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Currents in nonequilibrium statistical mechanics

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Nonzero currents characterize the nonequilibrium state in stochastic dynamics (or master equation) models of natural systems. In such models there is a matrix R of transition probabilities connecting the states of the system. We show that if the strength of a transition increases, so does the current along the corresponding bond. We also address the inverse problem: given a set of observed currents, we show the extent to which the original "R" can be recovered. These considerations lead to a general discussion of time scales and substance flows.

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I. INTRODUCTION

Nonequilibrium systems in statistical mechanics present an overwhelmingly wide array of phenomena. We have sought [1–8] a general approach based on the master equation in which many useful tautologies emerge—just as the second law of thermodynamics can emerge as a tautology (translate: *theorem*) once an appropriate framework is defined. The master equation (or stochastic dynamics) approach has been adopted by many investigators in recent years, although as early as 1976 one can find a review paper [9] advocating this perspective.

An important adjunct to this approach is the presence of *currents*. This is the hallmark of the departure from simple equilibrium, and with an appropriate choice of coarse grains the absence of currents is equivalent to detailed balance. It is our feeling that any approach to understanding complexity will involve dealing with currents in an essential way, and we offer as evidence the ubiquity of flow diagrams in studies of the biochemistry of the cell [10], of ecological systems [11–13], of economic systems [14], and in many, many other contexts. In recent papers [3,4] we proposed that it was precisely in the currents that the defining characteristics (and perhaps a definition!) of complexity could be found. Currents are also significant for the study of dissipation. From circuit theory's "*IV*" to the most general contexts, as visualized in, say, Refs. [3] or [9], currents play a role in generating dissipation. Yet another role for currents is in the study of chemical rate process. An example is Ref. [15] where there is enhancement of a process through the introduction of intermediate states (what we called a ladder), and the use of currents in the associated analysis is essential.

All these applications make it an essential physical objective to understand the general properties of currents. To this end, in the present paper we examine such properties with emphasis on the relation to the underlying dynamics. This feature is also important: often the experimentally observed quantity *is* the current, and the researcher's interest is in deducing its origins. Both physical and mathematical issues emerge. The purely mathematical questions are (1) given a matrix of transition probabilities and the associated currents, does (for example) the current increase if a relevant transition probability does? Such a relation would be reminiscent of the GHS inequalities [16] showing that the rate of change of magnetization decreases if coupling strength does (for the case of positive magnetization). As for those inequalities, proving such an "obvious" relation is not trivial. (2) Given a set of (probability) currents, how much can be known about the underlying matrix of transition probabilities? Can this information be further refined using currents on other time scales? The physical questions deal not only with the validity of the model, but also with the relation of the mathematical structure to experimentally accessible quantities. Thus, the models depend on a coarse graining of the truly microscopic variables into what could be called "mesoscopic" states, as well as the existence and selection of time scales on which transitions between these states are conceptually meaningful. Specifically with respect to currents, as remarked earlier, an important physical consideration is the fact that currents (of substances) can be measured in experiments, while the mesoscopic dynamics and even the stationary state are not directly measurable. We also remark that standard thermodynamics carefully avoids much of what concerns us here, making infinitely slow changes, although not in equilibrium.

An overview of our results follows. We refer to quantities to be defined more precisely in Sec. II, but hope that nevertheless this summary will be useful. In Sec. III we begin with a matrix of transition probabilities for a Markov process and prove that if a particular (off-diagonal) matrix element is increased, the current through the associated bond also increases. By current we mean the *net* transfer of probability in the steady state. This also implies a definite sign of change in several related currents.

Following that, in Sec. IV, we deal with the inverse problem: given currents and a stationary distribution for the Markov process, we produce a stochastic matrix with the same currents and stationary distribution. We also characterize the remaining freedom in the full specification of the underlying transition matrix.

By higher currents we mean those associated with higher powers of the matrix of transition probabilities. In Sec. V we

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show that with increasing information about higher currents one can learn more and more about the underlying transition matrix. In principle, given enough such data one can know extensive spectral information and in some cases determine the transition matrix completely. Note that we often use an assumption of genericity, since in many practical cases symmetries can cause certain currents to vanish, in which case there may be no further information to be gleaned. The fact that further information can be obtained from higher powers of the transition matrix makes it clear that its associated time interval is not arbitrary, and we discuss its physical significance in Sec. VI.

Finally, we provide a discussion of the relation between the currents at the level of the Markov process, namely, *probability* currents, and the currents measured in natural situations, for example, currents of heat along a metal bar or nitrogen flow in an ecosystem. These are in a sense projections of the probability currents and we make this relation precise.

At the end of the paper we provide a short summary of our results and a discussion of open problems.

II. NOTATION AND CONVENTIONS

The space of states is designated X and has cardinality $N<\infty$. Between states $x,y\in X$ there is a probability R_{xy} of transition, $x\leftarrow y$, in time Δt, which for now we take to be unity. The nature of the states and the appropriate time scale for individual time steps are mandated by the phenomena being described. In particular, the limit $\Delta t\to 0$ is not, in general, justified. We return to this later.

At a particular time t, the system can be described by a probability distribution $\rho(x,t)$. The matrix R will propagate this distribution, $\rho(x,t+1)=\Sigma_y R_{xy}\rho(y,t)$. Occasionally this will be written in matrix form with the state argument ("x") suppressed as $\rho(t+1)=R\rho(t)$. R has eigenvalues [17] $\lambda_0,\lambda_1,\ldots$ ordered by $1\equiv\lambda_0\geqslant|\lambda_1|\geqslant|\lambda_2|\geqslant\ldots$. The stationary state of R, i.e., the right eigenvector of eigenvalue 1, is $p_0(x)$, satisfying, in matrix form, $Rp_0=p_0$. We assume that R is irreducible, so that $p_0(x)$ is unique and strictly positive for all $x\in X$. The corresponding left eigenvector is $A_0(x)\equiv 1$ whose eigenvalue relation (namely, that the columns of R sum to unity) represents conservation of probability. Other eigenvectors are designated p_k (right) and A_k (left), $k=1,\ldots,N-1$, and satisfy the usual orthonormality conditions, $\langle A_k|p_\ell\rangle=\delta_{k\ell}$ [18]. With the matrix R we associate a graph whose vertices are the points of X and with edges connecting any pair having a nonzero transition probability. The matrix R may be *doubly stochastic*, which means that row sums are also 1. In this case $p_0(x)\equiv 1/N$.

For most of this paper, we assume that if any off-diagonal element R_{xy} is nonzero, so is R_{yx}. The latter assumption enters our graph-theoretical explicit form for the stationary state. (See [9] for how this assumption can be weakened.) In the opposite situation ($R_{xy}R_{yx}=0\ \forall\ x\neq y$), R is termed *completely irreversible*.

