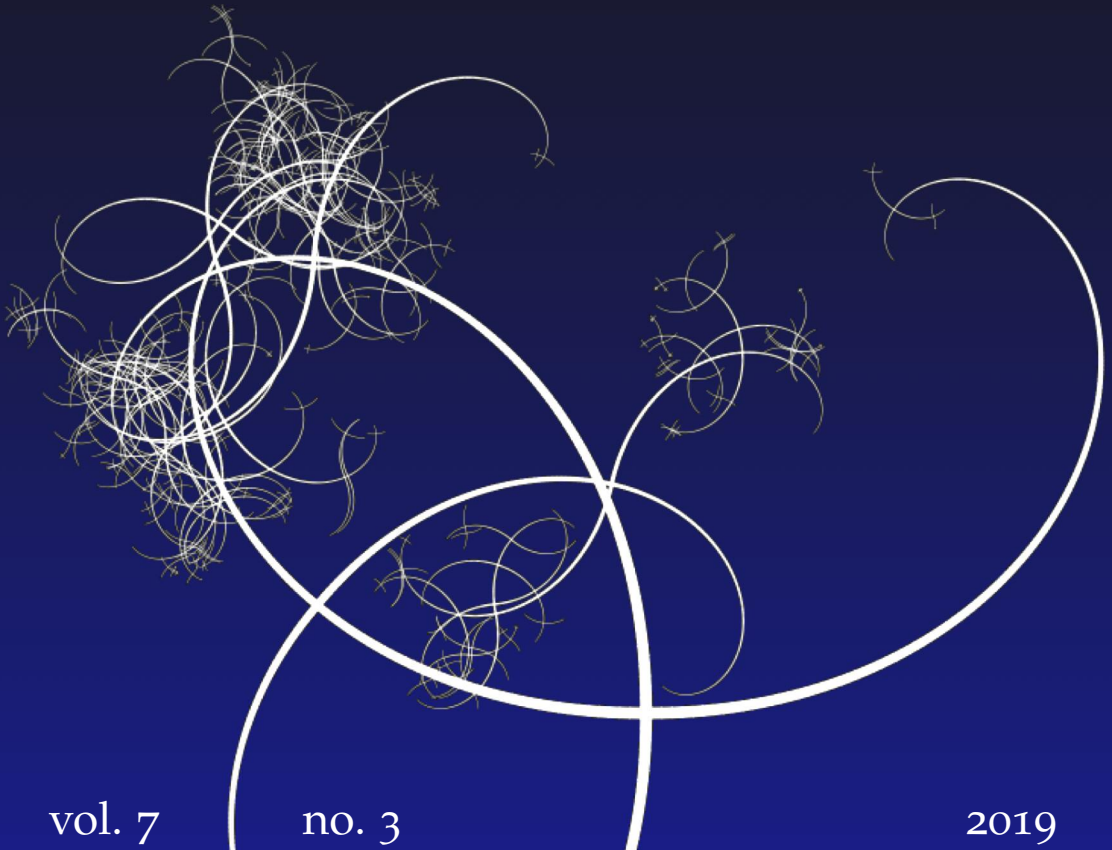


NISSUNA UMANA INVESTIGAZIONE SI PUO DIMANDARE VERA SCIENZA
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LEONARDO DA VINCI



vol. 7

no. 3

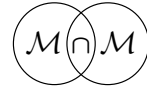
2019

MATHEMATICS AND MECHANICS
of
Complex Systems

JUSTINE LOUIS

LOW-TEMPERATURE RATCHET CURRENT





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JUSTINE LOUIS

We give an explicit expression for the low-temperature ratchet current in a multi-level system and find its numerical value as the number of states goes to infinity.

