The non-equilibrium steady state of sparse systems with non-trivial topology

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Abstract – We study the steady state of a multiply connected system that is driven out of equilibrium by a sparse perturbation. The prototype example is an $N$-site ring coupled to a thermal bath, driven by a stationary source that induces transitions with log-wide distributed rates. An induced current arises, which is controlled by the strength of the driving, and an associated topological term appears in the expression for the energy absorption rate. Due to the sparsity, the crossover from linear response to saturation is mediated by an intermediate regime, where the current is exponentially small in $\sqrt{N}$, which is related to the work of Sinai on “random walk in a random environment”.

The transport in a chain due to non-symmetric transition probabilities is a fundamental problem in statistical mechanics [1–6]. It can be regarded as a random walk in a random environment. The seminal observation is due to Sinai [2]: considering a chain of length $N$, the randomness implies a buildup of an exponentially large potential barrier $\exp(\sqrt{N})$, and consequently an exponential suppression of the current, reflecting a sub-diffusive $[\log(t)]^{4/3}$ spreading in time.

We would like to explore how this picture is modified if the chain is replaced by a configuration with a non-trivial topology, such as a ring, accounting for: 1) unavoidable telescopic correlations between the transition probabilities; 2) sparsity due to log-wide distribution of the transition rates as in glassy systems.

Let us expand on the roles played by these two ingredients: In the physical model that we would like to consider (fig. 1) the transition rates are not independent random variables. Rather they are determined by differences of uncorrelated on-site energies. These differences are strongly correlated: their sum does not grow with $N$.

Consequently the theory of Sinai does not apply. We shall see that in order to witness a “Sinai regime” we have to introduce into the model an additional ingredient: one may call it glassiness or sparsity. These terms emphasize complementary characteristics of the assumed log-wide distribution of the transition rates: the distribution spans several decades; accordingly the vanishingly small values constitute the majority; while the large values constitute a minority; which is reflected by having a median that is much smaller compared with the algebraic average.

Our focus is on the non-equilibrium steady-state (NESS) global current $I$ that circulates the whole ring,

\begin{figure}[h]
\centering
\includegraphics[width=0.5\textwidth]{ring_diagram}
\caption{(Colour on-line) A ring made up of $N$ isolated sites with on site energies $\epsilon_n$. The ring is coupled to a heat reservoir (represented by the blue “environment”) and subjected to a noisy driving field (represented by the red circle) that induces a current in the ring. In the numerical tests the energies occupy a band of width $\Delta = 1$, and the temperature of the bath is $T_B = 2$. The driving-source–induced rates $w_{\epsilon}^+$ are log-box distributed over 8 decades, while the bath-induced rates are all with $w_{\beta}^+ = 1$.}
\end{figure}
I lines (labeled as Eq. B) are the estimates for the SMF, eq. (19). The two straight dotted lines see fig. 2. For weak driving one observes a linear response $T$ considering a ring that is composed of $N$ sites (fig. 1). The ring is weakly coupled to a bath that has temperature $T_B$. In the absence of driving the average current $I$ is zero. The driving is modeled as a stationary noise source that has an intensity $\epsilon^2$. The driving breaks detailed balance, leading to a non-vanishing affinity along the ring. This affinity, which we call stochastic motive force (SMF), labeled as $\mathcal{E}_\omega$, induces a circulating steady-state current, see fig. 2. For weak driving one observes a linear response behavior $I \propto \mathcal{E}_\omega \propto \epsilon^2$. For very strong driving $I$ saturates.

Both the linear response for weak driving and the saturation for strong driving have a relatively simple explanation (see details later). But the crossover from linear response to saturation is more subtle, because it is related to the distribution of the transitions rates. If the distribution is log-wide we call the system sparse, implying that most of elements are much smaller compared with the average. Due to the sparsity one observes that there is an intermediate region where $\mathcal{E}_\omega \sim \sqrt{N}$, while the current becomes exponentially small, exhibiting fluctuations as a function of $\epsilon^2$.

**Outline.** We introduce the ring model and clarify its relation to the standard paradigm of NESS analysis. We derive expressions for the SMF, for the current, and for the EAR, illuminating their dependence on the driving intensity. With regard to the EAR, we highlight the manifestation of a topological term.