The current is the net flow between states:

$$J_{xy}\equiv R_{xy}p_0(y)-R_{yx}p_0(x) \tag{1}$$

(there is no summation over either x or y in this relation—in general, in this paper we do not use a summation convention). This is the current *in the stationary state* [19]. When J vanishes the system is said to satisfy *detailed balance*. For an equilibrium system and with time-symmetric coarse grains, J vanishes, and detailed balance obtains. Other currents may be considered. First, one may use other probability distributions, not just p_0. Of interest to us in this paper are the multistep currents

$$J^{(n)}_{xy}\equiv (R^n)_{xy}p_0(y)-(R^n)_{yx}p_0(x), \tag{2}$$

which we call "higher currents." At times we will emphasize the matrix of transition probabilities used in constructing a given current. The notation will be $J(R)$. Thus from Eqs. (1) and (2) it follows that $J(R)^{(n)}=J(R^n)$ (using the fact that they have the same stationary state). Note that $J(R^n)\equiv J^{(n)}$ is *not* the nth power of $J^{(1)}$.

Remark. See [2] for the effect of coarse graining on currents.

Remark. A matrix is said to satisfy "Kirchoff's law" if both row and column sums are zero. Any current matrix satisfies this: $\Sigma_x J_{xy}=\Sigma_y J_{xy}=0$. In words, current in equals current out. But non-skew-symmetric matrices can also satisfy Kirchoff's law, for example, $W\equiv R-1$, where R is doubly stochastic.

If R has a spectral expansion in eigenvectors (i.e., no Jordan form is needed), $J(R)=0$ if and only if

$$p_k(x)=A_k(x)p_0(x)\quad \text{for all } k \text{ and } x \tag{3}$$

(recall, no summation over x). Under the same assumption, $J(R)=0$ if and only if $J(R^n)=0$. These assertions are a consequence of the spectral expansion of $J(R^n)$. This can be obtained from the spectral expansion of R (hence of R^n) combined with Eq. (2), and takes the form [20]

$$J(R^n)_{xy}=\sum_{k\geqslant 1}\lambda_k^n[p_k(x)A_k(y)p_0(y)-p_k(y)A_k(x)p_0(x)], \tag{4}$$

from which our assertion is evident.

In Ref. [1] we proved that $J(R)=0$ if and only if for any closed path in X, $\gamma\equiv(x_1,x_2,\ldots,x_n,x_1)$, one has

$$R_{x_1x_2}R_{x_2x_3},\ldots,R_{x_nx_1}=R_{x_1x_n}R_{x_nx_{n-1}},\ldots,R_{x_2x_1}. \tag{5}$$

This theorem has the virtue that the existence of currents can be checked without knowing the stationary state, p_0.

Remark. The power of the requirement (5) can be seen in a quick demonstration that a system in contact with two reservoirs must have currents [21]. The context of this assertion is that X is a product of other spaces, which for convenience we write $X=\Pi_{k\in V}C_k$. V can be thought of as a coordinate space, with C_k a fiber at $k\in V$. X is thus a fiber space and a full specification of $x\in X$ corresponds to giving a value on each space in the product. Aside from the reservoirs, there is a dynamics R_0 that satisfies detailed balance, allowing transitions between different states of X. Introduction of reservoirs is achieved by appending to this dynamics the possibility of other transitions in two of the spaces in the product.

One could think of this as a bar of metal in contact with different temperatures at its ends. Imagine the bar partitioned into v little compartments going from one end to the other. Energy can pass symmetrically from compartment to neighboring compartment. The possible states of a single compartment form the fiber C_k, with k labeling the compartments in a one-dimensional fashion. We suppose there is a nondegenerate energy $e(c)$ associated with each state of a fiber. Energy conservation is satisfied, except for reservoir-induced transitions. Thus if $c_k \to c_k'$, then for either $k+1$ or $k-1$ there must be a transition with an energy change compensating for what happened in C_k. The exceptions occur at the ends of the bar. Suppose C_1 is in contact with a "cold" reservoir at temperature T_c. This means that energy nonconserving transitions are allowed *between* its states. Were this compartment cut off from the rest of the bar the distribution of its states would be $\Pr(c) \sim \exp[-e(c)/T_c]$, where Boltzmann's constant is taken to be unity. Hooking this compartment up to the rest of the bar creates an overall matrix of transition probabilities, call it R, with a stationary distribution $p_0(x) \sim \exp[-E(x)/T_c]$, where $x=(c_1,c_2,\ldots,c_v)$, [or $x=(c_1(x),c_2(x),\ldots,c_v(x))$] and $E(x)=\Sigma_k e(c_k)$. This R (together with its p_0) satisfies detailed balance.

Now we want to show that attaching another reservoir at temperature T_h ($>T_c$) to the other end of the bar forces there to be a current. Call this compartment C_v. First imagine that we *instead* attach the cold reservoir (temperature T_c) to it. (Previously, states within C_v could only change by a long series of transitions going back to C_1.) Nevertheless, we still have detailed balance and the equilibrium Boltzmann distribution $p_0(x) \sim \exp[-E(x)/T_c]$ is the same. This means the following. Take a path in X that begins with some $x_0 =(c_1,c_2,\ldots,c_v)$ and let there be a transition (due to the reservoir) $c_1 \to c_1'$, lowering the energy. Continue the path with nearest neighbor transitions along the bar, e.g., $(c_1',c_2,c_3,\ldots,c_v) \to (c_1,c_2',c_3,\ldots,c_v)$ with $e(c_1')+e(c_2) =e(c_1)+e(c_2')$ until we reach the other end. (In this example the fibers are all the same and the transitions are exchanges.) Now raise the last fiber state, using the currently attached T_c reservoir. This is a closed path in X. If we were to write down the probabilities of this and of the inverse transition [as in Eq. (5)], they would be equal (because this is a detailed balance state).

Here is the punch line: the only change in the above story if the hot reservoir is operating in C_v is that the temperature-T_c transition probability for that one transition is replaced by the temperature-T_h transition probability. Saying that this is at a different temperature means that the ratio of up-to-down transition probabilities is different. So the product is different and there must be a current, by the aforementioned theorem.

We confess that this was a long exposition for a proof that we said was quick. However, most of that exposition was concerned with defining the system and notation (which we will use later). The actual demonstration consisted of defining the path and observing that changing it destroys the detailed balance equality of the path product.

III. STRENGTHENING A BOND INCREASES THE CURRENT

In this section the original matrix of transition probabilities is designated $\bar{R}$. The stationary state of $\bar{R}$ is $\bar{p}_0$. One of its

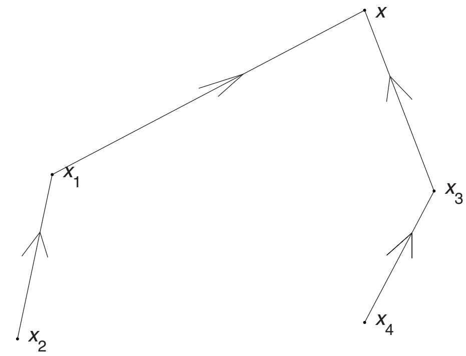

FIG. 1. Graph for the example.

matrix elements will be increased (with appropriate adjustment on the diagonal to conserve probability), and we will show that the new matrix, designated R, has strictly more current than did $\bar{R}$.