1. Introduction

In [Maes et al. 2014], the authors study stationary occupations in nonequilibrium multilevel systems at low temperatures. The system under consideration is an irreducible continuous time Markov jump process on a set of states K with transition rates $\lambda(x, y)$ expressed in terms of the reactivities $a(x, y)$ and depending on the inverse temperature β . It is assumed that the system is in contact with an environment at uniform temperature and also subject to external forcing which breaks the Boltzmann occupation statistics. Being away from detailed balance implies that a current can flow in the system. To achieve nonequilibrium conditions, different physical models exist such as flashing ratchets. This corresponds to a random flipping between a flat potential and a nontrivial energy landscape. This is known as a continuous time Parrondo game [Parrondo 1998] and is studied in [Maes et al. 2014] as an example of their asymptotic formula for the stationary occupations. The authors model the multilevel system by a graph consisting of two rings of N vertices which represent the states, and the edges stand for the preferred successors. This enables them to determine the direction of the ratchet current at low temperatures, which cannot be determined by entropic considerations only, and to evaluate it numerically while in the present paper we give an exact expression for it up to exponentially small corrections. This calculation confirms their result and in particular that the ratchet current is positive. The proof is based on an application of the Tutte matrix tree theorem. In the present section, we recall the definitions and results from [Maes et al. 2014, §3], and in the next section we give an explicit expression for the ratchet current and find its limit as the number of states goes to infinity.

Communicated by Raffaele Esposito.

The author acknowledges support from Swiss National Science Foundation grant 200021_132528/1.

MSC2010: primary 05C30, 82C03; secondary 05C05, 05C20, 05C50.

PACS2010: 05.70.Ln.

Keywords: nonequilibrium statistical mechanics, direction current, Tutte matrix tree theorem.

The zero-temperature logarithmic limit denoted by $\phi(x, y)$ is given by

$$\phi(x, y) := \lim_{\beta \rightarrow \infty} \frac{1}{\beta} \log \lambda(x, y).$$

The zero-temperature logarithmic limit of the escape rates of state x is denoted by $\Gamma(x)$ and given by

$$\Gamma(x) := - \lim_{\beta \rightarrow \infty} \frac{1}{\beta} \log \left(\sum_y \lambda(x, y) \right) = - \max_y \phi(x, y).$$

The logarithmic-asymptotic transition probability is given by $e^{-\beta U(x, y)}$ where

$$U(x, y) := -\Gamma(x) - \phi(x, y).$$

We have $U(x, y) \geq 0$ for all $x, y \in K$. The smaller $U(x, y)$ is, the larger is the probability of transition from state x to state y . Hence, the set of preferred successors of x is defined by

$$\{y \in K \mid U(x, y) = 0\}.$$

When $U(x, y) = 0$, the probability of transition from x to y is high. Thus, we consider the directed graph K^D defined by the vertex set K and edge set $\{(x, y) \mid U(x, y) = 0\}$ where (x, y) indicates an oriented edge from x to y . The transition rates are related to the reactivities by the relation

$$\lambda(x, y) = a(x, y)e^{-\beta(\Gamma(x)+U(x,y))}.$$

Using the Kirchhoff formula on K^D , the stationary occupation ρ is given by

$$\rho(x) = \frac{W(x)}{\mathfrak{L}}, \quad \text{where } W(x) = \sum_{\mathcal{T}_x} \prod_{(y,z) \in \mathcal{T}_x} \lambda(y, z) \text{ and } \mathfrak{L} = \sum_{x \in K} W(x)$$

where the sum runs over all oriented edges (y, z) in the in-tree \mathcal{T}_x . The low-temperature asymptotic of the stationary occupation is given in:

Theorem [Maes et al. 2014, Theorem 2.1]. *There is $\epsilon > 0$ so that as $\beta \rightarrow \infty$,*

$$\rho(x) = \frac{1}{\mathfrak{L}} A(x) e^{\beta(\Gamma(x) - \Theta(x))} (1 + O(e^{-\beta\epsilon}))$$

with

$$\Theta(x) := \min_{\mathcal{T}_x} U(\mathcal{T}_x) \quad \text{for} \quad U(\mathcal{T}_x) := \sum_{(y,y') \in \mathcal{T}_x} U(y, y'),$$

$$A(x) := \sum_{\mathcal{T}_x \in \mathcal{M}(x)} \prod_{(y,y') \in \mathcal{T}_x} a(y, y') = e^{\rho(\beta)}$$

where the last sum runs over all spanning trees minimizing $U(\mathcal{T}_x)$ (i.e., $\mathcal{T}_x \in \mathcal{M}(x)$ if $\Theta(x) = U(\mathcal{T}_x)$).

