretical level one can use the Green-Kubo linear response formulas to express the transport coefficient in terms of equilibrium autocorrelation function of the respective current [6]. However, calculating time-dependent correlation function is often too involved even for in principle solvable systems (like, e.g., Bethe ansatz solvable XXZ spin chain). One therefore has to resort to numerical calculations. For that two different frameworks are used: (i) closed Hamiltonian evolution calculating either the equilibrium current autocorrelation function, or spreading of inhomogeneous states, (ii) direct simulation of nonequilibrium steady state (NESS) transport by explicitly taking into account driving reservoirs at different potential. For classical systems there is plenty of different reservoir types available (Langvin, stochastic, Nose-Hoover, etc.) and both approaches have been used extensively [7,8]. In quantum domain efficiently describing reservoirs is trickier, one approach is using Lindblad master equation [9,10] which in general though is not easy to solve. Therefore, traditionally a unitary closed system setting has been prevalent [11,12]. With recent matrix-product based methods [13] though things are changing as direct NESS simulations of Lindblad master equations [9,10] are efficient and are thus becoming indispensable [14–22], especially when large 1d systems are required. An important question therefore is whether Hamiltonian and NESS approaches give the same transport coefficient? We stress that even for weak nonequilibrium driving resolution is far from obvious – sometimes doubts are expressed that an explicit driving could somehow modify transport properties – while on a formal mathematical level the expression for transport coefficients is completely different and no rigorous connection is known [4] neither for classical nor for quantum systems.

We address the relation between “equilibrium” and NESS transport coefficients for 1D quantum systems. By first writing a NESS Kubo-like formula for the transport coefficient in a form that makes comparison transparent, we see that the NESS transport coefficient is due to unitary spreading of a local disturbance and boundary leaks. We then show that, provided the unitary part is diffusive, the two approaches give the same transport type and in particular the same diffusion constant. Theoretical results which also predict a particular convergence with system size $L$ are verified in explicit models.

The setting.— A common way to account for an explicit coupling to reservoirs in 1D systems is by an appropriate boundary conditions on top of Hamiltonian bulk evolution. Any quantum evolution should preserve positivity of density matrices as well as its trace. If one in addition assumes that the reservoir is infinitely large and fast, i.e., induces Markovian evolution, one is led to the Lindblad master equation [9,10]

$$\frac{d\rho}{dt} = \mathcal{L}(\rho) = i[\rho, H] + \mathcal{L}_{\text{dis}}(\rho),$$

(1)

where $\mathcal{L}_{\text{dis}}(\rho) = \sum_k 2L_k \rho L_k^\dagger - \rho L_k^\dagger L_k - L_k^\dagger L_k \rho$ is a dissipator that depends on a set of Lindblad operators $L_k$. In transport studies one often employs Lindblad operators that act only at the chain boundaries inducing a unique NESS reached after a long time. Transport properties are in turn given by the scaling of the NESS current. Cou-
plied with MPS-based methods \cite{13} to encode the state $\rho(t)$ one is often able to simulate quantum systems of several hundred sites which is crucial in systems with weak integrability breaking due to e.g. small interactions \cite{24} or disorder \cite{21}. For weak driving we can write the Lindbladian as a sum of two linear operators

$$\mathcal{L} = \mathcal{L}_0 + \mu \mathcal{L}_1,$$

where $\mu$ is some small parameter and $\mathcal{L}_0$ is Lindbladian. The (unique) steady state of $\mathcal{L}_0$ is denoted by $\rho_0$, $\mathcal{L}_0 \rho_0 = 0$. For small $\mu$ we look for a perturbative NESS solution $\rho = \rho_0 + \mu \rho_1 + \cdots$, getting a standard expression for the linear correction $\mathcal{L}_0 \rho_1 = -\mathcal{L}_1 \rho_0 = -R$. Formally, one can write $\rho_1 = -\mathcal{L}_0^{-1}(R)$. This expression has a unique solution provided $R$ is orthogonal to the kernel of $\mathcal{L}_0$. Alternatively, one can do time-dependent perturbation theory \cite{24}, arriving at \cite{15}

$$\rho_1 = \rho_1(t \to \infty) = \int_0^\infty e^{\mathcal{L}_0^\tau} R d\tau = \int_0^\infty R(\tau) d\tau. \quad (3)$$

