Pumping-Restriction Theorem for Stochastic Networks.

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(Dated: September 2, 2008)

We formulate an exact result, which we refer to as the pumping restriction theorem (PRT). It imposes strong restrictions on the currents generated by periodic driving in a generic dissipative system with detailed balance. Our theorem unifies previously known results with the new ones and provides a universal nonperturbative approach to explore further restrictions on the stochastic pump effect in non-adiabatically driven systems.

PACS numbers: 03.65.Vf, 05.10.Gg, 05.40.Ca

Introduction. The stochastic pump effect (SPE), which is the rectification of classical stochastic currents under time-periodic excitations, manifests itself in various systems [1]. For example, it plays a fundamental role in the theory of molecular motors [2]. A theory of the SPE, developed in the limit of adiabatically slow perturbations [3, 4], provided qualitative insight as well as proposed quantitative approaches for pump-current calculations.

Beyond the adiabatic limit, such a unifying theory is yet to emerge. Although many specific systems have been studied in great detail, universal results in this domain have been very rare. The recently discovered Fluctuation Theorems proposed a new approach to the nonadiabatic regime [5]. They addressed such questions as work production or probability relations among single trajectories [6], but not the magnitude of the SPE.

In a recent work of Rahav, Horowitz and Jarzynski [7], a universal result for the non-adiabatic regime, called the “no-pumping” theorem, was formulated. One can parametrize kinetic rates of an arbitrary Markov chain, developed in the limit of adiabatically slow perturbations [5], provided qualitative insight as well as proposed quantitative approaches for pump-current calculations.

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In this Letter, we derive generic restrictions on the SPE, that include previously found theorems [3, 7] as a special case. We show that there is a wide class of stochastic models on graphs, where nonadiabatic but periodic modulation of some parameters leads to a zero time-averaged flux through any link. We also predict restrictions on the values of nonzero pump currents when they are allowed. Such restrictions are sensitive to the topology of the graph representing the system. Thus, we claim that it is possible to determine whether two given links on a graph belong to the same loop by merely measuring the presence of the SPE.

Representative examples. Consider a particle moving according to Markov chain rules on a graph with a finite number of states and the detailed balance. First, we note a trivial observation, that periodic variation of parameters on a tree-like graph would not produce a net current because any flux that passes through any given link would eventually return through the same link after driven parameters return to the initial values. Pump currents are possible only on graphs with loops, such as the one shown in Fig. 1. Note, however, that the previous analysis still applies to some of the links. Namely, the integrated over time fluxes through links 1-2 and 4-5 in Fig. 1 must be zero.

A less trivial problem is whether there are general conditions (beyond the situation discussed in [2]) under which the flow through any link belonging to the loop in Fig. 1 such as the link 2-3 can be zero. For the model in Fig. 1 we claim, that if one varies the rates related to the links 1-2 and 4-5 cyclically but otherwise arbitrarily, while other rates remain constant and satisfy the detailed balance condition, then the time integrated current through any link on the loop will be zero. To prove it, we split the set of links in Fig. 1 into two subsets {1-2, 4-5} ∈ X1 and {2-3, 3-4, 2-4} ∈ X0. Consider the evolution of probabilities p, on three sites connected by the links in X0, i.e. the sites with indexes i = 2, 3, 4. Conservation laws require that

\begin{align*}
\dot{p}_2 &= j_{12}(t) - j_{23}(t) - j_{24}(t), \\
\dot{p}_3 &= j_{23}(t) - j_{34}(t), \\
\dot{p}_4 &= j_{34}(t) + j_{24}(t) - j_{45}(t),
\end{align*}

(1)
where \( j_{ij}(t) \) is the current passing through the link \( i-j \). Requiring the final probability distribution to be equal to the initial one, we reach the conditions

\[
\int_0^T dt \rho_i = \int_0^T dt j_{i2}(t) = \int_0^T dt j_{45}(t) = 0, \tag{2}
\]

where the upper limit of the integration depends on the choice of the driving protocol. In case of a single localized pulse that drives kinetic rates on links in \( X_1 \), \( T \) must be formally infinite in order to allow the system to relax to equilibrium. In case of a steady periodic driving with the period \( \tau \), if the system already reached the steady regime with \( \rho_i(t) = \rho_i(t+\tau) \), one can choose the upper integration limit \( T = \tau \).