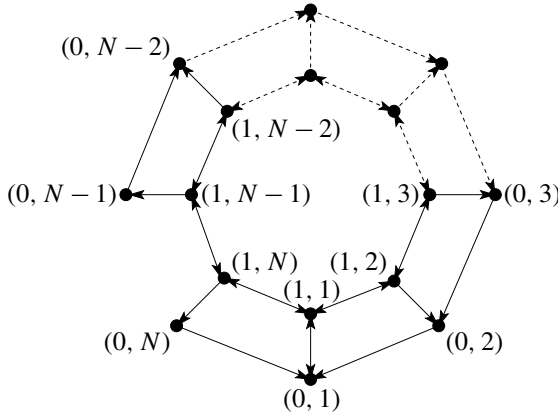


Figure 1. The directed graph K^D .

The case $a \gg 1$ satisfies detailed balance, and the model is then running on a single ring while in the case $a \ll 1$ the rings are uncoupled and detailed balance happens again for $a = 0$. We thus consider the case $a = 1$ corresponding to the nonequilibrium situation. The states, or energy levels, on the outer ring are denoted by $(0, i)$ and on the inner ring by $(1, i)$, where $i = 1, \dots, N$. The energies are denoted by $E_i, i = 1, \dots, N$, and are such that $E_1 < \dots < E_N$. The transition rates on the outer ring are thus given by

$$\lambda((i, 0), (i + 1, 0)) = e^{\beta(E_i - E_{i+1})/2}, \quad \lambda((i + 1, 0), (i, 0)) = e^{\beta(E_{i+1} - E_i)/2}.$$

On the inner ring, the transition rates are constant and equal to one, that is,

$$\lambda((i, 1), (i + 1, 1)) = \lambda((i + 1, 1), (i, 1)) = 1.$$

The two rings are connected with transition rates constant and equal to one:

$$\lambda((i, n), (i, 1 - n)) = 1, \quad \text{where } n \in \{0, 1\}.$$

The digraph K^D modeling the ratchet is represented in Figure 1. In the present case, for all $x \in K$, there exists an in-spanning tree \mathcal{T}_x in K^D , so that $U(\mathcal{T}_x) = 0$, and therefore, $\Theta(x) = 0$. Let \mathcal{D} be the set of states for which $\Gamma(x) = 0$; it is given by $\mathcal{D} = \{(1, 0), (i, 1), i = 1, \dots, N\}$. We denote $f \simeq g$ if $f = g + O(e^{-\beta\epsilon})$ as $\beta \rightarrow \infty$. For $x \in \mathcal{D}$, we have $\rho(x) \simeq |M(x)|/\mathcal{L}$, where $|M(x)|$ is the number of in-spanning trees in K^D . For $x \notin \mathcal{D}$, the stationary distribution is exponentially small since from the theorem it is given by $\rho(x) \simeq |M(x)|e^{\beta\Gamma(x)}/\mathcal{L}$, with $\Gamma(x) < 0$. The stationary ratchet current in the clockwise direction is given by

$$J_R = j((i + 1, 0), (i, 0)) + j((i + 1, 1), (i, 1)), \quad \text{for } i = 1, \dots, N,$$

where $j(x, y) = \lambda(x, y)\rho(x) - \lambda(y, x)\rho(y)$.

For $i = 1$,

$$J_R = j((2, 0), (1, 0)) + j((2, 1), (1, 1)).$$

On the outer ring, $j((2, 0), (1, 0)) = \lambda((2, 0), (1, 0))\rho(2, 0) - \lambda((1, 0), (2, 0))\rho(1, 0)$ with

$$\begin{aligned} \lambda((1, 0), (2, 0)) &\simeq 0, & \lambda((2, 0), (1, 0)) &= e^{(E_2 - E_1)\beta/2}, \\ \rho(2, 0) &\simeq \frac{|M(2, 0)|}{\mathfrak{Z}} e^{\beta\Gamma(2,0)} = \frac{|M(2, 0)|}{\mathfrak{Z}} e^{-(E_2 - E_1)\beta/2}, \end{aligned}$$

so that $j((2, 0), (1, 0)) \simeq |M(2, 0)|/\mathfrak{Z}$.