NESS Kubo. For the sake of concreteness let us illustrate everything on an important case of a boundary driven Lindblad dynamics that has been used extensively to numerically study high-energy magnetization (particle) transport in 1D lattice systems, e.g. \cite{15, 16, 20, 23, 25, 30}. One uses magnetization driving described by Lindblad operators: $L_1 = \sqrt{\Gamma} \sqrt{1 + \mu \sigma^z_1}$, $L_2 = \sqrt{\Gamma} \sqrt{1 - \mu \sigma^z_1}$, $L_3 = \sqrt{\Gamma} \sqrt{1 - \mu \sigma^z_2}$, $L_4 = \sqrt{\Gamma} \sqrt{1 + \mu \sigma^z_2}$. $\Gamma$ is the coupling strength while $\mu$ is the driving strength. The dissipator at the left end acts on boundary Pauli matrices as: $\mathcal{L}_L(\sigma^z_1) = -2\Gamma \sigma^z_1$, $\mathcal{L}_L(\sigma^z_2) = -2\Gamma \sigma^z_2$, $\mathcal{L}_L(\sigma^x_1) = -4\Gamma \sigma^x_1$, $\mathcal{L}_L(\sigma^x_2) = 4\Gamma \mu \sigma^y_1$, and similarly with a reversed sign of $\mu$ at the right end. The unique steady state of such 1-site dissipator is $\sim 1 + \mu \sigma^x$, i.e., driving tries to impose magnetization $+\mu$. The natural small parameter is $\mu$ so that the splitting is done into an equilibrium Lindbladian $\mathcal{L}_0 := \mathcal{L}(\mu = 0)$ (the steady-state of $\mathcal{L}_0$ is an infinite temperature state $\rho_0 \sim 1$) and perturbation $\mu \mathcal{L}_1 := \mathcal{L} - \mathcal{L}_0$ (such decomposition is exact, there are no higher order terms in $\mu$). To get $\rho_1$ we need $R = \mathcal{L}_1(\rho_0) = 4\Gamma(\sigma^x_1 - \sigma^x_2)$. Here we explicitly see that $R$ is indeed orthogonal to the kernel of $\mathcal{L}_0$. The expectation value of any traceless observable $A$ in the NESS is, for small $\mu$ \cite{3},

$$\langle A \rangle = 4\Gamma \mu \int_0^\infty \text{tr}(A e^{\mathcal{L}_0 t}(\sigma^x_1 - \sigma^x_2)) dt. \quad (4)$$

We remark that the limit of small $\mu$ is (always) well behaved in the sense that the convergence radius is finite (and typically large) in the thermodynamic limit (TDL).

In cases when $H$ is reflection symmetric, $PHP^t = H$, with $P$ being a reflection of site $k$ around the midpoint, $k \to L + 1 - k$, the full $\mathcal{L}_0$ is also, and so we can further desymmetrize and write $\rho_1 = \tilde{\rho}_1 - P \tilde{\rho}_1 P^t$, where $\tilde{\rho}_1 := -4\Gamma \mathcal{L}_0^{-1}(\sigma^x_1) = 4\Gamma \int_0^\infty \sigma^x_1(t) dt$ and $\sigma^x_1(t) := e^{\mathcal{L}_0 t} \sigma^x_1$. In particular, the NESS current is odd under $P$ and so the contributions from the $\sigma_2^x$ and $\sigma_1^x$ are the same, and one has $j = 8\Gamma \mu \int_0^\infty \text{tr}(j_{k,k+1} e^{\mathcal{L}_0 t} \sigma^x_2) dt$ (due to the continuity equation it is independent of $k$). Diffusion constant $D$ is defined via a Fick’s-like law relation in the NESS,

$$j = -D \frac{z_L - z_1}{L}, \quad D := \frac{\tilde{j}}{z_1 - z_L}, \quad (5)$$