The current through any link can be formally written in terms of instantaneous site probabilities and the kinetic rates, \( j_{ij} = k_{ij} \rho_i - k_{ij} \rho_j \). Denote \( \rho_i = \int_0^T \rho_i(t) dt \). Integrating (2) over time, using conditions (2) one arrives at a set of equations,

\[
-k_{32} + k_{42} \rho_2 + k_{23} \rho_3 + k_{34} \rho_4 = 0,
-k_{23} + k_{13} \rho_3 + k_{32} \rho_2 + k_{34} \rho_4 = 0,
-k_{24} + k_{34} \rho_4 + k_{42} \rho_2 + k_{33} \rho_3 = 0.
\tag{3}
\]

The set of equations (3) for \( \rho_i \) coincides with the one for probabilities on a 3-state Markov chain with the same topology and rates as for a subset \( X_0 \) at equilibrium state. Since all rates on this subset are time-independent and satisfy the detailed balance, the solution of (3) is \( \rho_i = Ce^{-E_i}, i = 2, 3, 4 \), where \( C \) is a constant that depends on the details of the driving protocol, but is equal for all three states on the loop. The total flux passed through e.g. the link 2-3 then reads

\[
J_{23}(T) = \int_0^T j_{23}(t) dt = C(k_{32}e^{-E_2} - k_{23}e^{-E_3}) = 0. \tag{4}
\]

This concludes our proof that varying the kinetic rates outside the loop only, does not lead to a net time averaged flux through any link on the graph in Fig. 1.

**Numerical check.** To test our predictions we performed numerical simulations for the graph shown in Fig. 1. In all examples we assume the kinetic rates to satisfy the detailed balance condition with the parametrization: \( k_{ij} = k \exp([E_j - W_{ij}]/k_B T) \). \( T \) we chose the energy scale so that \( k = 1, k_B T = 1 \). Fig. 2 shows the flux passed through the link 2-3 on the loop, when only parameters \( E_1 \) and \( W_{45} \) outside the loop are changing with time. After completion of the external driving, the system relaxes with a zero net current through the link 2-3, as we predicted.

Our numerical results show that if barriers are varied on the loop but potential depths \( E_j \) are varied only on external sites then nonzero pump current through the loop links appears, as shown in Fig. 3. However, the opposite is not true. Namely, if one varies well depths on the loop sites but barriers are varied along external links, numerically we always found no overall pump flux, as we show in Fig 4. The latter result is also easy to understand by introducing the quantities \( f_i = \int_0^T dt e^{E_i(t)} \rho_i(t) \), \( i = 2, 3, 4 \). The same analysis as before leads to the equilibrium master equation for \( f_i \) with equal forward/backward rates connecting any pair of sites, and a constant solution, ensuring the zero time-averaged current through any link on the loop. The previously found theorem 7 can be proved for any graph by the same steps and change of variables. We are now in a position to frame our result in a form of a general and rigorous mathematical statement.

**Pumping-Restriction Theorem (PRT).** For a graph \( X \) we denote the vector spaces of time averaged populations \( \rho \in C_0(X) \) and time-averaged currents \( J \in C_1(X) \), so that \( \rho = \{\rho_i\} \), \( J = \{J_{ab}\} \) with \( J_{ba} = -J_{ab} \) and \( J_{ab} = 0 \) when the nodes \( a \) and \( b \) are not connected by
produces the second no-pumping theorem of [7]. The PR T, pumped currents through different links on where the pumped current is restricted to a vector subspace $J \subseteq \mathcal{H}$, of populations that would be constant within the space of populations that would be constant within the connected components of $X$. Note that the conjugate operator $\hat{\partial}^\dagger : C_0(X) \rightarrow C_1(X)$ has a form $(\hat{\partial}^\dagger \rho)_{ab} = \rho_a - \rho_b$. In detailed balance the rates are given by $k_{ab} = g_{ba} e^{E_a}$, where $g_{ab} = g_{ba} = \kappa e^{-W_{ab}}$ is referred to as a metric on $X$. The Euler theorem claims [8]

$$\dim C_1 - \dim C_0 = \dim H_1 - \dim H_0.$$ \hfill (5)