There is a graph-theoretical way of producing p_0, going back to Kirchoff and presented in [9,1]. If $x \in X$, call $\mathcal{T}(x)$ the set of all spanning trees with root x, oriented towards x. If $T \in \mathcal{T}(x)$, call

$$\bar{R}_T = \text{product of } \bar{R}_{uv} \text{ over edges in } T.$$

Then

$$\bar{p}_0(x) = \frac{\sum_{T\in\mathcal{T}(x)} \bar{R}_T}{\bar{Z}}, \quad \text{with } \bar{Z} \equiv \sum_x \sum_{T\in\mathcal{T}(x)} \bar{R}_T. \tag{6}$$

$\bar{Z}$ is a kind of partition function.

Example. See Fig. 1. $\bar{R}_T = \bar{R}_{xx_1}\bar{R}_{xx_3}\bar{R}_{x_1x_2}\bar{R}_{x_3x_4}$.

To carry out this program, we first evaluate the derivatives of J, using formula (6).

A. Variation of currents

1. First derivative: $\partial J_{x_0y_0}/\partial R_{x_0y_0}$

Calculate this derivative directly. Start with

$$J_{x_0y_0} = \frac{1}{Z}\left[R_{x_0y_0} \sum_{\substack{T'\in\mathcal{T}(y_0)\\ (y_0,x_0)\notin T'}} R_{T'} - R_{y_0x_0} \sum_{\substack{T\in\mathcal{T}(x_0)\\ (x_0,y_0)\notin T}} R_T \right]. \tag{7}$$

Take the derivative with respect to $R_{x_0y_0}$.

$$\frac{\partial J_{x_0y_0}}{\partial R_{x_0y_0}} = \frac{-1}{Z^2}\frac{\partial Z}{\partial R_{x_0y_0}}\left[R_{x_0y_0} \sum_{\substack{T'\in\mathcal{T}(y_0)\\ (y_0,x_0)\notin T'}} R_{T'} - R_{y_0x_0} \sum_{\substack{T\in\mathcal{T}(x_0)\\ (x_0,y_0)\notin T}} R_T \right] + \frac{1}{Z} \sum_{\substack{T'\in\mathcal{T}(y_0)\\ (y_0,x_0)\notin T'}} R_{T'}. \tag{8}$$

Now

$$\frac{\partial Z}{\partial R_{x_0y_0}} = \sum_{\substack{\text{trees } T\\(x_0y_0)\in T}} \frac{R_T}{R_{x_0y_0}}, \tag{9}$$

and

$$\frac{\partial J_{x_0y_0}}{\partial R_{x_0y_0}} = \frac{1}{Z^2}\left(\sum_{\substack{T'\in\mathcal{T}(y_0)\\(y_0,x_0)\notin T'}} R_{T'}\right)\left(Z - \sum_{\substack{\text{trees } T\\(x_0y_0)\in T}} \frac{R_T}{R_{x_0y_0}}\right) + \frac{1}{Z^2}\frac{\partial Z}{\partial R_{x_0y_0}} R_{y_0x_0}\left(\sum_{\substack{T\in\mathcal{T}(y_0)\\(x_0,y_0)\notin T}} R_T\right). \tag{10}$$

Evidently, both terms are positive because $\frac{\partial J_{x_0y_0}}{\partial R_{x_0y_0}} > 0$ and

$$Z - \sum_{\substack{\text{trees } T\\(x_0y_0)\in T}} \frac{R_T}{R_{x_0y_0}} = \sum_{\substack{\text{trees } T\\(x_0y_0)\notin T}} \frac{R_T}{R_{x_0y_0}}. \tag{11}$$

Thus we conclude

$$\frac{\partial J_{x_0y_0}}{\partial R_{x_0y_0}} > 0. \tag{12}$$

2. *Second derivative*

We start from Eqs. (10) and (11). Note that a tree $T' \in \mathcal{T}(y_0)$ (with root y_0) cannot contain the bond (x_0y_0) (*no* path can have y_0 as a source), and in Eq. (11), $R_{x_0y_0}$ does not appear. Thus, by taking the derivative of Eq. (10),

$$\frac{\partial^2 J_{x_0y_0}}{\partial R_{x_0y_0}{}^2} = -\frac{2}{Z^3}\frac{\partial Z}{\partial R_{x_0y_0}}\left(\sum_{\substack{T'\in\mathcal{T}(y_0)\\(y_0,x_0)\notin T'}} R_{T'}\right)\left(\sum_{\substack{\text{trees } T\\(x_0y_0)\notin T}} R_T\right) - \frac{2}{Z^3}\left(\frac{\partial Z}{\partial R_{x_0y_0}}\right)^2 R_{y_0x_0}\left(\sum_{\substack{\text{trees } T\\(x_0y_0)\notin T}} R_T\right) = -\frac{2}{Z^3}\frac{\partial Z}{\partial R_{x_0y_0}}\left[\left(\sum_{\substack{T'\in\mathcal{T}(y_0)\\(y_0,x_0)\notin T'}} R_{T'}\right)\left(\sum_{\substack{\text{trees } T\\(x_0y_0)\notin T}} R_T\right) + \frac{\partial Z}{\partial R_{x_0y_0}} R_{y_0x_0}\sum_{\substack{\text{trees } T\\(x_0y_0)\notin T}} R_T\right]. \tag{13}$$

Since this is clearly negative we have

$$\frac{\partial^2 J_{x_0y_0}}{\partial R_{x_0y_0}{}^2} < 0. \tag{14}$$

From Eq. (13), because the bracket cannot contain $R_{x_0y_0}$, one sees that only $1/Z^3$ contains $R_{x_0y_0}$, and its derivative does not contain $R_{x_0y_0}$. Thus

$$(-1)^k \frac{\partial^k J_{x_0y_0}}{\partial R_{x_0y_0}{}^k} < 0. \tag{15}$$

B. Variation of $J_{y_0z_0}$

Let z_0 be a point from which current flows *into* y_0, where $R_{x_0y_0}$ is the matrix element that has been increased.

We consider the derivative of $J_{y_0z_0}$ with respect to $R_{x_0y_0}$. One has

$$J_{y_0z_0} = \frac{1}{Z}\left(R_{y_0z_0}\sum_{T\in\mathcal{T}(z_0)} R_T - R_{z_0y_0}\sum_{T\in\mathcal{T}(y_0)} R_T\right). \tag{16}$$

Note that a tree $T \in \mathcal{T}(y_0)$ with root y_0 oriented toward y_0, cannot contain the bond from y_0 to x_0, so that R_T cannot contain $R_{x_0y_0}$. Then by taking the derivative of $J_{y_0z_0}$ with respect to $R_{x_0y_0}$, one gets

$$\frac{\partial J_{y_0z_0}}{\partial R_{x_0y_0}} = -\frac{1}{Z}\frac{\partial Z}{\partial R_{x_0y_0}} J_{y_0z_0} + \frac{1}{Z} R_{y_0z_0} \sum_{\substack{T\in\mathcal{T}(z_0)\\(x_0,y_0)\in T}} \frac{R_T}{R_{x_0y_0}}, \tag{17}$$

and

$$\frac{\partial Z}{\partial R_{x_0y_0}} = \sum_{\substack{\text{all } T\\(x_0,y_0)\in T}} \frac{R_T}{R_{x_0y_0}}. \tag{18}$$

From this formula we deduce that if $\bar{J}_{y_0z_0} \le 0$, then $\frac{\partial J_{y_0z_0}}{\partial R_{x_0y_0}} > 0$.

