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

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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 [2–7]. It can be regarded as *a random walk in a random environment*. The seminal observation is due to Sinai [3]: 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 $[\log(t)]^4$ 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* [a] between the transition probabilities; (2) *sparsity* due to log-wide distribution of the transition rates as in glassy systems; (3) Global currents that reflect the non-trivial topology.

Our focus is on the non-equilibrium steady state (NESS) global current I that circulates the whole ring, and on the associated energy absorption rate (EAR). Let us present some numerical results that clarify the physical picture and motivate the subsequent analysis. We consider 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 ϵ^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 $\mathcal{E}_{\circlearrowleft}$, induces a circulating steady-state current, see Fig. 2. For weak driving one observes a linear response behavior $I \propto \mathcal{E}_{\circlearrowleft} \propto \epsilon^2$. For very strong driving I saturates.

The crossover from linear response to saturation 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 $\mathcal{E}_{\circlearrowleft} \sim \sqrt{N}$, while the current becomes exponentially small, exhibiting fluctuations as a function of ϵ^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.

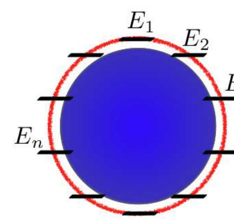

FIG. 1: A ring made up of N isolated sites with on site energies ϵ_n. The ring is coupled to a heat reservoir (represented by the blue "environment") and subjected to a noisy driving field (represented by the red circle) that induces a current in the ring. In the numerical tests the energies occupy a band of width $\Delta = 1$, and the temperature of the bath is $T_B = 2$. The driving source induced rates $w^{\epsilon}_{\overleftarrow{n}}$ are log-box distributed over 8 decades, while the bath induced rates are all with $w^{\beta}_{\overleftarrow{n}} = 1$.

Sparse networks.– Consider a general rate equation with transition rates w_{nm}. 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 $x \equiv (m \rightsquigarrow n)$, that connects site m to site n, we define the coupling $w(x)$ and the field $\mathcal{E}(x)$ as follows:

$$\mathcal{E}(x) \equiv \ln\left[\frac{w_{nm}}{w_{mn}}\right], \qquad w(x) \equiv [w_{nm}w_{mn}]^{1/2} \tag{1}$$

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 define the "potential variation" between two points x_1 and x_2 along a line segment as follows:

$$\mathcal{E}(x_1 \rightsquigarrow x_2) \;=\; \int_{x_1}^{x_2} \mathcal{E}(x)dx \tag{2}$$

This is identified as the medium entropy production [8] during a realization of a process where the system makes the transitions from x_1 to x_2. Given a loop, one defines the SMF (or mesoscopic affinity [9]) as follows:

$$\mathcal{E}_{\circlearrowleft} \equiv \sum_x \mathcal{E}(x) \equiv \oint \mathcal{E}(x)dx \quad (3)$$

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:

$$\mathcal{E}_{\cap} \equiv \text{maximum}\Big\{|\mathcal{E}(x_1 \rightsquigarrow x_2)|\Big\} \quad (4)$$

Referring to a Ring, it is important to realize that $\mathcal{E}_{\cap}$ cannot be smaller than $\mathcal{E}_{\circlearrowleft}$. See Fig.2. If the $\mathcal{E}(x)$ 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 ϵ^2, and by a bath that has a temperature T_B. Namely,

$$w_{nm} = w^{\epsilon}_{nm} + w^{\beta}_{nm} \quad (5)$$

where $w^{\epsilon}_{nm} = w^{\epsilon}_{mn} \propto \epsilon^2$, while the bath is detailed-balanced with $w^{\beta}_{nm}/w^{\beta}_{mn} = \exp[-(E_n - E_m)/T_B]$. This is formally a special case of the common non-equilibrium paradigm of 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 $T_B < \infty$.