**Sparse networks.** Consider a general rate equation for the occupation probabilities $p_m$, namely

$$\frac{dp_m}{dt} = \sum_n w_{mn} p_m - w_{nm} p_n,$$

where $w_{nm}$ is the transition rate from $m$ to $n$. We can regard it as describing a network that consists of “sites” connected by “bonds”. Specifically we consider later a ring that consists of $N$ sites (fig. 1). With regard to the bond $x \equiv (m \sim n)$, that connects site $m$ to site $n$, we define the coupling $w(x)$ and the field $\mathcal{E}(x)$ as follows:

$$\mathcal{E}(x) \equiv \ln \left[ \frac{w_{nm}}{w_{mn}} \right],$$

$$w(x) \equiv \left[ w_{nm} w_{mn} \right]^{1/2}.$$

We say that the system is sparse or glassy if either $w(x)$ or $\mathcal{E}(x)$ of the connecting bonds have a log-wide distribution. This means that there is a small fraction of bonds where the coupling or the field is strong, while in the overwhelming majority it is very small.

We can regard $\mathcal{E}(x)$ as the “potential difference” across the bond $x \equiv (m \sim n)$, The reason for this terminology becomes obvious if one considers bath-induced transitions (see the details after eq. (7)): then it equals $- (E_n - E_m) / T_B$. Note that optionally $\mathcal{E}(x)$ can be regarded as the entropy change of the bath during the $(m \sim n)$ transition [7]. Consequently it is natural to define the “potential variation” between two points $x_1$ and $x_2$ along a line segment as follows:

$$\mathcal{E}(x_1 \sim x_2) = \int_{x_1}^{x_2} \mathcal{E}(x) dx.$$
Given a loop, one defines the SMF (or mesoscopic affinity \([8]\)) as follows:

\[ E_0 \equiv \sum_x E(x) \equiv \oint E(x) dx. \] (5)

The summation above is over the bonds \(x\) along the loop, which becomes an integral in the continuum limit. For a detailed balanced system the SMF is zero for any loop. Otherwise the system relaxes to a NESS.

For the subsequent analysis we define “the effective potential barrier” along a segment as the maximal potential variation (see how it looks in fig. 3):

\[ E_{\text{eff}} \equiv \max \left\{ [E(x_1 \sim x_2)] \right\}. \] (6)

Referring to a ring, it is important to realize that \( E_{\text{eff}} \) cannot be smaller than \( E_0 \). If the \( E(x) \) were totally uncorrelated both the maximal potential variation and the SMF would be proportional to \( \sqrt{N} \).

**NESS paradigm.** – In the physical problem the network consists of \( N\) sites, with on-site energies \( E_n \). The transition rates \( w_{nm} \) from site \( n \) to site \( m \) are induced by a driving source that has an intensity \( \epsilon^2 \), and by a bath that has a temperature \( T_B \). Namely,

\[ w_{nm} = w^\epsilon_{nm} + w^\beta_{nm}, \] (7)

where \( w^\epsilon_{nm} = w^\epsilon_{mn} \propto \epsilon^2 \), while the bath is detailed-balanced with \( w^{\beta}_{nm}/w^{\beta}_{mn} = \exp[-(E_n - E_m)/T_B] \). One can define a symmetrized rate as \( w_{\text{sym}} = (w_{nm} + w_{mn})/2 \). Then it follows that

\[ w_{nm} = \frac{2w_{\text{sym}}}{1 + \exp\left(\frac{E_n - E_m}{T_B}\right)} \] (8)

Our setting as described above is formally a special case of the common non-equilibrium paradigm for a system that is coupled to two heat baths. The driving source is like a bath that has temperature \( T_A = \infty \), while the environment is a bath that has a finite temperature \( T_B < \infty \). As discussed in ref. \([1]\) the generalization of the detailed balance condition requires

\[ w_{nm}(Q_A, Q_B)/w_{nm}(-Q_A, -Q_B) = \exp\left(\frac{Q_A}{T_A} - \frac{Q_B}{T_B}\right), \] (9)

where \( Q_A \) and \( Q_B \) are the the amounts of energies that are transferred from the baths to the system. In our setting the two baths are independent of each other and therefore any event is either with \( Q_A = E_n - E_m \) and \( Q_B = 0 \), or with \( Q_B = E_n - E_m \) and \( Q_A = 0 \).

**Microscopic temperature.** – In the absence of driving the transitions that are induced by the bath satisfy detailed balance, and accordingly the steady state of the system is canonical with occupation probabilities \( p_n \propto \exp[-E_n/T_B] \). Once we add the driving this is no longer true. Still, there is a well defined NESS, so we can formally define a microscopic temperature for each transition separately via the formula

\[ \frac{p_n}{p_m} = \exp\left[\frac{E_n - E_m}{T_{nm}}\right]. \] (10)

Unlike a canonical state, here we may have a wide distribution of microscopic temperatures. Furthermore, in a NESS the local temperature can be negative, \( i.e. \), the occupation of a higher level can be larger than the occupation of a lower one.