where $z_k := \text{tr}(\rho \sigma^x_k)$ is the NESS expectation of magnetization. Besides the current we therefore also need boundary magnetization. Provided the system is not ballistic and the NESS current decays to zero in the TDL one will have $z_1 \to -\mu$ and $z_L \to -\mu$. To see that one writes the NESS condition at the boundary: taking the NESS as $\rho \sim 1 + (\sum_k z_k \sigma^x_k + \frac{1}{2} \sum_j \tilde{z}_j \sigma^x_{j+1} + \cdots)$, we get for our magnetization driving the exact stationarity condition $\mathcal{L}(\rho) = 0 = [4\Gamma \mu - 4\Gamma z_1 - j \sigma^x_1 + \cdots$, where the dots represent terms orthogonal to $\sigma^x_1$; the three terms in the bracket that in the NESS must sum to zero come from the injection of magnetization ($\mathcal{L}_L(1)$), absorption ($\mathcal{L}_L(\sigma^1_1)$), and continuity equation (current flowing from the 1st site due to $[j_{1,2}, H]$), respectively. We have an exact relation (independent of the details of $H$ and the value of $\mu$) $4\Gamma (\mu - z_1) = j$, and $4\Gamma (\mu + z_L) = j$. These relations show that, provided $j \to 0$, one has $z_1 \to \mu$ and $z_L \to -\mu$. Therefore, in the TDL $z_1 \to -2\mu$ and one can write a Kubo-like NESS expression (see Ref. \cite{31} for classical heat conduction and Ref. \cite{29} for quantum expression), abbreviating $\sigma^x_1(t) = e^{\text{C}0t} \sigma^x_1$,

$$D = \lim_{L \to \infty} 4\Gamma L \int_0^\infty \text{tr}(j_{k,k+1} e^{\text{C}0t} \sigma^x_1(t)) dt. \quad (6)$$

This expression can be transformed into an alternative form by using continuity equation for magnetization (see also latter derivations), obtaining \cite{29}

$$D = \lim_{L \to \infty} L \int_0^\infty \text{tr}(j_{k,k+1} e^{\text{C}0t} \sigma^x_2) dt, \quad (7)$$

holding for any $p$ and $k$. By trivially defining the extensive current $J := L j_{k,k+1}$ the above expression can also be recast into

$$D = \lim_{L \to \infty} \frac{1}{2} \int_0^\infty \text{tr}(J(t) dt) dt, \quad (8)$$

with $J(t) := e^{\text{C}0t} J_0$. Although this looks deceptively similar to the standard (equilibrium) Green-Kubo formula \cite{3} the content is formally completely different (unitary vs. dissipative evolution).

We now rewrite Eq.\,(6) to a form that is better for comparison with unitary setting. Let us denote expectation values in a dissipatively propagated operator $e^{\text{C}0t} \sigma^x_1$ as $z_k(0) := \text{tr}(\sigma^x_1 e^{\text{C}0t} \sigma^x_1)$ and $j_k(0) := \text{tr}(j_{k,k+1} e^{\text{C}0t} \sigma^x_1)$.

Taking time derivative and evaluating $\mathcal{L}_0(\sigma^x_1)$, one gets

$$\dot{z}_1(0) = -4\Gamma z_1(0) - j_1(0), \quad \dot{z}_L(0) = -4\Gamma z_L(0) + j_L(0), \quad (7)$$

while in the bulk one has $\dot{z}_k(0) = j_{k-1}(0) - j_k(0)$. These are nothing but the continuity equations. The initial conditions are $z_k^{(0)}(0) = \delta_{k,1}$. Integrating \,(7) over time from $0$ to $\infty$, noting that $z_k^{(0)}(\infty) = 0$, one sees that the integral of $j_{L-1}(t)$ needed for $D$ is in turn equal to
the integral of \( z_L^{(0)}(t) \), 
\[ \int_0^\infty j_k^{(0)}(t) dt = 4\Gamma \int_0^\infty z_L^{(0)}(t) dt = 1 - 4\Gamma \int_0^\infty z_1^{(0)}(t) dt. \]
The diffusion constant can therefore be written as
\[ D = \lim_{L \to \infty} 16\Gamma^2 \int_0^\infty \text{tr}(\sigma_L^z \sigma_1^z(t)) dt, \quad \sigma_k^z(t) = e^{\mathcal{L}_0 t} \sigma_k^z. \] (8)

