

Pumping Restriction Theorem for Stochastic Networks

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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, and provides a universal nonperturbative approach to explore the stochastic pump effect in nonadiabatically driven systems.

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Introduction.—The stochastic pump effect (SPE), which is the rectification of classical stochastic currents under time-periodic driving, manifests itself in a variety of systems [1,2]. A theory of the SPE, developed in the limit of adiabatically slow [3,4], and weak [5] perturbations provided qualitative insight as well as proposed quantitative approaches for pump-current calculations.

Beyond the perturbative limits universal results have been very rare, and a unifying theory is yet to emerge. The recently discovered fluctuation theorems proposed a new approach to the nonadiabatic regime [6]. They addressed such questions as work production or probability relations among single trajectories [7], but not the magnitude of the SPE. Steps have been made to develop efficient numerical algorithms for SPE evaluations [8].

In a recent work of Rahav, Horowitz, and Jarzynski [9], a universal result for the nonadiabatic regime, called the “no-pumping” theorem, was formulated. One can parametrize kinetic rates of an arbitrary Markov chain with detailed balance conditions, so that for any pair of sites i and j these rates are written as $k_{ij} = ke^{E_j - W_{ij}}$, where E_i can be called the depth of a potential well i , and $W_{ij} = W_{ji}$ is called the size of the potential barrier i - j . Energy scale is $k_B T = 1$. The theorem [9] states that to generate rectified currents during a cyclic process, both well depths and barrier sizes must be varied.

In this Letter, we derive generic restrictions on the SPE, that include previously found theorems [3,9] 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.

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 treelike 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 [9]) under which the flux 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 $\{1-2, 4-5\} \in X_1$ and $\{2-3, 3-4, 2-4\} \in X_0$. Consider the evolution of probabilities p_i on three sites connected by the links in X_0 , i.e., the sites with indexes $i = 2, 3, 4$. Conservation laws require that

$$\begin{aligned} \dot{p}_2 &= j_{12}(t) - j_{23}(t) - j_{24}(t), & \dot{p}_3 &= j_{23}(t) - j_{34}(t), \\ \dot{p}_4 &= j_{34}(t) + j_{24}(t) - j_{45}(t), \end{aligned} \quad (1)$$

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

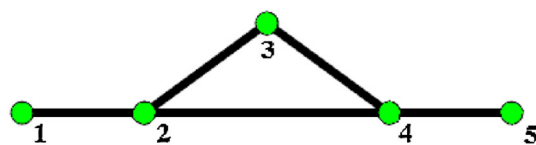


FIG. 1 (color online). Five-state graph with one loop [2342].

$$\int_0^T dt \dot{p}_i = \int_0^T dt j_{12}(t) = \int_0^T dt j_{45}(t) = 0, \quad (2)$$

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 the equilibrium. In case of a steady periodic driving with the period τ , if the system already reached the steady regime with $p_i(t) = p_i(t + \tau)$, 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, $j_{ij} = k_{ji}p_i - k_{ij}p_j$. Denote $\rho_i \equiv \int_0^T p_i(t)dt$. Integrating (1) over time, using (2), one arrives at

$$\begin{aligned} -(k_{32} + k_{42})\rho_2 + k_{23}\rho_3 + k_{24}\rho_4 &= 0, \\ -(k_{23} + k_{43})\rho_3 + k_{32}\rho_2 + k_{34}\rho_4 &= 0, \\ -(k_{24} + k_{34})\rho_4 + k_{42}\rho_2 + k_{43}\rho_3 &= 0. \end{aligned} \quad (3)$$

The set of Eqs. (3) for ρ_i coincides with the one for probabilities on a three-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

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

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 in Fig. 1. We assume the kinetic rates to satisfy the detailed balance condition [9]. Figure 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 $f_i = \int_0^T dt [e^{E_i(t)} p_i(t)]$, $i = 2, 3, 4$. The same analysis as before leads to the equilibrium master equation for f_i with equal forward/backward rates connecting any