C. Variation of other currents

From Kirchoff's law

$$\sum_x J_{xy} = 0. \tag{19}$$

We use this to deduce the variation of other currents in X, not only $J_{y_0x_0}$.

Indeed, if we assume that $J_{x_0y_0}$ increases, there must be a state x_1 such that $J_{x_1x_0}$ also increases in order to maintain Kirchoff's law at the node x_0. From this we deduce that there is a whole path $(x_0,x_1,\ldots,x_N)$ such that $J_{x_1x_0},\ldots,J_{x_Nx_{N-1}}$ all increase. In the same way, we see that there is a path $(y_0,y_1,\ldots,y_N)$ such that the currents $J_{y_1y_0},\ldots,J_{y_Ny_{N-1}}$ increase.

IV. FINDING R, GIVEN p_0 AND THE J'S: TRANSITION PROBABILITIES GIVEN THE STATIONARY DISTRIBUTION AND CURRENTS

This section and the next are devoted to an inverse problem. Given p_0 and a collection of J's, what can be said of the R that generated them? These "J's" are presumably those generated by R, R^2, etc.

We first establish properties of currents and auxiliary matrices built from some particular stochastic matrix R.

For given R, define

$$J(R)^+_{xy} = \frac{1}{2}[J(R)_{xy} + |J(R)_{xy}|] = \text{positively flowing current}. \tag{20}$$

Further define

$$\tilde{J}^+_{xy} = \begin{cases} J^+_{xy} & \text{for } x \neq y \\ -\sum_{z\neq x} J^+_{zx} & \text{for } x = y. \end{cases} \tag{21}$$

Then for any x,

$$\sum_y \tilde{J}^+_{yx} = 0. \tag{22}$$

Provided that $|\tilde{J}^+_{xx}| \leqslant 1$, it follows that $\mathbf{1}+\tilde{J}^+_{xy}$ is a stochastic matrix; it will be called $\tilde{R}$. The fact that the condition $|\tilde{J}^+_{xx}| \leqslant 1$ is satisfied follows from

$$0 \leqslant \sum_{z\neq x} J^+_{zx} \leqslant \sum_{\substack{z\neq x \\ \text{with } J_{zx}\geqslant 0}} R_{zx}p_0(x) \leqslant \sum_{z\neq x} R_{zx}p_0(x) \leqslant p_0(x). \tag{23}$$

That is, since the J's we have given actually arise from some R, they will satisfy this inequality.

Lemma. $\tilde{R}_{xy} \equiv \mathbf{1}+\tilde{J}^+_{xy}$ is a doubly stochastic matrix with stationary state $p_0^+(x) \equiv 1/N$ for any x (recall, $N=|X|$). Moreover, if $x\neq y$, at least one of $\tilde{J}^+_{xy}$ or $\tilde{J}^+_{yx}$ is 0 (so it is *completely irreversible*, in the terminology of Sec. II).

Proof. We already know that $\mathbf{1}+\tilde{J}^+_{xy}$ is stochastic. All we need show is the transposed condition

$$\sum_y \tilde{J}^+_{xy} = 0. \tag{24}$$

Indeed,

$$\sum_y \tilde{J}^+_{xy} = \sum_{y\neq x} J^+_{xy} - \sum_{z\neq x} J^+_{zx}. \tag{25}$$

But $J^+_{xy}=-J_{yx}$ if $J_{yx}\leqslant 0$ and $J^+_{zx}=J_{zx}$ if $J_{zx}\geqslant 0$ so that

$$\sum_y \tilde{J}^+_{xy} = -\left[\sum_{\{y|J_{yx}\leqslant 0\}} J_{yx} + \sum_{\{z|J_{zx}\geqslant 0\}} J_{zx}\right] = -\sum_y J_{yx} = 0. \tag{26}$$

In the first equality the sum over J^+_{xy} in Eq. (25) has been replaced by its transpose, while J^+_{zx} has been left alone. The last equality follows because the current is conserved at each node x.

Corollary. Let $\mathcal{J}^+_{xy}$ be the current obtained from $\mathbf{1}+\tilde{J}^+$ by the same method as in Eq. (21), so that $\mathcal{J}^+$ could be called $J^+(\tilde{R})$. Then

$$\mathcal{J}^+ = \frac{1}{N}\tilde{J}^+. \tag{27}$$

Proof. Indeed the normalized stationary state of $\tilde{J}^+$ is $p_0^+(x)=\frac{1}{N}$, so that obviously for $x\neq y$, $\mathcal{J}^+_{xy}=\tilde{J}^+_{xy}p_0^+(y)=\frac{1}{N}\tilde{J}^+_{xy}$, and for $x=y$, $\mathcal{J}^+_{xx}=-\Sigma_{z\neq x}\mathcal{J}^+_{zx}=-\frac{1}{N}\Sigma_{z\neq x}\tilde{J}^+_{zx}=\frac{1}{N}\tilde{J}^+_{xx}$.

Remark. This corollary is valid for any stochastic matrix R that is doubly stochastic and completely irreversible.

Corollary. Let K be such that $\mathbf{1}+K$ is doubly stochastic and completely irreversible. Then K is $N\tilde{J}(K^+)$.

A. Extracting R from J^+ and p_0

We return to our inverse problem.

Suppose there is a matrix $\tilde{J}^+$ such that (i) $\tilde{J}^+_{xy}\geqslant 0$ and $\tilde{J}^+_{xy} \mid \tilde{J}^+_{yx}=0$ for $x\neq y$; (ii) $\tilde{J}^+_{xx}=-\Sigma_{z\neq x}\tilde{J}^+_{zx}$; (iii) $\Sigma_{x\neq z}\tilde{J}^+_{zx}=\Sigma_{y\neq z}\tilde{J}^+_{yz}$ (this requirement is imposed in order that the underlying current satisfies Kirchoff's law); and (iv) $\tilde{J}^+_{xy}\leqslant 1$ for $x\neq y$ and $|\tilde{J}^+_{xx}|\leqslant 1$. Then $\mathbf{1}+\tilde{J}^+$ is doubly stochastic, as shown above.

We fix a probability distribution p_0 on X, with $p_0(x)>0$. We want to find a stochastic matrix R such that

$$Rp_0 = p_0, \tag{28}$$

$$\tilde{J}^+_{xy} = R_{xy}p_0(y) - R_{yx}p_0(x) \quad \text{for } x\neq y, \quad \text{when this quantity is positive}. \tag{29}$$

Before doing so, however, we note that besides conditions (i)–(iv), there is an additional requirement on the quantities J and p_0 that is necessary in order that the problem have a solution.