This equation has several nice features and is the central result that we build upon. Time integral always converges regardless of the system size or the transport type because \( \mathcal{L}_0 \) is contractive (all nonzero eigenvalues have negative real parts) and \( \mathcal{L}_0(\sigma_k^z) \neq 0 \). Transport type is reflected in the \( L \) dependence of the integral which is well defined even for anomalous transport. In equilibrium Green-Kubo formula on the other hand the question of (finite) transport coefficient boils down to whether the equilibrium autocorrelation function decays sufficiently fast with time, and if one deals with an anomalous transport it can not be applied straightforwardly [31][32]. While the NESS current \( j = \text{tr}(\dot{j}_{k,k+1}\rho) \) is an expectation in a complicated NESS \( \rho \), Eq. (8) gives a more natural interpretation of the same quantity: \( D \) is expressed as a certain transfer probability across the chain, with evolution \( \mathcal{L}_0 \) that is unitary except at the boundaries, and starting with all magnetization on the first site, \( \sigma_1^z \). It suggests that the transport type will be governed by the unitary evolution in the bulk. However, it is far from clear that such \( D \) is exactly the same as the one given by the equilibrium Green-Kubo formula. For instance, naively \( D \) looks proportional to \( \Gamma^2 \) (dependence on \( \Gamma \) has indeed been observed in small systems [32]). In the following we show that Eq. (8) gives exactly the correct diffusion constant.

Before that let us illustrate Eq. (8) by a numerical experiment. Taking the Heisenberg XXZ chain in a staggered field, \( H = \sum_j \sigma_j^x \sigma_{j+1}^x + \sigma_j^y \sigma_{j+1}^y + \Delta \sigma_j^z \sigma_{j+1}^z + \frac{1}{2}(h \sigma_j^x \sigma_{j+1}^y + h_{j+1} \sigma_j^y \sigma_{j+1}^x) \), with \( h_{3k} = -h, h_{3k+1} = -h/2, h_{3j+2} = 0 \), one has a quantum chaotic model (random matrix level spacing statistics [33]) for which diffusion is expected. We numerically [24] evaluate different expectations in \( e^{\mathcal{L}_0 t} \sigma_1^z \), shown in Fig. 1. The initial magnetization spreads from site 1 such that corresponding integrals result in \( D \).

**Equality of diffusion.**—To get \( D \) one needs \( z_L^{(0)}(t) \), which in turn means solving equilibrium dissipative evolution \( \mathcal{L}_0 \) of the initial \( \sigma_1^z \). In general this is not an easy problem and our aim here is not to get an exact solution for a particular \( H \), but instead to show in general that, provided the unitary dynamics is diffusive, the transport coefficient obtained in a boundary driven NESS [8] is the same as the “unitary” one.

To show that we take the exact conservation equations at the boundary [7] while we replace complicated evolution equation of the current \( j_k^{(0)} \) by a simpler one, assuming that the Fick’s law holds, \( j_k^{(0)} = -D_{eq}(z_k^{(0)} - z_{k+1}^{(0)}) \). This is to say that the dissipative part of \( \mathcal{L}_0 \) is treated exactly while the unitary evolution in the bulk is assumed to be perfectly diffusive. Here we specifically stress that \( D_{eq} \) is the unitary diffusion coefficient of bulk dynamics (e.g., obtained from the Green-Kubo formula) which could in principle be different than the NESS one \( D \). The Fick’s law in the bulk together with (7) constitutes a closed set of \( L \) coupled differential equations for \( z_k^{(0)}(t) \), which are nothing but a discrete diffusion equation \( \dot{z}_k = D_{eq}(z_{k+1}^{(0)} + z_{k-1}^{(0)} - 2z_k^{(0)}) \) plus a dissipative boundary condition [7]. We are especially interested in the large-\( L \) behavior where we write a partial differential equation (PDE) for \( z(x,t) \), \( \dot{z}(x,t) = D_{eq}z''(x,t) \), with boundary conditions,
\[
\dot{z}(0,t) = -4\Gamma z(0,t) - D_{eq}z'(0,t)
\]
\[
\dot{z}(L,t) = -4\Gamma z(L,t) + D_{eq}z'(L,t),
\] (9)
and the initial condition \( z(x,0) = \delta(x - 0^+) \). Absorbing boundary conditions [6] result in a slightly nonstandard boundary problem that can however still be solved by the standard separation of variables. Writing solution in terms of eigenfunctions \( X_n(x) \) as \( z(x,t) = \int_0^\infty X_n(x) \phi_n(t) dt \)
\[ \sum_n c_n X_n(x) e^{-D_{\text{eq}} k_n^2 t}, \]  
we get unnormalized \[24\]
\[ X_n(x) = \cos(k_n x) + \frac{4\Gamma - D_{\text{eq}} k_n^2}{D_{\text{eq}} k_n} \sin(k_n x), \]  
(10)
with transcendental eigenvalue equation for \( k_n \),
\[ \tan(k_n L) = -2D_{\text{eq}} k_n \left( \frac{4\Gamma - D_{\text{eq}} k_n^2}{(4\Gamma - D_{\text{eq}} k_n^2)^2 - D_{\text{eq}} k_n^2} \right). \]  
(11)