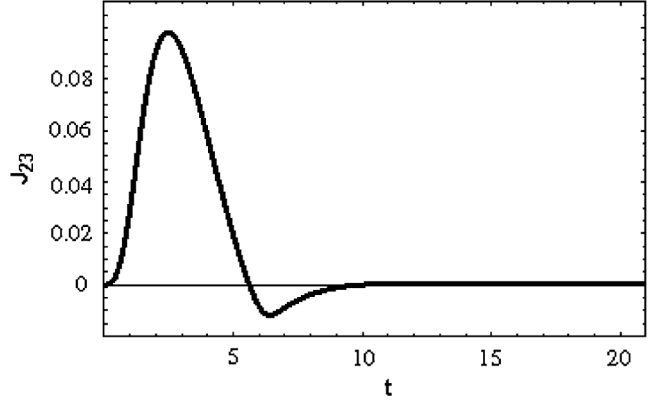


FIG. 2. The total flux passed through the link 2–3 by time t . Variable parameters are $E_1(t) = E_1 + E \sin(\omega t)$, and $W_{45}(t) = W_{45} + W \cos(\omega t)$, for $t \in (0, 2\pi/\omega)$, and $E_1(t) = E_1$, $W_{45}(t) = W_{45} + W$ for $t > 2\pi/\omega$, and we distinguish between $E_1(t)$ and E_1 etc. Choice of constant parameters is $\omega = 1$, $k = 1$, $E = 1$, $W = 2$, $E_1 = -1$, $E_2 = 0.2$, $E_3 = -0.05$, $E_4 = 0.1$, $E_5 = -0.25$, $W_{45} = 0.3$, $W_{12} = 0$, $W_{23} = 0.2$, $W_{34} = -0.2$, $W_{24} = 0.25$, $W_{ij} = W_{ji}$ for any $i-j$.

pair of sites, and a constant solution, ensuring the zero time-averaged current through any link on the loop.

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 $\mathbf{J} \in C_1(X)$, so that $\rho = \{\rho_a\}$, $\mathbf{J} = \{J_{ab}\}$ with $J_{ba} = -J_{ab}$ and $J_{ab} = 0$ when the nodes a and b are not connected by an edge. We further introduce the boundary operator $\partial: C_1(X) \rightarrow C_0(X)$ by $(\partial \mathbf{J})_a = \sum_b J_{ba}$. Let $H_1(X)$ be the subspace of physical time-averaged currents, i.e., satisfying the continuity condition, and $H_0(X)$ represent the space of populations that would be constant within the connected components of X . Note that the conjugate operator $\partial^\dagger: C_0(X) \rightarrow C_1(X)$ has a

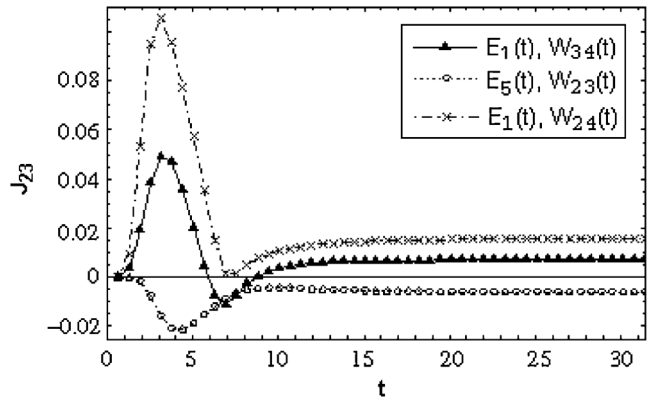


FIG. 3. The total flux passed through the link 2–3 by time t . W_{ij} is varied along one of the loop links. Variable parameters, indicated on a graph legend, change with time according to $E_i(t) = E_i + E \sin(\omega t)$, and $W_{ij}(t) = W_{ij} + W \cos(\omega t)$, for $t \in (0, 2\pi/\omega)$, and $E_i(t) = E_i$, $W_{ij}(t) = W_{ij} + W$ for $t > 2\pi/\omega$. Constant parameters are as in Fig. 2.

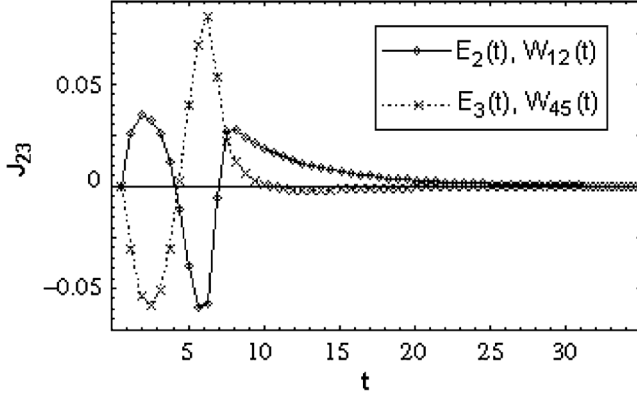


FIG. 4. The total flux passed through the link 2–3 by time t , when only E_i were allowed to vary on one of the loop sites and W_{ij} is varied along external links. Variable parameters, indicated on a graph legend, change with time according to $E_i(t) = E_i + E \sin(\omega t)$, and $W_{ij}(t) = W_{ij} + W \cos(\omega t)$, for $t \in (0, 2\pi/\omega)$, and $E_i(t) = E_i$, $W_{ij}(t) = W_{ij} + W$ for $t > 2\pi/\omega$. Constant parameters are as in Fig. 2.