Suppose that there is some stochastic R for which Eqs. (28) and (29) are satisfied. Then for that R and for any y

$$\sum_{x\neq y}\tilde{J}^+_{xy} = \left(\sum_{x\neq y} R_{xy}\right)p_0(y) - \left(\sum_{x\neq y} R_{yx}\right)p_0(x) \leqslant \left(\sum_{x\neq y} R_{xy}\right)p_0(y). \tag{30}$$

Therefore for any stochastic R and any $y\in X$,

$$\frac{\sum_{x\neq y}\tilde{J}^+_{xy}}{p_0(y)} \leqslant \left(\sum_{x\neq y} R_{xy}\right) \leqslant 1. \tag{31}$$

This yields a necessary condition for the existence of a solution to Eqs. (28) and (29),

$$\frac{\sum_{x\neq y}\tilde{J}^+_{xy}}{p_0(y)} \leqslant 1. \tag{32}$$

Now Eqs. (28) and (29) are a system of linear equations for R (given $\tilde{J}^+_{xy}$ and p_0), so that the general solution is the sum of a particular solution of Eqs. (28) and (29) and of a general solution of the homogeneous system associated with that same pair of equations. The homogeneous solution S thus satisfies

$$Sp_0 = 0, \tag{33}$$

$$S_{xy}p_0(y) - S_{yx}p_0(x) = 0 \quad (x\neq y). \tag{34}$$

B. Particular solution of Eqs. (28) and (29)

We assume that Eq. (32) is satisfied. The particular solution is defined by

$$R_{xy}^{(0)} = \frac{\tilde{J}_{xy}^{+}}{p_0(y)} \quad \text{for } x \neq y, \tag{35}$$

$$R_{xx}^{(0)} = 1 - \sum_{y\neq x} R_{yx}^{(0)}. \tag{36}$$

From Eqs. (31) and (32) we see that $0 \leqslant R_{xy}^{(0)} \leqslant 1$ for all x,y and that $R^{(0)}$ is a stochastic matrix. Then using Eqs. (35) and (36),

$$\sum_y R_{xy}^{(0)} p_0(y) = \sum_{y\neq x} R_{xy}^{(0)} p_0(y) + \left(1 - \sum_{z\neq x} R_{zx}^{(0)}\right) p_0(x)$$
$$= p_0(x) + \sum_{y\neq x} \tilde{J}_{xy}^{+} - \sum_{y\neq x} \tilde{J}_{zx}^{+}. \tag{37}$$

Recall that $\tilde{J}^{+}$ is such that $\mathbf{1}+\tilde{J}^{+}$ is doubly stochastic, which means precisely that

$$\sum_{y\neq x} \tilde{J}_{xy}^{+} = \sum_{y\neq x} \tilde{J}_{zx}^{+}, \tag{38}$$

so that

$$R^{(0)} p_0 = p_0. \tag{39}$$

Finally, the current associated with $R^{(0)}$ is

$$J_{xy} = R_{xy}^{(0)} p_0(y) - R_{yx}^{(0)} p_0(x). \tag{40}$$

For $x \neq y$, either $R_{xy}^{(0)}$ or $R_{yx}^{(0)}$ is zero. If $R_{xy}^{(0)} \neq 0$, then $R_{xy}^{(0)} = \tilde{J}_{xy}^{+}/p_0(y)$, and $R_{yx}^{(0)}=0$, so that

$$J_{xy}^{+} = \tilde{J}_{xy}^{+}, \tag{41}$$

and similarly for the other case.

C. General solution of the homogeneous system, Eqs. (33) and (34)

There are many matrices S satisfying Eq. (34). The general form is $S_{xy}=K_{xy}\sqrt{p_0(x)/p_0(y)}$, where K is any symmetric matrix. Take any one of these (for $x \neq y$) and set

$$S_{xx} = -\sum_{y\neq x} S_{yx}. \tag{42}$$

Clearly S satisfies Eq. (33). Now we define

$$R = R^{(0)} + S. \tag{43}$$

Note that S should be chosen small enough so that all matrix elements of R fall between zero and one. Then R is stochastic, has p_0 as its stationary state, and has the prescribed J^{+} as its current.

V. HIGHER ORDER CURRENTS IN THE RECOVERY OF THE MATRIX OF TRANSITION PROBABILITIES

We next explore information available through *higher order* currents. It is interesting that a single measurement of current, say after one time step, still can omit a great deal of information about the underlying transition matrix. This is because one has only observed *net* flow. The fact that further information about R can come from $J^{(2)}$, etc., makes this point at the physical level.

A. Recursion relation

We will show that

$$J_{xy}^{(n)} = (RJ^{(n-1)})_{xy} - (R^{n-1}J)_{xy}, \tag{44}$$

and

$$J^{(n)} = RJ^{(n-1)} + J(R^T)^{n-1}, \tag{45}$$

where (R^T) is the transpose of the matrix R [see Eq. (2) for notation].

Proof.

$$J_{xy}^{(n)} = \sum_z R_{xz}(R^{n-1})_{zy} p_0(y) - \sum_z (R^{n-1})_{yz} R_{zx} p_0(x)$$
$$= \sum_z R_{xz} J_{zy}^{(n-1)} + \sum_z R_{xz}(R^{n-1})_{yz} p_0(z)$$
$$- \sum_z (R^{n-1})_{yz} R_{zx} p_0(x). \tag{46}$$

For assertion (45) use the fact that J is skew symmetric.

Case J=0

From Eq. (44) it follows that if $J=0$, then $J^{(n)}=0$ for all n.

B. Relation of $J^{(n)}$ and the characteristic polynomial of R

Define the characteristic polynomial of R:

$$P_R(\lambda) = \det(\lambda I - R) \equiv \lambda^N + a_1\lambda^{N-1} + \cdots + a_N. \tag{47}$$

Equation (47) holds for R (replacing λ) and, in particular, for any specific x,y. Right multiplying by $p_0(y)$ implies

$$R_{xy}^N p_0(y) + a_1 R_{xy}^{N-1} p_0(y) + \cdots + a_N \delta_{xy} p_0(y) = 0. \tag{48}$$

Exchanging x and y and subtracting implies

$$0 = J_{xy}^{(N)} + a_1 J_{xy}^{(N-1)} + \cdots + a_{N-1} J_{xy}^{(1)}. \tag{49}$$

In the same way one can multiply the characteristic equation by any power r of R, to obtain

$$J^{(N+r)} + a_1 J^{(N+r-1)} + \cdots + a_{N-1} J^{(r+1)} + a_N J^{(r)} = 0 \tag{50}$$

(with $J^{(0)} \equiv 0$).

A number of facts follow from this relation.

(1) For each r, $r=-1,0,1,\ldots,N-2$, and for any collection of pairs (x_r,y_r)

$$a_1 J_{x_r y_r}^{(N+r)} + a_2 J_{x_r y_r}^{(N+r-1)} + \cdots + a_{N-1} J_{x_r y_r}^{(r+2)} + a_N J_{x_r y_r}^{(r+1)} = -J_{x_r y_r}^{(N+r+1)}. \tag{51}$$

We take the perspective that the $J^{(n)}$'s are given, so that this is a system of N equations for the N unknowns $a_1,a_2,\ldots,a_N$. If there is a collection of points (x_r,y_r), for $-1 \leqslant r \leqslant N-2$, for which the determinant of this system is not zero, then one can obtain the a's. These are symmetric functions of the eigenvalues of R.

(2) It further follows from Eq. (50) that for $r \geqslant 2N$, all $J^{(k)}$ for $k \geqslant 2N$ are known recursively.