Consider a partition $X = X_0 \cup X_1$, where $X_0$ consists of edges (and adjacent nodes) where the rates are given by $k_{ab} = g_{a,b} e^{E_a}$, whereas $X_1$ represents the rest of the edges with arbitrary rates $k_{ab}(t)$. Note that $X_0 \cap X_1$ does not have any edges, whereas its nodes provide the currents between $X_0$ and $X_1$. The PRT claims that

(i) for the described periodic driving the generated pumped current is restricted to a vector subspace $V$ such that $\mathbf{J} \in V \subset H_1(X)$, with the dimension

$$\dim V = \dim H_1(X) - \dim H_1(X_0) = \dim C_1(X_1) - \dim H_0(X_0) - \dim C_0(X) + \dim C_0(X) + 1.$$ \hfill (6)

(ii) given a set of links with driven barriers, the embedding $V \subset H_1(X)$ is totally determined by the (time-independent) metric $g_{ab}$ on $X_0$.

The statement (ii) implies that if there are constraining equations that determine relations among possible pumped currents through different links on $X_0$, then coefficients in these equations will depend only on the metric on $X_0$. Note also that the choice $X_0 = X$ reproduces the second no-pumping theorem of [7]. The PRT, however, claims more: starting with the no-pumping situation, at least one of $E_i$ driven, and also driving the barriers at a certain number $n$ of links, the number of independent generated currents may not exceed $n$, i.e., $\dim V \leq \dim C_1(X_1)$, that follows from second equality in (6). The PRT T can be interpreted as the claim of the number of independent generated currents to be equal to the maximum number of driven barriers, which removal does not split the remaining graph into disjoined components.

The proof of PRT is based on the Master Equation and the expression for the current $\dot{\mathbf{p}}(t) = \hat{\partial} \mathbf{j}(t)$, $\mathbf{j}(t) = \hat{\partial}^\dagger e^{E(t)} \mathbf{p}(t)$, \hfill (7)

where the second equality is valid on $X_0$. Representing the current $\mathbf{j}(t) = \mathbf{j}_0(t) + \mathbf{j}_1(t)$ as the sum of the $X_0$ and $X_1$ components and averaging (integrating) Eq. (7) over time we obtain for the time-integrated quantities $\hat{\partial} \dot{\mathbf{j}}$, $\mathbf{j}_0 = \hat{\partial}^\dagger \mathbf{f}$, \hfill (8)

where $\mathbf{f} = \int_0^T e^{E(t)} \mathbf{p}(t)$, $\mathbf{j}_0 = \int_0^T \mathbf{j}_1(t)$, and $\mathbf{j} \in H_0(X_0 \cap X_1)$ describes the flux passed between $X_0$ and $X_1$. Since the operator $\hat{\partial} \dot{\mathbf{j}}$ can be viewed as the discrete Laplacian in $X_0$ associated with the metric $g$, the first two equations in (8) have a solution if and only if the total flux entering any connected component of $X_0$ and $X_1$ is zero. Let $V_0 \subset H_0(X_0 \cap X_1)$ is the vector subspace of $\mathbf{f}$ that satisfies these conditions. The solution of the first equation in (8) is unique up to an additive constant distribution, which does not affect the value of $\mathbf{j}_0$, i.e., the latter is uniquely determined by $\mathbf{f} \in V_0$ and metric on $X_0$. On the other hand, given $\mathbf{f} \in V_0$, the component $\mathbf{j}_1$ is defined up to a current that circulates completely within $X_1$ and is represented by an element of $H_1(X_1)$. Thus we proved that the metric on $X_0$ and topology of $X_1$ determine the restrictions on $\mathbf{j}$, which implies the statement (ii) of PRT. In addition our analysis implies

$$\dim V = \dim V_0 + \dim H_1(X_1).$$ \hfill (9)

To derive the explicit expression (9), which completes the proof we combine Eqs. (9) with the identity

$$\dim H_1(X) = \dim H_1(X_0) + \dim H_1(X_1) + \dim V_0,$$ \hfill (10)

which results in the first equality in (6). The second equality follows from (5) and that $\dim H_0(X) = 1$. Note
that the identity \[10\] has a very simple physical meaning: For any physical current \(J \in H_1(X)\) on our graph we can identify the current \(J^{(0)} \in V_0\) that flows from \(X_0\) to \(X_1\), and once the exchange current \(J^{(01)}\) is identified, the complete current \(J\) is defined up to the currents \(J^{(0)} \in H_1(X_0)\) and \(J^{(1)} \in H_1(X_1)\) that circulate strictly within \(X_0\) and \(X_1\), respectively.

