Current Fluctuations in 1D Diffusion-Reaction Systems via Tensor Networks

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Fluctuation Relation for Currents

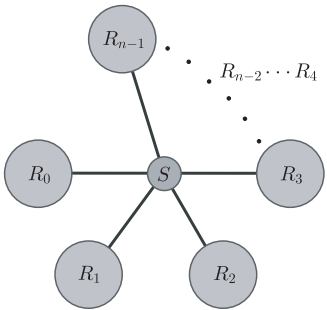

Figure: Schematic representation of a system S in contact with n particle reservoirs $R_0,\ R_1,\ R_2, \cdots, R_{n-1}$.

- R_i denotes particle reservoir with chemical potential μ_i.
- Z_i denotes particle transfers flowing from reservoir R_i to system S.
- A_i denotes affinity between the reservoir R_i and R_0 (taken as the reference); If the whole system is isothermal, then $A_i = \beta(\mu_i - \mu_0)$, where $\beta \equiv (k_{\mathrm{B}} T)^{-1}$ is inverse temperature, and k_{B} the Boltzmann's constant.
- $\mathbf{Z} = (Z_1, \cdots, Z_{n-1})$, $\mathbf{A} = (A_1, \cdots, A_{n-1})$.
- $\mathcal{P}_{\mathbf{A}}(\mathbf{Z}, t)$ denotes the probability distribution of particle transfers $\mathbf{Z}$ during the time interval $[0,\ t]$.

$\mathcal{P}_{\mathbf{A}}(\mathbf{Z}, t)$ obeys the multivariate fluctuation relation, reading

$$\frac{\mathcal{P}_{\mathbf{A}}(\mathbf{Z}, t)}{\mathcal{P}_{\mathbf{A}}(-\mathbf{Z}, t)} \simeq_{t\to\infty} \exp\left(\mathbf{A} \cdot \mathbf{Z}\right).$$

Fluctuation Relation for Currents

We define the cumulant generating function in terms of the counting parameters $\boldsymbol{\lambda} = \{\lambda_i\}$ as

$$Q(\boldsymbol{\lambda}; \mathbf{A}) \equiv \lim_{t\to\infty} -\frac{1}{t} \ln \sum_{\mathbf{Z}} \mathcal{P}_{\mathbf{A}}(\mathbf{Z}, t)\, \mathrm{e}^{-\boldsymbol{\lambda}\cdot\mathbf{Z}},$$

then the fluctuation relation can be written in the following form,

$$Q(\boldsymbol{\lambda}; \mathbf{A}) = Q(\mathbf{A} - \boldsymbol{\lambda}; \mathbf{A}).$$

The mean currents and their diffusivities can be obtained by taking the successive derivatives of the cumulant generating function with respect to the counting parameters:

$$J_i(\mathbf{A}) \equiv \lim_{t\to\infty} \frac{1}{t} \langle Z_i(t) \rangle_{\mathbf{A}} = \left. \frac{\partial Q(\boldsymbol{\lambda}; \mathbf{A})}{\partial \lambda_i} \right|_{\boldsymbol{\lambda}=\mathbf{0}},$$

$$D_{ij}(\mathbf{A}) \equiv \lim_{t\to\infty} \frac{1}{2t} \langle [Z_i(t) - J_i t]\, [Z_j(t) - J_j t] \rangle_{\mathbf{A}} = -\frac{1}{2} \left. \frac{\partial^2 Q(\boldsymbol{\lambda}; \mathbf{A})}{\partial \lambda_i \partial \lambda_j} \right|_{\boldsymbol{\lambda}=\mathbf{0}},$$

where the notation $\langle \cdot \rangle$ stands for the sample average over the data from the counting statistics.

Application of Tensor Networks to Nonequilibrium Physics

Study the dynamical fluctuations in systems with stochastic dynamics.

- exploit tensor networks to obtain the long-time statistics, i.e. the large deviations, of trajectory observables from tilted generators (in analogy with finding quantum ground states);
- exploit tensor networks to efficiently sample rare events;
- extend tensor-network approach to finite time trajectories.

Table: Comparison Between Markov Jump Process and Quantum Dynamics.