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

$$\frac{p_n}{p_m} = \exp\left[-\frac{E_n - E_m}{T_{nm}}\right] \quad (6)$$

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 $w_{\overrightarrow{n}} = w_{n,n-1}$, and $w_{\overleftarrow{n}} = w_{n-1,n}$, and $w_{\overline{n}} = (w_{\overrightarrow{n}} + w_{\overleftarrow{n}})/2$. The superscripts β and ϵ are used in order to distinguish the bath and driving source contributions. Inspired by the analogy to "connectors in series" we define the "average" transition rate as

$$w \equiv \left(\frac{1}{N}\sum_x \frac{1}{w_{\overline{n}}(x)}\right)^{-1} \quad (7)$$

with similar definitions for w^{β} and w^{ϵ}. It is now natural to define a dimensionless driving intensity ϵ^2 and dimensionless coupling parameters g_n, such that the latter reflect the relative exposure of the bonds to the driving:

$$\frac{w^{\epsilon}}{w^{\beta}} \equiv \epsilon^2, \qquad \frac{w^{\epsilon}_{\overline{n}}}{w^{\beta}_{\overline{n}}} \equiv g_n \epsilon^2 \quad (8)$$

Note that if the $w^{\beta}_{\overline{n}}$ are identical, as assumed in our numerical tests, then the harmonic average over the g_n is unity. The 1st and 2nd moments are always larger, and in particular for sparse $w^{\epsilon}_{\overline{n}}$ they satisfy the strong inequality $1 \ll \overline{g_n} \ll \overline{g_n^2}$. The variance is $\text{Var}(g_n) = \overline{g_n^2} - \overline{g_n}^2$. In the numerics we assume that the g_n are log-box distributed over several decades in the range $[g_{\min}, g_{\max}]$.

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

$$\mathcal{E}_{\circlearrowleft} = T_B \ln\left[\frac{\prod_x^{\circlearrowleft} w_x}{\prod_x^{\circlearrowright} w_x}\right] \equiv \ln\frac{[\circlearrowleft]}{[\circlearrowright]} \quad (9)$$

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

$$\mathcal{E}_{\circlearrowleft} \approx -\sum_n \left[\frac{1}{1 + g_n\epsilon^2}\right]\frac{\Delta_n}{T_B} \quad (10)$$

Recall that we have $\sum_n \Delta_n = 0$. Additionally we define

$$\Delta^{(0)} \equiv \sum_n g_n \Delta_n \sim \pm\Big[2N\,\text{Var}(g)\Big]^{1/2}\Delta \quad (11)$$

$$\Delta^{(\infty)} \equiv \sum_n \frac{1}{g_n}\Delta_n \sim \pm\Big[2N\,\text{Var}(g^{-1})\Big]^{1/2}\Delta \quad (12)$$

The RMS-based estimate of the sums follows from the observation that, say, $\Delta^{(0)}$ can be rearranged as $\sum_n (g_{n+1} - g_n)E_n$, which is a sum of N independent random variables. Consequently we get for the SMF the following approximation

$$\mathcal{E}_{\circlearrowleft} \approx \frac{1}{T_B}\begin{cases} \Delta^{(0)}\epsilon^2, & \epsilon^2 < 1/g_{\max} \\ -\Delta^{(\infty)}/\epsilon^2, & \epsilon^2 > 1/g_{\min} \\ \sim [\pm]\Delta^{(*)}, & \text{otherwise} \end{cases} \quad (13)$$

where $\Delta^{(*)} \equiv N^{1/2}\Delta$, and the $\sim$ implies that the the result exhibit fluctuations as ϵ^2 is varied. Looking in Fig.3 at the plot of $|\mathcal{E}_{\circlearrowleft}|$, 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 Δ_n.

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

$$\dot{p}_n \ = \ w_{\overleftarrow{n+1}} p_{n+1} + w_{\overrightarrow{n}} p_{n-1} - 2 w_{\overline{n}} p_n \tag{14}$$

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

$$w_{\overrightarrow{n}} p_{n-1} - w_{\overleftarrow{n}} p_n = I, \qquad \sum_n p_n = 1 \tag{15}$$

This set of equations can be solved for the current using elementary algebra, or alternatively using the network formalism for stochastic systems [9–11]. The result may be written in compact notation as follows:

$$I \ = \ \frac{\prod_x^{\circlearrowleft} w_x - \prod_x^{\circlearrowright} w_x}{\sum_{x,n} \prod_{x'}^{(x\leadsto n)} w_{x'}} \ \equiv \ \frac{[\circlearrowleft] - [\circlearrowright]}{[\leadsto]} \tag{16}$$

where $\prod^{(x\leadsto n)}$ is the product of the $N{-}1$ rates that lead from the cut at bond x to the target site n. In continuum limit notations the expression can be written as

$$I \ = \ \frac{\mathrm{e}^{\mathcal{E}_{\circlearrowleft}/2} - \mathrm{e}^{-\mathcal{E}_{\circlearrowleft}/2}}{\sum_x \frac{1}{w(x)} \int dx' \mathrm{e}^{\mathcal{E}(x\leadsto x')/2}} \tag{17}$$