\( X_n \) are orthogonal with respect to a modified inner product
\[ \langle X_n, X_m \rangle := \int_0^L X_n(x) X_m(x) dx + X_n(0) X_m(0) + X_n(L) X_m(L). \]  
The initial condition gives \( c_n = \frac{1}{\langle X_n, X_n \rangle} \).

We can now express finite-\( L \) NESS transport coefficient \( D_{\text{eq}} \) as
\[ D = 16\Gamma^2 L \int_0^\infty z(L, t) dt = \frac{16\Gamma^2 L}{D_{\text{eq}}} \sum_{n=1}^\infty \frac{(-1)^n}{k_n^2(\langle X_n, X_n \rangle)}. \]  
(12)

In the TDL one can replace the sum with an integral (we checked \[24\] that this describes the exact sum \[12\] well even for not too large \( L \sim 16 \), resulting in \[24\]
\[ D = \frac{D_{\text{eq}}}{1 + \frac{D_{\text{eq}}}{2\Gamma L}} \approx D_{\text{eq}}(1 - \frac{D_{\text{eq}}}{2\Gamma L}). \]  
(13)

The NESS transport coefficient \( D_{\text{eq}} \) defined via NESS current scaling \[5\], is in the leading order in \( L \) exactly equal to the bulk unitary transport coefficient \( D_{\text{eq}} \) defined via unitary evolution. Furthermore, finite size corrections should scale as \( \sim 1/L \) for weak driving \( \mu \) and fixed coupling \( \Gamma \) one always has \( D = D_{\text{eq}} \) in the TDL. The only assumption going into deriving this expression is that in the bulk, where one has only unitary evolution, the Fick’s law holds. If the Fick’s law holds only on some hydrodynamic lengthscale of \( l_s \) lattice spacings, not on a single one as assumed above, we expect that the above expression is modified to
\[ D \approx D_{\text{eq}} \left( 1 - \frac{\alpha(\Gamma)}{L/l_s} \right), \]  
(14)

with possibly complicated \( \alpha(\Gamma) \) that is not necessarily \( 1/\Gamma \). If the Fick’s law \( D_{\text{eq}} \) has subleading corrections in \( L \) (either due to the boundary, or due to bulk dynamics) this can modify convergence of \( D_{\text{eq}} \) \[13\], however, one will still have \( D = D_{\text{eq}} \) in the TDL. The correct order of limits does matter: if one instead takes a fixed \( L \) and \( \Gamma \rightarrow 0 \) the diffusion constant goes to zero, while if one takes first \( \Gamma \rightarrow 0 \) and only then weak driving \( \mu \rightarrow 0 \) and \( L \rightarrow \infty \) the diffusion constant diverges \[31\].