(3) If one knows $a_1, \ldots, a_N$ and $J^{(1)}, \ldots, J^{(N-1)}$, then all $J^{(k)}$ are known for $k \geqslant N$.

Remark. If $1 > |\lambda_1| > |\lambda_2| > \ldots > |\lambda_{N-1}|$, one could also prove this result in the following manner. Use the spectral expansion of R,

$$J_{xy}^{(\ell)} = \sum_{k=1}^{N-1} \lambda_k^{\ell} [p_k(x) A_k(y) p_0(y) - p_k(y) A_k(x) p_0(y)]. \quad (52)$$

If we assume that for all k there exist (x,y) with $p_k(x)A_k(y)p_0(y) - p_k(y)A_k(x)p_0(y) \neq 0$, one can deduce the eigenvalues $\lambda_1, \lambda_2, \ldots, \lambda_{N-1}$. Indeed, for $\ell \to \infty$,

$$J_{xy}^{(\ell)} \sim \lambda_1^{\ell} [p_1(x) A_1(y) p_0(y) - p_1(y) A_1(x) p_0(y)]. \quad (53)$$

Choosing x and y such that the coefficient is nonzero,

$$\lambda_1 = \lim_{\ell \to \infty} \frac{J_{xy}^{(\ell+1)}}{J_{xy}^{(\ell)}}. \quad (54)$$

Next subtract the λ_1 term to obtain λ_2, etc.

Remark. The set of stochastic matrices with given $J^{(k)}$ is an isospectral set. N.B. This assumes that R is generic.

Remark. It can happen that for generic R one gets complex conjugate eigenvalue pairs. The above procedure then requires a slight modification, but the essential conclusion stands. As above, the limiting process can give eigenvalue magnitudes. Then one looks at ratios of J's. This requires that no more than two magnitudes are equal (which is generic). It should also be noted that we are focusing on in-principle recovery of information, since the calculational precision required here is daunting.

C. Determination of R using the $J^{(n)}$

We suppose that we know the spectrum of R, perhaps using the first $(2N-1)$ $J^{(n)}$'s, or perhaps in some other way. It is also assumed that the stationary state p_0 is known. We now show that with the first $(N-1)$ $J^{(n)}$'s we can recover all of R—again assuming that R is generic.

We rewrite the spectral expansion of J, Eq. (4), as

$$\sum_{k=1}^{N-1} \lambda_k^n U_{xy}^{(k)} = J_{xy}^{(n)}, \quad 1 \leqslant n < N-1, \quad (55)$$

where

$$U_{xy}^{(k)} \equiv p_k(x) A_k(y) p_0(y) - p_k(y) A_k(x) p_0(x). \quad (56)$$

For given x,y, Eq. (55) is a linear system of $N-1$ equations for the $N-1$ unknowns $U_{xy}^{(k)}$, with coefficients λ_k^n. For distinct λ's (the generic hypothesis), one can solve Eq. (55) (the determinant is nonzero) for the $U_{xy}^{(k)}$'s in terms of the $J_{xy}^{(n)}$ and the λ_k.

Next we wish to extract the p's and A's from the U's. Generically we expect that there are (at least) two y's such that the equations $U_{xy_\ell}^{(k)} = p_k(x) A_k(y_\ell) p_0(y) - p_k(y_\ell) A_k(x) p_0(x)$, $\ell = 1,2$, can be solved for the functions $p_k(x)$ and $A_k(x)p_0(x)$, $k>0$. Now, knowing p_0 and the eigenvalues, one can reconstruct R.

D. Case of doubly stochastic matrices

We now assume that R is doubly stochastic; this implies $p_0 = 1/N$. Then

$$J = (R - R^T)/N \quad \text{and} \quad J^{(2)} = [R^2 - (R^T)^2]/N. \quad (57)$$

Let $W \equiv \frac{1}{2}(R + R^T) - 1$, so that W is symmetric, non-negative off the diagonal, and has both rows and columns summing to zero. Then by direct calculation

$$J^{(2)} = \{1 + W, J^{(1)}\}, \quad (58)$$

where curly brackets indicate the anticommutator.

We specialize to the case $N=3$ to see a specific example of the use of higher currents to find R. Suppose that we know $J^{(k)}$ for $k=1,2,3,4$. The assumption that R is doubly stochastic simplifies the discussion, inasmuch as one immediately knows p_0.

For three-state systems there is (up to factors) only one skew symmetric matrix that satisfies Kirchoff's law. This is

$$\sigma \equiv \begin{pmatrix} 0 & 1 & -1 \\ -1 & 0 & 1 \\ 1 & -1 & 0 \end{pmatrix}. \quad (59)$$

The most general form for a 3-by-3 doubly stochastic matrix is thus

$$R = \begin{pmatrix} 1-a-b & a & b \\ a & 1-a-c & c \\ b & c & 1-b-c \end{pmatrix} + \alpha\sigma \equiv 1 + W + \alpha\sigma, \quad (60)$$

so that we wish to determine the four parameters, a, b, c, and α. The given information is $J^{(k)} \equiv j_k \sigma$, for $k=1,\ldots,4$. It is immediate that $\alpha = 3j_1$ (the "3" is N). Computing

$$\{1 + W, J^{(1)}\} = 2j_1(1 - a - b - c)\sigma \quad (61)$$

yields one constraint on a, b, and c, provided $j_1 \neq 0$. This provides Tr W, which is a_1, a coefficient in the characteristic polynomial. Clearly there remains missing information. We next turn to determining the other coefficients a_k. From Eq. (50) one obtains

$$j_3 = -(a_1 j_2 + a_2 j_1), \quad (62)$$

$$j_4 = -(a_1 j_3 + a_2 j_2 + a_3 j_1). \quad (63)$$

This determines the spectrum of R. To go directly to a, b and c we note that the coefficients a_k are the three fundamental symmetric functions of the elements of R. a_1 is the trace, which we already have. The other two a's are the determinant and the sum of the minors of the diagonal elements. This gives equations for a, b, and c, which is as good as is possible, since Eq. (50) as well as Eq. (58) are insensitive to a permutation of the state labels.

In the next example we look at a *completely irreversible* doubly stochastic matrix and show that it is fully determined by its currents in the 3-by-3 case. We suppose there is some matrix $\bar{R}$ such that

$$\bar{R}_{xy}\bar{R}_{yx}=0 \quad \text{for all } x\neq y. \tag{64}$$

Since $\bar{R}$ is doubly stochastic, its associated p_0 is $1/N$. Then

$$J(R)_{xy}=\begin{cases}\bar{R}_{xy}/N & \text{if } \bar{R}_{xy}\neq 0\\ -\bar{R}_{yx}/N & \text{if } \bar{R}_{yx}\neq 0.\end{cases} \tag{65}$$

We now seek a doubly stochastic R with the same currents as $\bar{R}$, so that it is convenient to write

$$R=\bar{R}+S, \tag{66}$$

where S is necessarily symmetric and satisfies Kirchoff's law. We will show that, given $J^{(1)}$ and $J^{(2)}$, S must be zero.