	Markov Jmmp Process	Quantum Dynamics
state distribution	$\mathcal{P}(X,t)$ (probability)	$\|\Psi(X,t)\rangle$ (probability amplitude)
normalization	$\sum_X \mathcal{P}(X,t) = 1$	$\sum_X \langle\Psi^\dagger(X,t)\|\Psi(X,t)\rangle = 1$
evolution equation	master equation	Schrödinger equation
generator	L (not necessarily Hermitian)	H (Hamiltonian, always Hermitian)
propagator	$\exp(Lt)$	$\exp(-\mathrm{i}Ht/\hbar)$
stable distribution	steady state (eigenvector of L corresponding to the largest eigenvalue 0)	ground state (eigenvector of H corresponding to smallest eigenvalue)
state space	grows exponentially with the degree freedoms (number of state variables)	grows exponentially with the degree freedoms (number of state variables)

Two kinds of species

- holes h^+, positive charged, density p
- electrons e^-, negative charged, density n

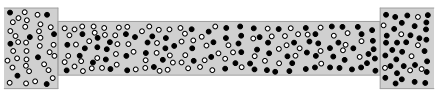

Figure: Schematic representation of the system. The white dots represent holes and the black ones represent electrons. At the two ends are the resevoirs with fixed densities, p_{L}, n_{L}, p_{R}, n_{R}.

Elementary process:

- hole diffusion, D
- electron diffusion, D
- generation and recombination reaction

$$\emptyset \underset{k_-}{\overset{k_+}{\rightleftharpoons}} h^+ + e^-,$$

where k_+ and k_- are respectively rate constants.

We neglect the long-ranged electrostatic interactions!!

The balance equations are

$$\partial_t n + \boldsymbol{\nabla} \cdot \mathbf{j}_n = \sigma_n,$$
$$\partial_t p + \boldsymbol{\nabla} \cdot \mathbf{j}_p = \sigma_p,$$

with the current densities

$$\mathbf{j}_n = -D\boldsymbol{\nabla} n + \delta\mathbf{j}_n,$$
$$\mathbf{j}_p = -D\boldsymbol{\nabla} p + \delta\mathbf{j}_p,$$

and reaction rate densities

$$\sigma_n = \sigma_p = k_+ - k_- np + \delta\sigma.$$

$\delta\mathbf{j}_n$, $\delta\mathbf{j}_p$, and $\delta\sigma$ are Gaussian white noises characterized by

$$\langle \delta\mathbf{j}_n(\mathbf{r},t) \otimes \delta\mathbf{j}_n(\mathbf{r}',t') \rangle = \Gamma_{nn}(\mathbf{r},t)\delta^3(\mathbf{r}-\mathbf{r}')\delta(t-t')\mathbf{I},$$
$$\langle \delta\mathbf{j}_p(\mathbf{r},t) \otimes \delta\mathbf{j}_p(\mathbf{r}',t') \rangle = \Gamma_{pp}(\mathbf{r},t)\delta^3(\mathbf{r}-\mathbf{r}')\delta(t-t')\mathbf{I},$$
$$\langle \delta\sigma(\mathbf{r},t)\, \delta\sigma(\mathbf{r}',t') \rangle = \Gamma_{\sigma\sigma}(\mathbf{r},t)\delta^3(\mathbf{r}-\mathbf{r}')\delta(t-t'),$$

where $\mathbf{I}$ is the 3×3 identity matrix and

$$\Gamma_{nn}(\mathbf{r},t) \equiv 2Dn(\mathbf{r},t),$$
$$\Gamma_{pp}(\mathbf{r},t) \equiv 2Dp(\mathbf{r},t),$$
$$\Gamma_{\sigma\sigma}(\mathbf{r},t) \equiv k_+ + k_- n(\mathbf{r},t)p(\mathbf{r},t),$$

are the spectral densities of the noises.

Spatial Discretization

- L cells
- each of length $\Delta x = l/L$, section area Σ, and volume $\Omega = \Sigma \Delta x$
- numbers of electrons and holes: $N_i = n(x_i)\Omega$, $P_i = p(x_i)\Omega$, with $x_i = (i - 0.5)\Delta x - l/2$ $(i = 1, 2, \cdots, L)$
- numbers of electrons and holes in reservoirs: $N_0 \equiv \bar{N}_{\rm L} = n_{\rm L}\Omega$, $N_{L+1} \equiv \bar{N}_{\rm R} = n_{\rm R}\Omega$, $P_0 \equiv \bar{P}_{\rm L} = p_{\rm L}\Omega$, and $P_{L+1} \equiv \bar{P}_{\rm R} = p_{\rm R}\Omega$.