Which can be roughly estimated as

$$I \ \sim \ \frac{1}{N} w \ \exp\left[-\frac{\mathcal{E}_{\cap}}{2}\right] \ 2\sinh\left(\frac{\mathcal{E}_{\circlearrowleft}}{2}\right) \tag{18}$$

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

$$I \ \approx \ \frac{1}{N} \begin{cases} -[\Delta^{(0)}/T_B] w^{\epsilon}, & \text{linear regime} \\ [\Delta^{(\infty)}/T_B] w^{\beta}, & \text{Saturation} \end{cases} \tag{19}$$

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.3. The small ϵ result is independent of w^{β}, 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^{ϵ}.

In the intermediate regime $|\mathcal{E}_{\circlearrowleft}| \sim N^{1/2}$. The maximal potential variation $\mathcal{E}_{\cap}$ 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.– Let us define the average occupation of the sites in the nth bond as $\bar{p}_n = (p_{n-1}+p_n)/2$. It follows from Eq.(15) that the occupation difference is

$$p_{n-1} - p_n = \left[\frac{w_{\overleftarrow{n}} - w_{\overrightarrow{n}}}{w_{\overleftarrow{n}} + w_{\overrightarrow{n}}}\right] 2\bar{p}_n + \left[\frac{2}{w_{\overleftarrow{n}} + w_{\overrightarrow{n}}}\right] I \tag{20}$$

For zero SMF the current is zero, and we can define microscopic temperatures using Eq.(6). For $T_B \gg \Delta$ one easily obtains the following practical approximation:

$$\frac{1}{T_n^{(0)}} \ \approx \ \left[\frac{w_{\overleftarrow{n}} - w_{\overrightarrow{n}}}{w_{\overline{n}}}\right] \frac{1}{\Delta_n} \ \approx \ \left[\frac{1}{1+g_n\epsilon^2}\right] \frac{1}{T_B} \tag{21}$$

If the current I were zero, the system would be locally heated, with microscopic temperatures $T_n^{(0)} > T_B$ that are non-uniform due to the dispersion in the couplings. We keep using the notation $T_n^{(0)}$ even if $I \neq 0$. Using Eq.(20) the heat flow through the system is

$$\dot{\mathsf{Q}} \ = \ \sum_n \left[w^{\beta}_{\overleftarrow{n}} p_n - w^{\beta}_{\overrightarrow{n}} p_{n-1}\right] \Delta_n \tag{22}$$

$$= \ \sum_n \left[(w_{\overleftarrow{n}} - w_{\overrightarrow{n}})\bar{p}_n + w^{\beta}_{\overline{n}}(p_n - p_{n-1})\right] \Delta_n \tag{23}$$

$$= \ \sum_n \left[\frac{\bar{p}_n w^{\beta}_{\overline{n}} \Delta_n^2}{T_B} - \frac{\bar{p}_n w^{\beta}_{\overline{n}} \Delta_n^2}{T_n^{(0)}} - I \frac{w^{\beta}_{\overline{n}}}{w_{\overline{n}}} \Delta_n\right] \tag{24}$$

In order to gain physical insight into this expression we assume $T_B \gg \Delta$, and identify the sum in the last term as the SMF of Eq.(10). Then we write the expression schematically as in Ref.[12] with an additional *topological term* due to the current:

$$\dot{\mathsf{Q}} \ \approx \ \left[\frac{D_B}{T_B} - \frac{D_B}{T^{(0)}}\right] + T_B \mathcal{E}_{\circlearrowleft} \ I \tag{25}$$

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.(24). It is interesting to point out that Eq.(25) connects between the entropy production obtained under different levels of coarse graining [8]. The term $\mathcal{E}_{\circlearrowleft} I$ 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.– The topological term in Eq.(25) is due to the current. However, one should realize that also the p_n in Eq.(24) depend implicitly on the current. Nevertheless, it makes sense to assume that the contribution of the second term can be experimentally distinguished. To confirm this conjecture we calculate in Fig.3 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 realize that this difference is correlated with the current.