It is immediate that $\{J^{(1)},S\}=0$. Moreover, S must have the form

$$S=\begin{pmatrix}-a-b & a & b\\ a & -a-c & c\\ b & c & -b-c\end{pmatrix}, \tag{67}$$

so that by the preceding section $\{J^{(1)},S\}=2(a+b+c)J^{(1)}$. Since $J^{(1)}$ is not zero, we must have $a+b+c=0$. We also know that the nondiagonal elements of S must be nonnegative, because of Eq. (66). Therefore $S=0$.

We note without proof that for any fully reversible doubly stochastic matrix the first two currents determine it uniquely, within the class of doubly stochastic matrices.

VI. COARSE GRAINING AND TIME SCALES

In previous sections we examined the possibility of recovering an underlying matrix of transition probabilities from currents. The motivation is that in examining a system it is generally the currents that one observes, rather than the individual transitions. We found that a study of the lowest order current, that associated with the transition matrix R (rather than higher powers of it), what we call $J^{(1)}$, does not provide full information; it is also useful to examine currents when two or three or more times steps have taken place.

At a mathematical level this makes sense: currents only measure net transfer. Transfers—not *net* transfers—that are invisible on a single time step may change the currents when several time steps are involved. But at a physical level it implies that "Δt," the time interval for the transitions described by R, is significant. For most of this paper we have taken Δt to equal 1, thereby downgrading its importance. However, there is real physical meaning to the size of this interval. In particular, when one seeks to derive the master equation, it is known that one cannot take Δt too small. A short statement of the physical significance is given in Ref. [22]. In particular, to justify the smearing within a coarse grain that is implicit in the use of the master equation it is necessary that Δt be long enough for the grain to be more or less uniformly occupied under the underlying dynamics, whether classical or quantum, within that time interval. So Δt is a relaxation time. Obviously the coarse grains themselves play a role in determining this time scale.

It follows that in trying to learn the internal dynamics of a system it is appropriate, if possible, to measure its currents for many different time intervals.

VII. SUBSTANCE FLOW

In many disciplines one illustrates the behavior of a complex system by showing the flow of various substances. These "substances" can be resources (e.g., energy, negentropy, water), materials (e.g., water, CO_2), or more abstract notions (e.g., money). The currents we have described until now are usually not the currents of these substances, but rather currents of probability, from which the usual flows can be constructed, as we now show. Note, however, that sometimes it is helpful to construct a model "R" directly from the usual flows. For example, in studying the flows of nutrients in ecology [11–13] it may be useful to take those flows as the matrix R itself. The interpretation is different, but many of the techniques we have introduced (e.g., the observable representation [6–8]) can be worth implementing. We took a similar approach to the use of R in finding communities in Ref. [5]. However, in the present section, we maintain the interpretation of the present paper, namely, that R is a matrix of transition probabilities.

The flows take place between what we will call "components." These may be physical locations along an iron bar, as in heat flow, or chemical species, etc. The space X has the structure of a product of these components: $X=C_1C_2\ldots$ Each $x\in X$ has the form $x=(c_1,c_2,\ldots)$, with c_k describing the state of component k. We sometimes write c_k as $c_k(x)$.

The "substances" that do the flowing are functions on the C's and we look at their sums. Let F refer to a particular substance and let $f_k(c_k)$ be the amount of that substance associated with component k when it is in the state c_k. The total amount of this substance when the (entire) system is in state x is

$$F(x)=\sum_k f_k(c_k). \tag{68}$$

To make this concrete, consider a model of heat transfer: a string of boxes stretching from a reservoir at temperature T_h (hot) to one at temperature T_c (cold). Each box has K possible states; state k, $0\leqslant k\leqslant K-1$ has energy $f(k)$. (In this case all components are isomorphic and the functions f_k are the same, so there is a simplification of notation.) Between the boxes we allow exchange of energy; randomly, energy can flow between adjacent boxes. The boxes at the ends have an additional random process: they can go up or down in energy, in such a way that—if disconnected from the other boxes—they would reach the Boltzmann distribution $\sim\exp[-f(k)/T_u]$, with $u=c,h$. In this case the total energy in the system at any moment is the function $F(x)$ given above. Because of the reservoirs at the ends, this need not be conserved. However, once the system has reached a steady state, it will be conserved on the average. (In Sec. II we also discussed this model.)

As in the example just given, it is worth distinguishing possible kinds of transitions. The dynamics can conserve a substance, or it may not, or it may only do so in the stationary state. We focus on a particular transition $y \to x$.

(1) A material is microconserved if $[R_{x,y} \neq 0] \Rightarrow [F(x) = F(y)]$. The *total amount of the substance remains the same in this transition*).

(2) A material is de facto conserved if, despite the fact that $F(x) \neq F(y)$ (with $R_{x,y} \neq 0$), nevertheless, $J_{x,y}=0$. The *total amount of the substance can fluctuate, but there is no net transfer in the stationary state*. Away from the stationary state there might be changes in total substance amount.

Furthermore, it may also be useful to break R into separate processes (see [3]). Some microconserve, some do not. In our heat conduction example, there was a breakdown in microconservation only at the reservoirs; the "internal" energy transfer process is conservative.

Consider a transition under an element of R that microconserves. For a particular pair x and y, for which $J^+_{x,y} > 0$, we can have a transfer of the substance F from component 1 to component 2 as follows: before the transition, component 1 had $f_1(c_1(y))$ of substance F; after, component 1 has $f_1(c_1(x))$ of substance F, where $c_k(x)$ means the state of the kth component in the global state x. Then the flow *from 1 to 2* due to this one nonzero current is

$$J^+_{x,y}[f_1(c_1(x)) - f_1(c_1(y))]. \tag{69}$$

We could have used $f_2(c_2(y)) - f_2(c_2(x))$, which by conservation has the same value. For total 1-to-2 flow, add this quantity over all transitions (with $J^+ > 0$) from 1 to 2. That is, let $L(F,2,1) \equiv$ flow of F from 1 to 2. Then

$$L(F,2,1) = \sum_{x,y} J^+_{xy}[f_1(c_1(x)) - f_1(c_1(y))], \tag{70}$$

where the transition $y \to x$ is assumed to be such that $c_k(x) = c_k(y)$ for all k except $k=1$ and $k=2$.

One can then verify that in the iron bar example there are the following features: (1) temperature decreases linearly along the bar, from T_h to T_c; and (2) flow of heat is constant from compartment to compartment.

Equation (70) can yield far more interesting structure than it does in the iron bar case. For complex systems one can expect the diagrams that generations of biologists and many others have found useful.

In the Appendix we discuss another way of looking at current that sheds further light on Eq. (69).