The system state is specified by the hole numbers $\mathbf{P} = \{P_i\}_{i=1}^{L}$ and the electron numbers $\mathbf{N} = \{N_i\}_{i=1}^{L}$ in the cells and they evolve in time according to the network

$$
\begin{array}{ccccccccccccccc}
\bar{P}_{\rm L} & \underset{W_0^{(-P)}}{\overset{W_0^{(+P)}}{\rightleftarrows}} & P_1 & \underset{W_1^{(-P)}}{\overset{W_1^{(+P)}}{\rightleftarrows}} & P_2 & \underset{W_2^{(-P)}}{\overset{W_2^{(+P)}}{\rightleftarrows}} & \cdots & \underset{W_{L-2}^{(-P)}}{\overset{W_{L-2}^{(+P)}}{\rightleftarrows}} & P_{L-1} & \underset{W_{L-1}^{(-P)}}{\overset{W_{L-1}^{(+P)}}{\rightleftarrows}} & P_L & \underset{W_L^{(-P)}}{\overset{W_L^{(+P)}}{\rightleftarrows}} & \bar{P}_{\rm R} \\
 & & W_1^{(+)} \updownarrows W_1^{(-)} & & W_2^{(+)} \updownarrows W_2^{(-)} & & \cdots & & W_{L-1}^{(+)} \updownarrows W_{L-1}^{(-)} & & W_L^{(+)} \updownarrows W_L^{(-)} & & \\
\bar{N}_{\rm L} & \underset{W_0^{(-N)}}{\overset{W_0^{(+N)}}{\rightleftarrows}} & N_1 & \underset{W_1^{(-N)}}{\overset{W_1^{(+N)}}{\rightleftarrows}} & N_2 & \underset{W_2^{(-N)}}{\overset{W_2^{(+N)}}{\rightleftarrows}} & \cdots & \underset{W_{L-2}^{(-N)}}{\overset{W_{L-2}^{(+N)}}{\rightleftarrows}} & N_{L-1} & \underset{W_{L-1}^{(-N)}}{\overset{W_{L-1}^{(+N)}}{\rightleftarrows}} & N_L & \underset{W_L^{(-N)}}{\overset{W_L^{(+N)}}{\rightleftarrows}} & \bar{N}_{\rm R}
\end{array}
.
$$

Master Equation

The probability $\mathcal{P}(\mathbf{P}, \mathbf{N}, t)$ is ruled by the master equation

$$\frac{\mathrm{d}\mathcal{P}}{\mathrm{d}t} = \hat{L}\mathcal{P} = \sum_{i=0}^{L} \Big[\left(\mathrm{e}^{+\partial_{P_i}} \mathrm{e}^{-\partial_{P_{i+1}}} - 1\right) W_i^{(+P)} \mathcal{P} + \left(\mathrm{e}^{-\partial_{P_i}} \mathrm{e}^{+\partial_{P_{i+1}}} - 1\right) W_i^{(-P)} \mathcal{P} + \left(\mathrm{e}^{+\partial_{N_i}} \mathrm{e}^{-\partial_{N_{i+1}}} - 1\right) W_i^{(+N)} \mathcal{P} + \left(\mathrm{e}^{-\partial_{N_i}} \mathrm{e}^{+\partial_{N_{i+1}}} - 1\right) W_i^{(-N)} \mathcal{P} \Big] + \sum_{i=1}^{L} \Big[\left(\mathrm{e}^{-\partial_{P_i}} \mathrm{e}^{-\partial_{N_i}} - 1\right) W_i^{(+)} \mathcal{P} + \left(\mathrm{e}^{+\partial_{P_i}} \mathrm{e}^{+\partial_{N_i}} - 1\right) W_i^{(-)} \mathcal{P} \Big],$$

where the transition rates are

$$W_i^{(+P)} = kP_i, \qquad W_i^{(-P)} = kP_{i+1},$$
$$W_i^{(+N)} = kN_i, \qquad W_i^{(-N)} = kN_{i+1},$$
$$W_i^{(+)} = \Omega k_+, \qquad W_i^{(-)} = \Omega k_- \frac{N_i}{\Omega} \frac{P_i}{\Omega},$$

and $k \equiv D/\Delta x^2$ for brevity.