Let us test the result \[13\] on three microscopic models. XX chain with bulk dephasing is an exactly solvable diffusive model in single-particle \[33\] as well as in many-particle \[36\] situation, with an exact expression \[36\] for the NESS \( D := j(L-1)/(2\mu) \) being \( D = D_{\text{eq}}/(1 + \frac{D_{\text{eq}}(\Gamma+1/\Gamma)}{2(L-1)}) \), where we defined \( D_{\text{eq}} := \lim_{L \rightarrow \infty} jL/2\mu = 2/\gamma \). For small \( \Gamma \) this form is exactly the same as the above general relation \[13\]. Next, we take the chaotic staggered XXZ model. In Fig. 2 we see that the finite-size correction indeed scales as \( 1/L \), however, the dependence on \( \Gamma \) is not as in Eq. \[13\] but rather more general \[14\]. We can see in Fig. 1 (dashed curves) that the solution \( z(x,t) \) of the PDE \[9\] describes full quantum evolution rather well for not too short times when diffusion is expected to emerge. Last, we take the integrable XXZ chain with \( h = 0 \) and \( \Delta = 1.5 \) at half-filling, where previous results indicate high-temperature diffusion, see e.g. Refs. \[16, 37–42\]. Our data show \[24\] that convergence is in this case not \( \sim 1/L \) as predicted for diffusive systems \[14\], but rather slower \( \sim 1/L^\alpha \) with the power around \( \alpha \approx 0.5 \) (see also data in the Supplement of \[24\] for similar slow convergence in a different model). Significance of that is at present not clear \[24\].

**Conclusion.**— Studying nonequilibrium steady state physics of 1D quantum systems we derive a weak driving Kubo-like expression for the diffusion constant that lends itself to comparison with unitary transport calculation. We show that provided the unitary evolution is diffusive the nonequilibrium transport coefficient is exactly the same as the one obtained for a closed system. We also predict a universal \( \sim 1/L \) convergence with system size in diffusive systems.

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SUPPLEMENTAL MATERIAL

Lindbladian perturbation theory

Let us write the Lindbladian as a sum of two linear operators (in concrete examples $\mathcal{L}_0$ is also Lindbladian while $\mathcal{L}_1$ is only linear but not Lindbladian),

$$\mathcal{L} = \mathcal{L}_0 + \mu \mathcal{L}_1,$$

(S1)

where $\mu$ is some small parameter. The (unique) steady state of $\mathcal{L}_0$ is denoted by $\rho_0$, $\mathcal{L}_0 \rho_0 = 0$. For small $\mu$ we look for perturbative solution

$$\rho = \rho_0 + \mu \rho_1 + \cdots,$$

(S2)

giving a standard perturbation theory expression for the steady-state linear correction $\rho_1$,

$$\mathcal{L}_0 \rho_1 = -\mathcal{L}_1 \rho_0 =: -R,$$

(S3)

where we use $R := \mathcal{L}_1 \rho_0$. Formally, one can write

$$\rho_1 = -\mathcal{L}_0^{-1}(R).$$

(S4)

This expression is well defined (has a unique solution) provided $R$ is orthogonal to the kernel of $\mathcal{L}_0$, in other words, if $\mathcal{L}_1 \rho_0$ is orthogonal to $\rho_0$ (this holds true for cases of interest discussed latter).

Alternatively, one can write the linear-response equation for a time-dependent perturbation $\rho_1(t)$,

$$\dot{\rho}_1(t) = \mathcal{L}_0 \rho_1 + \mathcal{L}_1 \rho_0,$$

(S5)

which is a linear inhomogeneous equation for $\rho_1(t)$. Formal solution satisfying $\rho_1(0) = 0$ is $\rho_1(t) = \int_0^t e^{\mathcal{L}_0(t-T)} R \d T$, where $R := \mathcal{L}_1 \rho_0$. The steady-state correction can therefore also be written as [15]

$$\rho_1 = \rho_1(t \to \infty) = \int_0^\infty e^{\mathcal{L}_0 \tau} R \d \tau = \int_0^\infty R(\tau) \d \tau,$$

(S6)

which is a formal way of writing the (pseudo)inverse in Eq. (S4). Note that $R(t) = e^{\mathcal{L}_0 t} R$ goes to zero (in any norm) at long times because of contractivity of $\mathcal{L}_0$ and the fact that $R$ is orthogonal to the kernel of $\mathcal{L}_0$. In a finite system the integral converges regardless of the dynamics.