VIII. SUMMARY AND OUTLOOK

This paper has two principal themes. First, we showed that increasing the transition probability along a bond increases the current along that same bond. This "obvious" relation is not trivial and our proof required control over the stationary state in the case of a general transition matrix. Second, we studied the inverse problem of deducing the nature of an underlying transition matrix based on its currents and stationary state. To wit (using our earlier notation), given p_0 and J, take only the positive part of J (called J^+) and let the off-diagonal elements of a matrix $\bar{R}$ be given by $J^+_{xy}/p_0(y)$ (no summation). Adjusting the diagonal for stochasticity (set column sums to 1), then $\bar{R}$'s current will be the original one and it will have the correct stationary state. The most general R satisfying the inverse problem is then given by $\bar{R} + K_{xy}\sqrt{p_0(x)/p_0(y)}$, where K is an arbitrary symmetric matrix such that R's matrix elements stay within [0,1]. This result is of physical significance, since it is the currents (or substance flows) that are observable. The latter issue also led us to explore both the time scales for the definition of the transition matrix and the way in which one goes from transitions and probability currents to substance flows (e.g., flow of carbon in an ecosystem). The general inverse problem, beginning from substance flows, has not been solved, so that model construction inevitably will depend on an independent understanding of the dynamics of a specific system.

Finally, in response to a query by a referee we comment on the relation of our work to the concept of *pairwise balance* [23]. The stationary state of a system satisfying this condition has the following property: for each $x, y \in X$ for which there is positive flow from x to y (i.e., $J_{yx} = J^+_{yx} > 0$), there is a state z for which $J^+_{yx} = J^+_{xz}$. (If $z=y$ for all x, then one has detailed balance.) A number of model systems have been found to possess this property. From our present and previous analyses of currents there is a sense in which one can consider such a stationary state to be closer to equilibrium than to full complexity. In [4] we relate complexity to topological and other features of the currents. One tool in this discussion is the loop expansion, in which the positive component of a general current matrix J^+_{xy} is expressed as a sum, $J^+_{xy} = \Sigma_\alpha u_\alpha J^{+(\alpha)}_{xy}$, with each $J^{+(\alpha)}_{xy}$ the current corresponding to a *loop* (so for each α, all $J^{+(\alpha)}_{xy}$ are equal and α can be thought of as a permutation). The collection of acceptable (real, positive) u_α's form a simplex, and the properties [e.g., log(log(dimension))] of that simplex were proposed as a definition of complexity. With *pairwise balance* the loop structure is easy to unravel. Pick an $x \in X$, say x_0, with a nonzero current and its matching, unequal pairs, say x_1 and x_{-1}. These have at least one additional matching pair (which could be x_0); keep going; the finiteness of X guarantees that one returns to x_0 (thus realizing a loop). If x_0 has another nonzero current, form its loop. Continue. If the magnitudes of currents out of x_0 are nondegenerate, and if this is true for all points in X (which generically should be the case), then the loop decomposition is unique—a far cry from the general situation. Moreover, even with degeneracy, the loop expansion has quite restricted possibilities. Of course, the study of pairwise balance systems has shown them to exhibit rich behavior not available in equilibrium systems, suggesting that either far more elaborate properties are possible when this condition is relaxed, or that our criteria for complexity are too restrictive.

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APPENDIX: ANOTHER INTERPRETATION OF THE PROBABILITY CURRENT

Consider trajectories of length n,

$$\gamma_n = (x_0, x_1, \ldots, x_{n-1}, x_n). \tag{A1}$$

If the initial point is weighted according to the stationary state, its weight is

$$w(\gamma_n) = R_{x_n x_{n-1}}, \ldots, R_{x_{k+1} x_k}, \ldots, R_{x_1 x_0} p_0(x_0), \tag{A2}$$

which is a probability distribution on the space of paths.

Fix a bond $\overline{xy}$. The number of times that this bond is traversed, in the direction $\bar{y}\to\bar{x}$, by the trajectory γ_n is

$$\sum_{k=0}^{n-1} \delta_{\bar{x}x_{k+1}} \delta_{\bar{y}x_k}. \tag{A3}$$

The quantity in Eq. (A3) is a random variable on the space of paths of length n and its average with respect to the weight $w(\gamma_n)$ is

$$\left\langle \sum_{0}^{n-1} \delta_{\bar{x}x_{k+1}} \delta_{\bar{y}x_k} \right\rangle_n = \sum \sum_{k=1}^{n-1} R_{x_n x_{n-1}}, \ldots, R_{x_{k+2}\bar{x}} R_{\bar{x}\bar{y}} R_{\bar{y}x_{k-1}}, \ldots, R_{x_1 x_0} p_0(x_0) + \sum R_{x_n x_{n-1}}, \ldots, R_{x_2 \bar{x}} R_{\bar{x}\bar{y}} p_0(\bar{y}), \tag{A4}$$

where the unmarked summations ("Σ") above are sums over all numerically indexed x's. We next make use of

$$\sum_u R_{uv} = 1 \quad \text{and} \sum_v R_{uv} p_0(v) = p_0(u), \tag{A5}$$

leading to

$$\left\langle \sum_{0}^{n-1} \delta_{\bar{x}x_{k+1}} \delta_{\bar{y}x_k} \right\rangle_n = n R_{\bar{x}\bar{y}} p_0(\bar{y}). \tag{A6}$$

Suppose that in the transition $\bar{y}\to\bar{x}$ a certain quantity $q(x)$ changes from $q(\bar{x})$ to $q(\bar{y})$ (with the opposite change in the opposite direction), then the net amount of q released when $\bar{x}\rightleftharpoons\bar{y}$ is, on the average, for trajectories of length n,

$$[q(\bar{x}) - q(\bar{y})] \left\langle \sum_{k=0}^{n-1} \delta_{\bar{x}x_{k+1}} \delta_{\bar{y}x_k} - \sum_{k=0}^{n-1} \delta_{\bar{y}x_{k+1}} \delta_{\bar{x}x_k} \right\rangle_n, \tag{A7}$$

and by Eq. (A6),

$$n J_{\bar{x}\bar{y}} [q(\bar{x}) - q(\bar{y})]. \tag{A8}$$

Thus the average of q released during transitions $\bar{x}\rightleftharpoons\bar{y}$ per unit time is $J_{\bar{x}\bar{y}}[q(\bar{x})-q(\bar{y})]$.

Remark. Note that this does *not* require higher currents, $J^{(2)}, \ldots, J^{(N)} \ldots$.

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[17] A matrix is *stochastic* if its columns sum to 1 and all its matrix elements are between 0 and 1. (For a slightly different definition of the matrix it's the rows that sum to 1.) By definition our R is stochastic and as such a great deal is known about it, in particular, that its spectrum $\{\lambda\}$ must satisfy $|\lambda_k| \leq 1$; $\forall\, k$. See [24,25] or many other references.
[18] At this level of generality R need not have N eigenvectors, and a Jordan form may be required in a spectral representation.
[19] The term "state" is used in two senses: elements of X and probability distributions on X. The intended meaning should be clear from the context.

[20] Recall that we here discuss only matrices R that are not completely irreversible. For example, a permutation matrix, which does not satisfy this condition, does not have the property that nonzero lower currents imply nonzero $J^{(n)}$ for arbitrarily large n.

[21] Three reservoirs (rather than two) can be set up to oppose each other and can yield zero current.

[22] L. S. Schulman, in *Time-Related Issues in Statistical Mechanics* lectures given at Institut de Physique Théorique, Direction des Sciences de la Matière, CEA-Saclay and at the Physics Dept., Technion (Haifa), (2005), Sec. III, p. 25; URL http://people.clarkson.edu.~schulman

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