Operator Definitions (in Doi-Peliti Formalism)

The state of a local cell is denoted by $|P_i N_i\rangle$, then we define the operators

$$\langle P_i' N_i' | a_i^- | P_i N_i \rangle = k P_i \delta_{P_i', P_i - 1} \delta_{N_i', N_i}, \qquad \langle P_i' N_i' | a_i^+ | P_i N_i \rangle = \delta_{P_i', P_i + 1} \delta_{N_i', N_i},$$
$$\langle P_i' N_i' | b_i^- | P_i N_i \rangle = k N_i \delta_{P_i', P_i} \delta_{N_i', N_i - 1}, \qquad \langle P_i' N_i' | b_i^+ | P_i N_i \rangle = \delta_{P_i', P_i} \delta_{N_i', N_i + 1}.$$

For reservoir cells, the operators should defined separately

$$a_0^- = k \bar{P}_{\mathrm{L}}, \qquad a_0^+ = a_{L+1}^+ = 1, \qquad a_{L+1}^- = k \bar{P}_{\mathrm{R}}.$$
$$b_0^- = k \bar{N}_{\mathrm{L}}, \qquad b_0^+ = b_{L+1}^+ = 1, \qquad b_{L+1}^- = k \bar{N}_{\mathrm{R}}.$$

Besides, we define

$$\langle P_i' N_i' | a_i | P_i N_i \rangle = k P_i \delta_{P_i', P_i} \delta_{N_i', N_i},$$
$$\langle P_i' N_i' | b_i | P_i N_i \rangle = k N_i \delta_{P_i', P_i} \delta_{N_i', N_i},$$

- a_i^+ (b_i^+) is called local creation operator for holes (electrons);
- a_i^- (b_i^-) is called local annihilation operator for holes (electrons);
- a_i (b_i) is called local number operator for holes (electrons).

The Doi-Peliti formalism is the classical version of second quantization.

Operator Definitions

For the generation and recombination reaction, we can define the following operators:

$$\langle P_i' N_i' | c^+ | P_i N_i \rangle = k_+ \Omega \delta_{P_i'-1,P_i} \delta_{N_i'-1,N_i},$$

$$\langle P_i' N_i' | c^- | P_i N_i \rangle = k_- \Omega \frac{P_i}{\Omega} \frac{N_i}{\Omega} \delta_{P_i'+1,P_i} \delta_{N_i'+1,N_i},$$

$$\langle P_i' N_i' | c | P_i N_i \rangle = \left(k_+ \Omega + k_- \Omega \frac{P_i}{\Omega} \frac{N_i}{\Omega} \right) \delta_{P_i',P_i} \delta_{N_i',N_i}.$$

- c_i^+ is called local generation operator for hole-electron pair;
- c_i^- is called local recombination operator for hole-electron pair;
- c_i is called local xx operator for hole-electron pair.

Tilted Generator for the Master Equation

$$\begin{aligned}\hat{L}_\lambda =& a_0^- \otimes a_1^+ \mathrm{e}^{-\lambda} + a_0^+ \otimes a_1^- \mathrm{e}^{+\lambda} + \sum_{i=1}^{L} \left(a_i^- \otimes a_{i+1}^+ + a_i^+ \otimes a_{i+1}^- \right) - \sum_{i=0}^{L} \left(a_i + a_{i+1} \right) \\ &+ b_0^- \otimes b_1^+ \mathrm{e}^{+\lambda} + b_0^+ \otimes b_1^- \mathrm{e}^{-\lambda} + \sum_{i=1}^{L} \left(b_i^- \otimes b_{i+1}^+ + b_i^+ \otimes b_{i+1}^- \right) - \sum_{i=0}^{L} \left(b_i + b_{i+1} \right) \\ &+ \sum_{i=1}^{L} \left(c_i^+ + c_i^- - c_i \right)\end{aligned}$$

the parameter λ is included to count transfers of unit charge

the cumulant generating function turns out to be the leading eigenvalue of the tilted generator

Table: The values of quantities and parameters specified in numerical computations.

diffusion coefficient, D	0.01
width of each cell, Δx	0.1
number of cells in discretized channel, L	10
number of holes in left-reservoir cell, $\bar{N}_{\mathrm{L}}$	8
number of holes in right-reservoir cell, $\bar{N}_{\mathrm{R}}$	2
number of electrons in left-reservoir cell, $\bar{N}_{\mathrm{L}}$	2
number of electrons in right-reservoir cell, $\bar{N}_{\mathrm{R}}$	8
truncation parameter, M	25

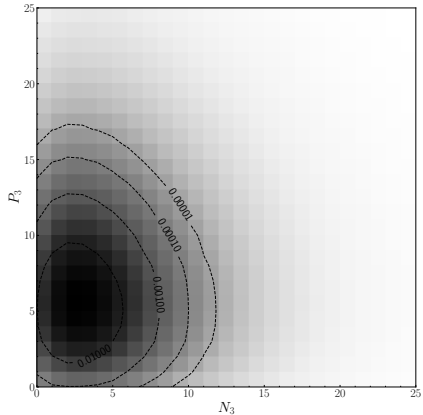

Figure: Probability distribuiton $\mathcal{P}(P_3, N_3)$ in the steady state. $k_+ = k_- = 10.0$.