**The ring model.** – As a specific example we consider a ring with random on-site energies \( E_n \in [0, \Delta] \), and near-neighbor transitions. We use the notations \( \Delta_n = E_n - E_{n-1} \), and \( w^\Delta_{mn} = w_{n,n-1} \) and \( w^\perp = w_{n-1,n} \) and \( w = (w^\Delta + w^\perp)/2 \). The superscripts \( \beta \) and \( \epsilon \) are used in order to distinguish the bath and driving source contributions. It is useful to notice that in the high-temperature limit eq. (8) takes the form

\[ \{ w^\beta_{mn}, w^\perp_{mn} \} = \left[ 1 \pm \frac{\Delta_n}{2T_B} \right] w^\beta_{mn} \] (11)

The rate equation (1) is formally identical to an electrical network where the \( p_n \) are like voltages, and the \( w_{nm} \) represent conductors. Inspired by this formal analogy, we regard the conductivity of the network as an “average” transition rate, which we call \( w \). Consequently for a network with near-neighbor transitions, which is like having “connectors in series”, we get

\[ w = \left( \frac{1}{N} \sum_x \frac{1}{w(x)} \right)^{-1} \] (12)

with similar definitions for \( w^\beta \) and \( w^\perp \). It is now natural to define a dimensionless driving intensity \( \epsilon^2 \) and dimensionless coupling parameters \( g_n \), such that the latter reflect the relative exposure of the bonds to the driving:

\[ \frac{w^\beta}{w^\perp} = \epsilon^2, \quad \text{(definition of } \epsilon^2\text{)}, \] (13)

\[ \frac{w^\beta}{w^\perp} = g_n \epsilon^2, \quad \text{(definition of } g_n\text{)}. \] (14)

**Sparsity** means that the coupling to the driving source are log-wide distributed. In the numerics we have assumed log-box distribution of the \( g_n \) over several decades. Namely, the values \( \ln(g_n) \) were generated such that they form a uniform distribution in the range \([g_{\text{min}}, g_{\text{max}}]\). As for the bath: the \( w^\beta_{mn} \) were assumed identical. Accordingly note that \( \sum_n g_n = 1 \), while \( 1 < g_n < g_{\text{max}} \). The variance is \( \text{Var}(g_n) = g_{\text{max}} - g_{\text{min}} \).

**Estimating the SMF.** – In the presence of driving the SMF is non-zero:

\[ E_0 = \ln \frac{\prod_x w_x^{\perp}}{\prod_x w_x^{\beta}} \equiv \ln \frac{[\perp]}{[\beta]}, \] (15)

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where $\prod^\circ$ is the product of all the $N$ anticlockwise rates, and $\prod^\bullet$ is similarly defined. If $T_B \gg \Delta$ we get

$$\mathcal{E}_\circ \approx \frac{1}{T_B} \begin{cases} \Delta(0)^2/\epsilon^2, & \epsilon^2 < 1/g_{\text{max}}, \\ -\Delta(\infty)/\epsilon^2, & \epsilon^2 > 1/g_{\text{min}}, \\ \Delta(\ast)/\epsilon^2, & \text{otherwise,} \end{cases}$$

(19)

where $\Delta(\ast) = N^{1/2}\Delta$, and the $\sim$ implies that the result exhibit fluctuations as $\epsilon^2$ is varied. Looking in fig. 2, at the plot of $|\mathcal{E}_\circ|$, we notice that there are dips that indicate that the SMF changes sign. These sign reversals depend on the specific realization of $g_n$ and $\Delta_n$.

The NESS current. – The rate equation for nearest-neighbor transitions is

$$\dot{p}_n = w_n^{\ast} p_{n+1} + w_n p_{n-1} - 2 w_n p_n.$$  

(20)

This set of equations is redundant because of conservation of probability. At steady state $\dot{p}_n = 0$, and there is some current $I$ in the system. So we can write the equivalent non-redundant set of $N+1$ equations,

$$w_n^{\ast} p_{n-1} - w_n p_n = I, \quad \sum_n p_n = 1.$$  

(21)