On the inner ring, $j((2, 1), (1, 1)) = \lambda((2, 1), (1, 1))\rho(2, 1) - \lambda((1, 1), (2, 1))\rho(1, 1)$ with

$$\begin{aligned} \lambda((2, 1), (1, 1)) &= \lambda((1, 1), (2, 1)) = 1, \\ \rho(2, 1) &\simeq \frac{|M(2, 1)|}{\mathfrak{Z}}, & \rho(1, 1) &\simeq \frac{|M(1, 1)|}{\mathfrak{Z}}, \end{aligned}$$

so that $j((2, 1), (1, 1)) \simeq (|M(2, 1)| - |M(1, 1)|)/\mathfrak{Z}$. The ratchet current is thus given by

$$J_R \simeq \frac{1}{\mathfrak{Z}} (|M(2, 0)| + |M(2, 1)| - |M(1, 1)|).$$

Considering converging arborescences, the Laplacian matrix of a directed graph is defined by $L = D - A$ where D is the diagonal out-degree matrix and $A = (A_{ij})$ is the adjacency matrix such that A_{ij} is the number of directed edges from i to j . The rows and columns of L are indexed by the vertices of the graph. Here, we index it first by the states on the outer ring and then the ones on the inner ring, that is $(1, 0), (2, 0), \dots, (N, 0), (1, 1), (2, 1), \dots, (N, 1)$. The Tutte matrix tree theorem [Aigner 2007] relates the number of spanning arborescences converging to x in K^D to the cofactors of the Laplacian $\det L_{x,y}$. Let $x \in K$. Then for all $y \in K$,

$$|M(x)| = (-1)^{x+y} \det L_{x,y}.$$

In particular, for $y = x$, we have $|M(x)| = \det L_x$. Therefore, we have

$$J_R \simeq \frac{1}{\mathfrak{Z}} (\det L_{(2,1)} + \det L_{(2,0)} - \det L_{(1,1)}).$$

The Laplacian matrix is given by

$$L = \left(\begin{array}{c|c} F & G \\ \hline \text{Id} & C \end{array} \right)$$

where F is the $N \times N$ lower triangular matrix given by

$$F = \begin{pmatrix} 1 & & & & \\ -1 & 1 & & & \\ & \ddots & \ddots & & \\ & & & -1 & 1 \\ -1 & & & 0 & 1 \end{pmatrix},$$

G is the $N \times N$ matrix such that all coefficients are zero except $G_{(1,0),(1,1)} = -1$, the matrix Id is the $N \times N$ identity matrix, and C is the circulant matrix

$$C = \begin{pmatrix} 3 & -1 & & & -1 \\ -1 & 3 & \ddots & & \\ & \ddots & \ddots & \ddots & \\ & & \ddots & \ddots & -1 \\ -1 & & & -1 & 3 \end{pmatrix}.$$

2. Calculation of the ratchet current

From [Maes et al. 2014], the numerator of J_R is given by

$$\det L_{(2,1)} + \det L_{(2,0)} - \det L_{(1,1)} = \det B_{N-1} - 2 \det B_{N-2} - 2$$

where B_N is the $N \times N$ tridiagonal matrix with 3 on the diagonal and -1 on the two off-diagonals which satisfies the recurrence relation $\det B_N = 3 \det B_{N-1} - \det B_{N-2}$ with $\det B_1 = 3$ and $\det B_2 = 8$. By solving the associated characteristic equation, we get

$$\det B_N = \frac{5 - 3\sqrt{5}}{10} \left(\frac{3 - \sqrt{5}}{2} \right)^N + \frac{5 + 3\sqrt{5}}{10} \left(\frac{3 + \sqrt{5}}{2} \right)^N.$$