The driving induces non-vanishing current I, hence the EAR of a closed ring is larger than that of a linear chain. However, the dependence of the EAR on the driving intensity remains sub-linear, even if the topological term is included. To establish this observation we further simplify the expression for the EAR in the linear-response regime:

$$\dot{\mathrm{Q}} = \sum_n \frac{\bar{p}_n w_n^{\beta} \Delta_n^2}{T_B}\left[1 - \frac{1}{1+g_n\epsilon^2}\right] + T_B \mathcal{E}_{\circlearrowleft}\, I \quad (26)$$

$$\approx \frac{D_B}{T_B}\left[\overline{(g_n\epsilon^2) - (g_n\epsilon^2)^2} + \mathrm{Var}(g)\epsilon^4\right] \quad (27)$$

We realize that without the current the non-linear term in the EAR expression has the coefficient $-\overline{g_n^2}$, while with current the coefficient becomes $-\overline{g_n}^2$, 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 [13], 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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[a] This follows from the observation that the rates depend on *differences* of uncorrelated energies. These differences are strongly correlated: their sum does not grow with N.
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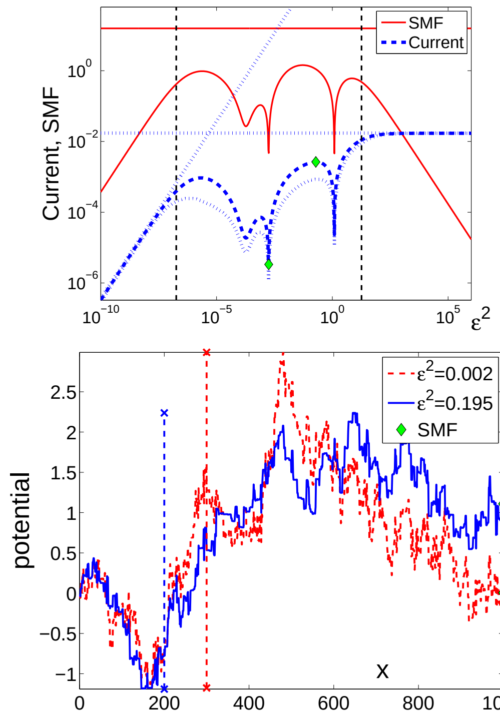

FIG. 2: We consider a Ring with N=10^3 sites, as defined in Fig. 1. In the upper panel the absolute values of the SMF (solid curve) and the current (thick dashed curve) are plotted as a function of the scaled driving intensity. The dotted lines and the solid horizontal line are the estimates for the SMF Eq. (13). Also the global approximation Eq. (18) is displayed (thin dashed curve). The vertical lines are $1/g_{\max}$ and $1/g_{\min}$. In the Lower panel the potential difference $\mathcal{E}(0 \rightsquigarrow x)$ is plotted against x, for two values of the driving intensity. Note that the SMF is $\mathcal{E}_{\circlearrowleft} \equiv \mathcal{E}(0 \rightsquigarrow N)$. The vertical lines correspond to the maximal potential variation $\mathcal{E}_{\cap}$.

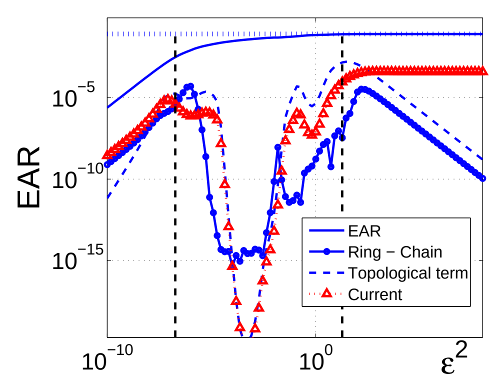

FIG. 3: The energy absorption rate (EAR) versus the driving intensity for a Ring with $N = 10^6$ sites, while the other parameters are the same as in the previous figure. The solid curve is the total EAR. The dotted horizontal line is the expected saturation value. The dashed curve is the topological term $\mathcal{E}_{\circlearrowleft} I$. The dash-dot curve is the EAR difference if the Ring is disconnected at one point. The current in the ring is also drawn (triangular markers).