This set of equations can be solved for the current using elementary algebra, or alternatively using the network formalism for stochastic systems [8–10]. The result may be written in compact notation as follows:

$$I = \prod_{x=1}^N w_x - \prod_{x=1}^N w_{x-1} w_x \prod_{x=1}^{N-1} w_{x+1} = \left[ \frac{0}{[\ast]} - \frac{[\ast]}{[\ast]} \right] (22)$$

where the denominator has a sum over bonds $x$ and target sites $n$. In each term the bond $x$ is disconnected to open the ring. The product $\prod_{n=1}^{x=n} w_{x-1}$ denotes the multiplication of the $N-1$ rates that are directed from the cut point towards the target site $n$. Note that the $N-1$ rates belong to the two paths that lead from $x$ to $n$. In continuum-limit notations the expression can be written as

$$I = \frac{e^{\mathcal{E}_\circ/2} - e^{-\mathcal{E}_\circ/2}}{\sum_x \frac{1}{w(x)} \int dx' e^{\mathcal{E}_\circ(x-x')/2}},$$

(23)

which can be roughly estimated as

$$I \approx \frac{1}{N} w \exp\left[ \frac{\mathcal{E}_\circ}{2} \right] 2 \sinh\left( \frac{\mathcal{E}_\circ}{2} \right).$$

(24)

This rough estimate is tested in fig. 2, and is in fact quite satisfactory.

Let us discuss in more detail the current for very weak and very strong driving. In both limits the SMF becomes very small, the Sinai factor exp[] becomes of order unity, and the sinh() can be approximated by a linear function. Accordingly we get

$$I \approx \frac{1}{N} \left[ \frac{-\Delta(0)/T_B}{w^\epsilon}, \frac{\Delta(\infty)/T_B}{w^B} \right],$$

(25)

As evident from these expressions, and as implied by the numerics, the direction of the current can change as the strength of the driving is increased, hence the dips in $|I|$ in fig. 4. The small $\epsilon$ result is independent of $w^B$, in spite of the bath dominance. The fingerprints of the bath show up only for strong driving, where the result becomes saturated, independent of $w^\epsilon$. The saturation by
itself could have been anticipated: it is due to having SMF \( \propto 1/e^2 \) with rates \( \propto e^2 \).

In the intermediate regime \( |E_{\psi}| \sim N^{1/2} \). The maximal potential variation \( E_{\psi} \) is of the same order of magnitude, but always lager, typically by some factor of order unity. Hence the current becomes exponentially small in \( \sqrt{N} \), as in the model by Sinai. Sparsity is the crucial requirement in order to observe this intermediate Sinai regime, otherwise there is merely a crossover from the linear response regime to the saturation regime.

The EAR formula. – By construction it is obvious that for zero driving intensity the system is detailed balanced with the temperature that is dictated by the bath: hence eq. (10) is satisfied with \( T_{nm} = T_B \). Also for non-zero driving the system is detailed balanced, provided the current is zero. This is implied by eq. (21). Consequently, in the absence of current, eq. (10) is still satisfied, but the microscopic temperature of the \( n \)-th transition is

\[
\frac{1}{T_n(0)} = 1 - \frac{\ln \left[ \frac{w_n}{w_{\pi}} \right]}{\Delta_n}.
\]

For \( T_B \gg \Delta \) one easily obtains the following practical approximation:

\[
\frac{1}{T_n} \approx \frac{w_n - w_{\pi}}{w_{\pi}} \frac{1}{\Delta_n} \approx \frac{1}{1 + g_n e^2} \frac{1}{T_B}.
\]

One observes that in the absence of current the system is locally heated, with microscopic temperatures \( T_n(0) \gg T_B \) that are non-uniform due to the dispersion in the couplings.

Let us see what happens if the current is non-zero. Again we can try to use eq. (10) in order to define a set of microscopic temperatures \( T_n \). One should notice that unlike \( T_n(0) \), some \( T_n \) might be smaller than \( T_B \) or even negative reflecting a probability occupation inversion (in the sense of Laser physics). For the following analysis it is useful to observe that eq. (21) provides an explicit expression for the occupation difference:

\[
p_{n-1} - p_n = \left[ \frac{w_{\pi} - w_n}{w_{\pi} + w_n} \right] 2 \tilde{p}_n + \left[ \frac{2}{w_{\pi} + w_n} \right] I,
\]

where \( \tilde{p}_n = (p_{n-1} + p_n)/2 \) is defined as the average occupation of the sites in the \( n \)-th bond. Note also that \( w_{\pi} - w_n \) originates exclusively from the bath, because the driving induces symmetric transitions.