The normalization factor is given by

$$\mathcal{Z} = \sum_{x \in K} \sum_{\mathcal{T}_x} \prod_{(y,z) \in \mathcal{T}_x} \lambda(y, z) \simeq \sum_{x \in \mathcal{D}} |M(x)| = \sum_{x \in \mathcal{D}} \det L_x.$$

The sum is over the states in \mathcal{D} since the contribution of the states which are not in \mathcal{D} is exponentially damped. Therefore, we have

$$\mathcal{Z} \simeq \det L_{(1,0)} + \sum_{i=1}^N \det L_{(i,1)}. \tag{1}$$

We have

$$\det L_{(1,0)} = \det C.$$

The circulant matrix C has eigenvalues $\mu_j = 3 - 2 \cos(2\pi j/N)$, $j = 0, 1, \dots, N-1$ [Biggs 1993]. Hence,

$$\det L_{(1,0)} = \prod_{j=0}^{N-1} (3 - 2 \cos(2\pi j/N)) = U_{N-1}^2(\sqrt{5}/2)$$

where U_N is the N -th degree Chebyshev polynomial of the second kind. Thus,

$$\det L_{(1,0)} = \left(\frac{3 + \sqrt{5}}{2}\right)^N + \left(\frac{3 - \sqrt{5}}{2}\right)^N - 2. \quad (2)$$

From the Tutte matrix tree theorem, the cofactor $(-1)^{N+i} \det L_{(i,1)}$ is equal to the number of converging arborescences to $(i, 1)$ and is equal to the cofactor of the Laplacian where row $(i, 1)$ and any column are removed. Since the only nonzero element of G is in column indexed by $(1, 1)$, we choose to remove that one, so that

$$|M(i, 1)| = (-1)^{(N+i)+(N+1)} \det L_{(i,1),(1,1)} = (-1)^{i+1} \det C_{(i,1),(1,1)} \quad (3)$$

since F is lower triangular. On the other hand, by adding to the first column of C all the other ones, we have

$$\det C = \begin{vmatrix} 1 & -1 & & -1 \\ 1 & 3 & \ddots & \\ & -1 & \ddots & \ddots \\ & & \ddots & \ddots & -1 \\ 1 & & & -1 & 3 \end{vmatrix} = \sum_{i=1}^N (-1)^{i+1} \det C_{(i,1),(1,1)}. \quad (4)$$

Putting (1), (2), (3), and (4) together, we have

$$\mathcal{L} \simeq 2 \det C = 2 \left(\frac{3 + \sqrt{5}}{2}\right)^N + 2 \left(\frac{3 - \sqrt{5}}{2}\right)^N - 4.$$

Up to exponentially small corrections $e^{-\beta\epsilon}$, the ratchet current is given for all N by

$$J_R \simeq \left(\frac{5+3\sqrt{5}}{10} \left(\frac{3+\sqrt{5}}{2}\right)^{N-1} + \frac{5-3\sqrt{5}}{10} \left(\frac{3-\sqrt{5}}{2}\right)^{N-1} - \frac{5+3\sqrt{5}}{5} \left(\frac{3+\sqrt{5}}{2}\right)^{N-2} - \frac{5-3\sqrt{5}}{5} \left(\frac{3-\sqrt{5}}{2}\right)^{N-2} - 2 \right) / \left(2 \left(\frac{3+\sqrt{5}}{2}\right)^N + 2 \left(\frac{3-\sqrt{5}}{2}\right)^N - 4 \right).$$

As a consequence, in the large system size limit the current saturates and has the limit

$$\lim_{N \rightarrow \infty} J_R \simeq \frac{1}{2} - \frac{1}{\sqrt{5}}.$$

Acknowledgements

The author thanks Anders Karlsson for suggesting this problem to her. She also thanks the referee for useful comments.

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Received 8 Jul 2019. Revised 12 Aug 2019. Accepted 24 Sep 2019.

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MEMOCS (ISSN 2325-3444 electronic, 2326-7186 printed) is a journal of the International Research Center for the Mathematics and Mechanics of Complex Systems at the Università dell'Aquila, Italy.

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