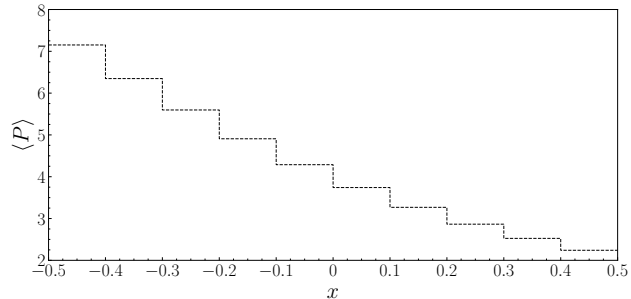

Figure: Mean number of holes $\langle P \rangle$ in the steady state. $k_+ = k_- = 10.0$.

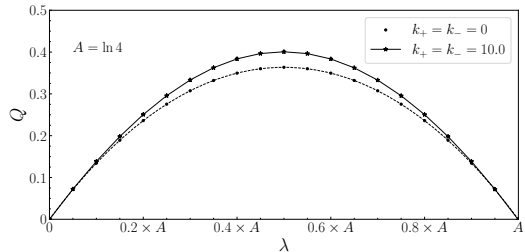

Figure: Cumulant generating function. The dash line is the analytical solution in the case $k_+ = k_- = 0$.

Gallavotti-Cohen symmetry: $Q(\lambda) = Q(A - \lambda)$.

In the case $k_+ = k_- = 0$ (the reaction is turned off), the cumulant generating function reads

$$Q(\lambda) = \overbrace{\frac{k\bar{P}_\mathrm{L}}{L+1}\left(1-\mathrm{e}^{-\lambda}\right) + \frac{k\bar{P}_\mathrm{R}}{L+1}\left(1-\mathrm{e}^{+\lambda}\right)}^{\text{hole contribution}} + \underbrace{\frac{k\bar{N}_\mathrm{L}}{L+1}\left(1-\mathrm{e}^{+\lambda}\right) + \frac{k\bar{N}_\mathrm{R}}{L+1}\left(1-\mathrm{e}^{-\lambda}\right)}_{\text{electron contribution}}.$$

So we have

$$A = \ln\frac{\bar{P}_\mathrm{L}}{\bar{P}_\mathrm{R}} \equiv \ln\frac{\bar{N}_\mathrm{R}}{\bar{N}_\mathrm{L}},$$

$$J = \overbrace{\frac{k(\bar{P}_\mathrm{L}-\bar{P}_\mathrm{R})}{L+1}}^{\text{hole contribution}} + \underbrace{\frac{k(\bar{N}_\mathrm{R}-\bar{N}_\mathrm{L})}{L+1}}_{\text{electron contribution}},$$

$$D = \overbrace{\frac{k(\bar{P}_\mathrm{L}+\bar{P}_\mathrm{R})}{2(L+1)}}^{\text{hole contribution}} + \underbrace{\frac{k(\bar{N}_\mathrm{L}+\bar{N}_\mathrm{R})}{2(L+1)}}_{\text{electron contribution}}.$$

We arrive at the equality:

$$A = \ln\frac{2D+J}{2D-J},$$

or equivalently

$$D = J\left(\frac{1}{\mathrm{e}^A-1}+\frac{1}{2}\right).$$

In the case $k_+ = k_- = 10.0$ (the reaction is turned on):

- A is the same;
- J is the same (first derivative of $Q(\lambda)$, with some analysis);
- D is smaller (second derivative of $Q(\lambda)$).

We arrive at inequality

$$D < J\left(\frac{1}{e^A - 1} + \frac{1}{2}\right).$$

A new thermodynamic uncertainty relation (upper bound)??

Conclusion and Perspectives

Conclusion:

- We demonstrate the power of tensor networks in their application to nonequilibrium physics.
- The cumulant generating function (or large deviation function) for the current in 1D diffusion-reaction systems is for the first time evaluated with DMRG approach.
- The current fluctuations is dampened by the nonlinear reactions between two species of charge carriers.

Perspectives

- The power of tensor networks in the application to nonequilibrium physics is far from being fully exploited, I hope more Chinese scientists can enter into this field.

Thank You!