We now can proceed to derive an expression for the EAR, which equals to the rate in which energy goes from the system to the bath. Accordingly we have to calculate the rate of energy flow \( \dot{Q} \) that is associated with the bath-induced transitions:

\[
\dot{Q} = \sum_n \left[ w_{\beta n}^b p_n - w_{\beta n}^b p_{n-1} \right] \Delta_n.
\]

Note that in steady state this should equal the rate of work \( W \), that is associated with the driving-source–induced transitions. We would like now to simplify the above expression. The first step is to rewrite \( a_1 b_1 - a_2 b_2 \) as the combination of \( (a_1 - a_2)(b_1 + b_2) \) and \( (a_1 + a_2)(b_1 - b_2) \). This gives

\[
\dot{Q} = \sum_n \left[ (w_{\beta n}^b - w_{\beta n}^b) p_n + w_{\beta n}^b (p_n - p_{n-1}) \right] \Delta_n.
\]

For the calculation of the differences in the above expression we use eq. (8) and eq. (28), respectively, and further simplify by assuming \( T_B \gg \Delta \), leading to

\[
\dot{Q} = \sum_n \left[ \tilde{p}_n^b w_{\beta n}^b \Delta_n^2 - \tilde{p}_n w_{\beta n}^b \Delta_n - I w_{\pi}^b \Delta_n \right].
\]

In the above expression it was convenient to keep using the notation \( T_n(0) \) even if the current is non-zero.

The last term in the EAR expression, eq. (31), arises because we have a non-trivial topology that can support non-zero current. We therefore name it “topological term”. We see that this term depends on the ratio \( w_{\beta n}^b/(w_{\beta n}^a + w_{\beta n}^b) \). Using the definition of eq. (14) and the expression for the SMF, eq. (16), it takes the form \( T_B E_{\psi} I \). Consequently we can write the expression for the EAR schematically as in ref. [11] with an additional topological term:

\[
\dot{Q} \approx \frac{D_B}{T_B} - \frac{D_B}{T_B(0)} + T_B E_{\psi} I.
\]

The first term represents the heat flow due to a temperature gradient. The definitions of the diffusion coefficient \( D_B \) and the induced temperature \( T(0) \) are implied by a comparison with eq. (31).

It is interesting to point out that eq. (32) connects between the entropy production obtained under different levels of coarse graining [7]. The term \( E_{\psi} I \) is a coarse-grained entropy production for a setup in which one can not distinguish between transitions mediated by the thermal bath and noise. In contrast, \( \dot{Q}/T_B \) is the entropy production rate when the two types of transitions are distinguishable.

EAR vs. current. – We would like to inquire whether the EAR is correlated with the current. At a superficial glance one may be tempted to say that there is a linear correlation due to the topological term \( \propto I \) in eq. (32). However, one should realize that also the \( p_n \) in eq. (31) depend implicitly on the current. Hence one should not expect a strict linear relation, but, speculatively, a weaker correlation. To confirm this conjecture we calculate in fig. 4 the difference between the EAR of a connected ring, and the EAR of the same ring after it had been disconnected at one point. We indeed observe that there is an unambiguous correlation.

The driving induces non-vanishing current \( I \), hence the EAR of a closed ring is larger than that of a linear chain. In the linear response regime one may expand the EAR in powers of \( e^2 \). One should observe that the \( I \) related corrections are of order \( e^4 \). Let us write the explicit
expression:

$$\dot{Q} = \sum_n \frac{\dot{p}_n \omega_n^{\alpha} \Delta n}{T_B} \left[ 1 - \frac{1}{1 + g_n \epsilon^2} \right] + T_B E \otimes I,$$

(33)

$$\approx \frac{D_B}{T_B} \left[ (g_n \epsilon^2) - (g_n \epsilon^2)^2 + \text{Var}(g) \epsilon^4 \right].$$

(34)

When comparing a closed ring to a disconnected ring, one should be aware that the last term, which we call “topological term”, should be either included or excluded, respectively. Compared with a disconnected ring the topological term obviously increases the EAR, but from the expression above we see that the global dependence of the EAR on the driving intensity remains sub-linear. Namely, one realizes that without the topological term the $\epsilon^4$ component in the EAR expression has the coefficient $-\gamma_n^2$, while with the topological term the net coefficient becomes $-\gamma_n^2$, which implies larger EAR but still sub-linear.

Summary. – The study of transport in network systems has numerous applications, notably in physical chemistry, where the dynamics is commonly described by a rate equation. There is much interest in studying NESS currents that are induced either by periodically varying system parameters [12], or by stochastic driving. Assuming the latter, we have considered the NESS of a driven ring that is coupled to a bath, and found both the steady-state current and the EAR. We have demonstrated how the ring-like topology and the sparsity lead to a glassy NESS with a non-trivial current dependence, exhibiting an interesting crossover from linear response to saturation via an intermediate Sinai-type regime.

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