We further illustrate the PRT using a graph in Fig. 3 with \(\dim C_1(X) = 7\) (the number of links), \(\dim C_0(X) = 6\) (the number of sites), and two independent loops, e.g., [2342] and [2462] that form a basis in \(H_1(X)\) with \(\dim H_1(X) = 2\). If only one barrier is driven we can generate not more than a 1D subspace of currents, i.e. \(\dim V \leq 1\). If the barrier at links 1-2 or 4-5 are driven, we are in the no-pump situation, since \(\dim V = 0\) (the subgraph \(X_0\) obtained upon elimination of the link 1-2, or 4-5, has two loops, hence \(\dim H_1(X_0) = 2\)). Driving the barrier at another single link yields \(\dim V = 1\), since the graph \(X_1\) in this case is connected. When a pair of barriers is driven we have \(\dim V = 0\) for \(\{1-2, 4-5\}\); \(\dim V = 1\) for \(\{2-3, 3-4\}, \{2-6, 6-4\}\), and when one of 1-2, 4-5 and one of the rest are driven. In all other cases we have \(\dim V = 2\) (all currents may be generated). Consider in more detail the \(\{2-3, 3-4\}\) driving. The subgraph \(X_1\) includes these two links and the vertices \(\{2, 3, 4\}\), \(X_0\) includes the rest of the links and the vertices \(\{1, 2, 6, 4, 5\}\), whereas \(X_0 \cap X_1\) has the vertices \(\{2, 4\}\) and no links. The exchange goes through two nodes \(\{2, 4\}\); the exchange currents satisfy relations \(J_{23} + J_{43} = 0\) that yields \(\dim V_0 = 2 - 1 = 1\), i.e. while allowed elements of \(X_0 \cap X_1\) have the form \(\{\rho_2, \rho_1\}\), elements in \(V_0\) are restricted to be of the form \(\{J, -J\}\). The subgraph \(X_1\) has no loops, and, therefore, no internal currents, which yields \(\dim V = 1\), which agrees with the PRT.

We also note that similar arguments lead to continuous (Langevin dynamics) counterparts of the no-pumping theorems of \[7\]. Let \(g^{ij}(x)\) be a metric in a compact oriented manifold \(M\) that describes bath-induced fluctuations/dissipation. If parametrized as \(g^{ik}(x) = h^{ik}(x)e^{V(x, t)}\), where \(h\) is time-independent and \(V\) is a periodic in time potential, then \(J^P(x) = 0\).

**Conclusion.** Many emerging mesoscopic devices, including molecular motors \[3\] and nanoscale electronic circuits \[8\] can be modeled as discrete connected entities with stochastic transitions among different states. The control over such new devices is impossible without deep understanding of non-adiabatic strongly driven regimes of their operation. Our result is a step toward such a theory. The PRT, presented here, determines the restrictions in the space of pumped current values on a graph. No-pumping conditions follow as its special consequences. The restrictions on the pump current space suggest, for example, that an application of a periodic stimulus can be used to induce a localized rectified effect without perturbing the whole circuit on average even if all its components are connected. It should be useful to explore how the PRT is modified by quantum effects. Violation of the “no-pumping” conditions due to quantum corrections can be employed to detect the quantum pump effect \[10\] by cooling the electronic circuit in the “no-pumping” regime down to the quantum domain.

Another possible application for this work is the reconstruction of the stochastic network topologies, e.g. in biochemical reactions. Standard measurement techniques, such as those based on the linear response, appear insufficient. One would expect to find a nonzero signal anywhere on an ergodic Markov chain in response to a time-dependent current inducing perturbation. However, we showed that measuring rectified current in response to external periodic stimulus can help one to identify whether or not two given links belong to the same loop. One of the perturbed links must belong to a common loop with the measured one in order to observe the SPE. Even without a quantitative understanding of the data, detecting only the presence of the SPE can be sufficient to deduce the topological structure of the network completing only a small number of measurements.

We thank the authors of Ref. \[7\] for sharing their results prior to publication, and also B. Munsky and I. Nemenman for useful discussions. This material is based upon work supported by the National Science Foundation under CHE-0808910 and in part by DOE under Contract No. DE-AC52-06NA25396.

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