form $(\partial^\dagger \rho)_{ab} = \rho_a - \rho_b$. In detailed balance the rates are given by $k_{ab} = g_{ab} e^{E_b}$, where $g_{ab} = g_{ba} = ke^{-W_{ab}}$ is referred to as a metric on X . The Euler theorem claims [10]

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

Consider a partition $X = X_0 \cup X_1$, where X_0 consists of edges (and adjacent nodes) where the rates are given by $k_{ab}(t) = g_{ab} e^{E_b(t)}$, 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

$$\begin{aligned} \dim V &= \dim H_1(X) - \dim H_1(X_0) \\ &= \dim C_1(X_1) - \dim H_0(X_0) - \dim C_0(X) \\ &\quad + \dim C_0(X_0) + 1. \end{aligned} \quad (6)$$

(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 [9]. The PRT, however, claims more: starting with the no-pumping situation with 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) and obvious inequalities $\dim H_0(X_0) \geq 1$, and $[-\dim C_0(X) + \dim C_0(X_0)] \leq$

0. Each of the driven links can be viewed as either responsible for an independent cycle or for connecting two disconnected parts. Therefore, the PRT 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 disjointed components.

The proof of PRT is based on the Master Equation and the expression for the current

$$\dot{\mathbf{p}}(t) = \partial \mathbf{j}(t), \quad \mathbf{j}(t) = \hat{g} \partial^\dagger e^{\hat{E}(t)} \mathbf{p}(t), \quad (7)$$

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 equations for the time-integrated quantities

$$\partial \hat{g} \partial^\dagger \mathbf{f} = -\boldsymbol{\zeta}, \quad \boldsymbol{\zeta} = \partial \mathbf{J}_1|_{X_0 \cap X_1}, \quad \mathbf{J}_0 = \hat{g} \partial^\dagger \mathbf{f}, \quad (8)$$

where $\mathbf{f} = \int_0^T e^{\hat{E}(t)} \mathbf{p}(t)$, $\mathbf{J}_{1/0} = \int_0^T \mathbf{j}_{1/0}(t)$, and $\boldsymbol{\zeta} \in H_0(X_0 \cap X_1)$ describes the flux passed between X_0 and X_1 . Since the operator $\partial \hat{g} \partial^\dagger$ 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 $\boldsymbol{\zeta}$ 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 $\boldsymbol{\zeta} \in V_0$ and metric on X_0 . On the other hand, given $\boldsymbol{\zeta} \in V_0$, 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

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

Combining Eq. (9) with the identity

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

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 $\mathbf{J} \in H_1(X)$ on our graph we can identify the current $\mathbf{J}^{(01)} \in V_0$ that flows from X_0 to X_1 , and once the exchange current $\mathbf{J}^{(01)}$ is identified, the complete cur-

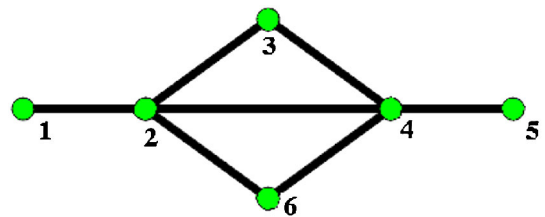


FIG. 5 (color online). A six state Markov chain.

rent 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. 5, 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 at 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 any other 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 $\{\rho_2, \rho_4\}$, 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 [9]. Let $g^{ij}(\mathbf{x})$ be a metric in a compact oriented manifold M that describes bath-induced fluctuations/dissipation. If parametrized as $g^{ik}(\mathbf{x}) = h^{ik}(\mathbf{x})e^{V(\mathbf{x},t)}$, where h is time independent and V is a periodic in time potential, then $J^j(\mathbf{x}) = 0$.

Conclusion.—Many emerging mesoscopic devices, including molecular motors [3] and nanoscale electronic circuits [11] 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 nonadiabatic strongly driven regimes of their operation. Our result is a step toward the theory of such a control. 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 [12] 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. 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.

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