Solving the PDE

We solve for time evolution by $\mathcal{L}_0$ by using exact dissipative boundary conditions while for a constitutive relation that connects local current to other local observables (like magnetization), and which is in principle complicated and depends on specifics of $H$, we take the Fick’s law,

$$j_k^{(0)} = -D_{eq}(\dot{z}_k^{(0)} - \dot{z}_k^{(0)}).$$

(S7)

This makes for a close set of equations for magnetizations $\dot{z}_k^{(0)}$. In the continuum limit we can replace a set of $L$ coupled differential equations by a PDE. Namely, we want to solve (dot denotes time derivatives, primes spatial derivatives)

$$\dot{z}(x,t) = D_{eq} \ddot{z}(x,t),$$

(S8)

with boundary conditions,

$$\dot{z}(0,t) = -4\Gamma z(0,t) - D_{eq} \dot{z'}(0,t)$$

(S9)

and the initial condition $z(x,0) = \delta(x - 0^+)$. We write the solution as

$$z(x,t) = \sum_n c_n X_n(x)e^{-D_{eq} k_n^2 t}$$

(S10)

in terms of eigenfunctions $X_n(x)$ satisfying the eigenequation $X_n'' + k_n^2 X_n = 0$. Eigenfunctions are $X_n(x) = A \cos(k_n x) + B \sin(k_n x)$ and have to satisfy boundary conditions $(4\Gamma - D_{eq} k_n^2) X_n(0) - D_{eq} X_n'(0) = 0$ and $(4\Gamma - D_{eq} k_n^2) X_n(L) + D_{eq} X_n'(L) = 0$. Choosing $A = 1$ and $B = (4\Gamma - D_{eq} k_n^2)/(D_{eq} k_n)$ satisfies the first boundary condition, so that the unnormalized eigenfunctions are

$$X_n(x) = \cos(k_n x) + \frac{4\Gamma - D_{eq} k_n^2}{D_{eq} k_n} \sin(k_n x),$$

(S11)

while the second one leads to a transcendental equation for the eigenvalues $k_n$,

$$\tan(k_n L) = -2 D_{eq} k_n \frac{(4\Gamma - D_{eq} k_n^2)}{(4\Gamma - D_{eq} k_n^2)^2 - D_{eq} k_n^2}. $$

(S12)

Because the boundary conditions depend on the eigenvalue $k_n$ (not one of the usual simpler Sturm-Liouville homogeneous boundary conditions with fixed coefficients)
one gets a modified inner product. Using standard procedure, multiplying the eigenequation for \( X_n \) by \( X_m \), integrating over \( x \) and making one per-parts integration, one ends up with \((k_n^2 - k_m^2)(X_n, X_m) = 0\), leading to orthogonality of different eigenfunctions \( X_n \) with respect to the inner product defined as,

\[
(X_n, X_m) := \int_0^L X_n(x) X_m(x) dx + X_n(0) X_m(0) + X_n(L) X_m(L).
\]

The initial condition in turn fixes the expansion coefficients \( c_n \) to simple \( c_n = 1/\langle X_n, X_n \rangle \) because one always has \( X_n(0) = 1 \). At the other end one has \( X_n(L) = (-1)^{n+1} \).

We can now express the NESS finite-\( L \) diffusion constant \( D \) as

\[
D = 16\Gamma^2 \int_0^\infty z(L, t) dt = \frac{16\Gamma^2 L}{D_{eq}} \sum_{n=1}^\infty k_n^2 (X_n, X_n),
\]

where \( k_n \) are solutions of Eq. (11). The norm of \( X_n \) is

\[
\langle X_n, X_n \rangle = \frac{L}{2} \left( 1 + \frac{4\Gamma - k_n^2 D_{eq}}{k_n^2 D_{eq}} \right) + 1 + \frac{4\Gamma}{D_{eq} k_n^2}.
\]

Denoting \( f(k_n) := \frac{1}{k_n^2 (X_n, X_n)} \), in the limit of large \( L \), when \( k_n \approx n\pi/L \), we are dealing with a sum of terms like \( f(n\pi/L) - f((n + 1)\pi/L) \approx -f'(k)\pi/L \). Replacing the sum with an integral one gets

\[
D = \frac{16\Gamma^2 L}{D_{eq}} \int_0^\infty \frac{-f'(k)}{2} dk.
\]

Despite complicated \( f'(k) \) the integral can be evaluated in closed form, resulting in

\[
D = \frac{D_{eq}}{1 + \frac{D_{eq}}{2\Gamma}}.
\]

In Fig. S3 we compare the continuum formula (S17) and the exact sum (S14), seeing that the replacement of a sum with an integral gives good results already for small \( L = 16 \).

It is instructive to understand where does the \( \sim 1/L \) correction in \( D \) come from. It is due to the last term in the norm (S15), namely, due to \( \frac{4\Gamma}{D_{eq} k_n^2} \). In the norm (S15) the first term proportional to \( L \) is simply due to the length of the interval while the last, \( L \)-independent \( 4\Gamma/D_{eq} k_n^2 \) is due to the fact that one does not have an integer number of oscillations in \( x \in [0, L] \) (see Fig. S2).

For instance, integrating \( \cos^2(k_n x) = (1 + \cos(2k_n x))/2 \) one gets “boundary” terms like \( \sin(2k_n L) \). In other words, the last term responsible for \( \sim 1/L \) correction is due to the boundary condition that causes a “phase shift” such that \( X_n(0, L) = \pm 1 \). Writing this term as \( \frac{8a}{k_n^2} \) one would get \( D_{eq}/D = 1 + \frac{aD_{eq}}{4\Gamma} \). The stronger the effect of the boundary, i.e., larger \( a \), the larger is finite-size correction.

**FIG. S2.** First eight eigenfunctions \( X_n(x) \) (S11). (a) shows unnormalized and (b) normalized eigenfunctions, both for \( \Gamma = 1 \), \( D_{eq} = 2.3 \) and \( L = 16 \).
FIG. S4. Convergence of the NESS diffusion constant with $L$ for the integrable XXZ Heisenberg chain with $\Delta = 1.5$ ($h = 0$). Full line is the asymptotic value $D(L \rightarrow \infty) \approx 2.6$. The inset shows relative error at finite $L$, i.e. $1 - D(L)/D(\infty)$, that here decays slower than prediction of diffusive theory [14]. Namely, two black lines are $1/L^{0.5}$ (full) and $0.8/L^{0.3}$ (dashed).

Using time-dependent density-matrix renormalization group (tDMRG) method and the mentioned Lindblad magnetization driving we study spin transport in a class of XXZ spin chains,

$$H = \sum_{j=1}^{L-1} \sigma_j^x \sigma_{j+1}^x + \sigma_j^y \sigma_{j+1}^y + \Delta \sigma_j^z \sigma_{j+1}^z + \frac{1}{2} (h_j \sigma_j^z + h_{j+1} \sigma_{j+1}^z),$$

(S18)

with $h_{3k} = -h$, $h_{3k+1} = -h/2$, $h_{3l+2} = 0$. For $h = 1$ we have quantum chaotic model [33], while for $h = 0$ the model is integrable. Spin current operator is $j_{k,k+1} = 2(\sigma_k^x \sigma_{k+1}^y - \sigma_k^y \sigma_{k+1}^x)$. For small driving $\mu$, we typically use $\mu = 0.01$, the NESS is close to the identity operator and one therefore studies infinite-temperature transport at half-filling (zero magnetization). Details of numerical implementation can be found in e.g. [16, 21] and references cited therein.

In the main text we presented data for a chaotic system, here we study the integrable case, $h = 0$ and $\Delta = 1.5$, where diffusion was observed. Indeed, we see (Fig. S4) that with system size $D$ converges to a constant independent of $\Gamma$. However, the convergence is slower. Finite-size correction does not scale as $\sim 1/L$, predicted by our theory for diffusive bulk evolution, but as $\sim 1/L^\alpha$ with $\alpha \approx 0.5$ (precise value is hard to determine due to limited data). We do not presently understand the origin of such slow convergence. Remember that $\sim 1/L$ correction in the case of diffusion was due to boundary effects, which in a diffusive system are expected to extend to a fixed distance into the bulk. Stronger finite-size effects like $1/L^{0.5}$ could either suggest that the effect of a boundary extends further into the system, or that the Fick’s law has $\sim 1/L^{0.5}$ corrections in the bulk. It is not clear if it signals some non-diffusive physics; we note that in higher NESS current fluctuations non-diffusive scaling has indeed been observed [43]. What is puzzling is that similar slow convergence has also been observed in a weakly perturbed XXZ model [23] (which is not integrable anymore), so it could be an effect having origin in some particular property of the XXZ model. An alternative explanation could also be that in the XXZ model finite size effects are simply larger, and at $L = 128$ we might not yet be in the asymptotic regime of $\sim 1/L$ scaling (magnetization profiles though are nicely linear for studied sizes).