Upper Bounded Current Fluctuation in One-Dimensional Driven Transport Systems

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Figure 1: 张凡，2023 年北京大学博士毕业，目前在日本做博后。

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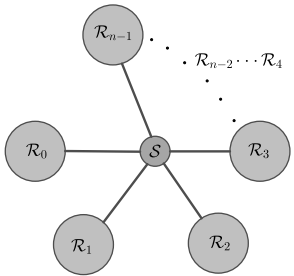

Figure 2: Schematic representation of a system S in contact with n particle reservoirs $R_0,\ R_1,\ R_2, \cdots, R_{n-1}$.

- 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.
- $\mathbf{Z} = (Z_1, \cdots, Z_{n-1})$, $\mathbf{A} = (A_1, \cdots, A_{n-1})$.
- $\mathcal{P}_{\mathbf{A}}(\mathbf{Z}, t)$ 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

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

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.

According to the multivariate fluctuation relation, the entropy production rate is given by

$$\frac{1}{k_{\mathrm{B}}}\frac{\mathrm{d}_{\mathrm{i}}S}{\mathrm{d}t} = \mathbf{A}\cdot\mathbf{J}(\mathbf{A}) = \lim_{t\to\infty}\frac{1}{t}\sum_{\mathbf{Z}}\mathcal{P}_{\mathbf{A}}(\mathbf{Z},t)\ln\frac{\mathcal{P}_{\mathbf{A}}(\mathbf{Z},t)}{\mathcal{P}_{\mathbf{A}}(-\mathbf{Z},t)}$$

in terms of the Kullback-Leibler divergence between the distributions $\mathcal{P}_{\mathbf{A}}(\mathbf{Z},t)$ and $\mathcal{P}_{\mathbf{A}}(-\mathbf{Z},t)$. It is always non-negative, which is in accord with the second law of thermodynamics.

- The entropy production implied by the fluctuation relation can serve as a measure of the breaking of the time-reversal symmetry of nonequilibrium probability distribution $\mathcal{P}_{\mathbf{A}}(\mathbf{Z},t)$.
- In equilibrium where $\mathbf{A}=\mathbf{0}$, detailed balance is recovered since $\mathcal{P}_{\mathbf{0}}(\mathbf{Z},t)\simeq\mathcal{P}_{\mathbf{0}}(-\mathbf{Z},t)$ by the fluctuation relation, and the entropy production rate is vanishing together with the affinities and the mean currents.

Introduction – Thermodynamic Uncertainty Relation (TUR)

The steady state TUR for a general Markovian dynamics is expressed as

$$\epsilon^2(\tau) \equiv \frac{\mathrm{var}(\Theta)}{\langle\Theta\rangle^2} \geq \frac{2k_{\mathrm{B}}}{\langle\Sigma\rangle},$$

where

- Θ is an arbitrary time-integrated current over some observation time $[0, \tau]$,
- $\mathrm{var}(\Theta) \equiv \langle\Theta^2\rangle - \langle\Theta\rangle^2$ the variance of Θ,
- $\langle\Sigma\rangle$ the total entropy production accumulated by τ.

For one-dimensional transport systems, the original TUR can be developed to yield an equivalent form

$$\frac{D}{J} \geq \frac{1}{A}.$$

Upper Bounded Current Fluctuation

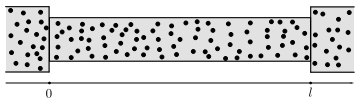

Figure 3: Schematic representation of a system in contact with 2 particle reservoirs.

We conjecture a upper bound for the current fluctuation:

$$\boxed{\frac{2D}{J} \leq \coth(A/2)}$$

- $J \equiv \lim_{t\to\infty}\langle Z_t\rangle/t$ is the mean current
- $D \equiv \langle (Z - Jt)\rangle/(2t)$ is the current diffusivity
- A is the affinity

Coarse-Grained Model

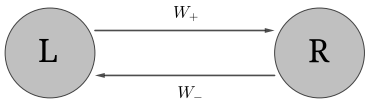

Figure 4: The system consisting of only two reservoirs with particles stochastically exchanging between them.

$$\frac{2D}{J} = \coth(A/2)$$

$$Q(\lambda) = W_+ \left(1 - \mathrm{e}^{-\lambda}\right) + W_- \left(1 - \mathrm{e}^{+\lambda}\right)$$

$$A = \ln \frac{W_+}{W_-}$$

$$J = \left.\frac{\partial Q}{\partial \lambda}\right|_{\lambda=0} = W_+ - W_-,$$

$$D = -\frac{1}{2}\left.\frac{\partial^2 Q}{\partial \lambda^2}\right|_{\lambda=0} = \frac{W_+ + W_-}{2}$$

Quantum Ballistic Transport

One-dimensional nonequilibrium system for fermionic ballistic transport.

- atomic chain, a nanowire, or a series of quantum dots
- a nanowire
- a series of quantum dots

The mean current and its diffusivity are given by the Landauer-Buttike formula

$$J = \int \frac{\mathrm{d}\omega}{2\pi} \mathbb{T}(\omega) \left(n_{\mathrm{L}} - n_{\mathrm{R}}\right),$$

$$D = \int \frac{\mathrm{d}\omega}{4\pi} \mathbb{T}(\omega) \left[(n_{\mathrm{L}}\bar{n}_{\mathrm{R}} + \bar{n}_{\mathrm{L}} n_{\mathrm{R}}) - \left(n_{\mathrm{L}} - n_{\mathrm{R}}\right)^2\right],$$

where the transmission function $\mathbb{T}(\omega) \in [0, 1]$ is determined by the microscopic model of the system and calculated by the nonequilibrium Green's function. The Fermi distribution of the electron with the energy ω of the reservoir $\alpha = \mathrm{L}, \mathrm{R}$ is

$$n_\alpha(\omega) = \frac{1}{\mathrm{e}^{\beta(\omega - \mu_\alpha)} + 1},$$

and

$$\bar{n}_\alpha(\omega) = 1 - n_\alpha(\omega).$$

We obtain

$$\frac{2D}{J} = \frac{\int \frac{\mathrm{d}\omega}{2\pi}\mathbb{T}(\omega)(n_{\mathrm{L}}\bar{n}_{\mathrm{R}} + \bar{n}_{\mathrm{L}}n_{\mathrm{R}})}{\int \frac{\mathrm{d}\omega}{2\pi}\mathbb{T}(\omega)(n_{\mathrm{L}}\bar{n}_{\mathrm{R}} - \bar{n}_{\mathrm{L}}n_{\mathrm{R}})} - \frac{\int \frac{\mathrm{d}\omega}{2\pi}\mathbb{T}(\omega)(n_{\mathrm{L}} - n_{\mathrm{R}})^2}{\int \frac{\mathrm{d}\omega}{2\pi}\mathbb{T}(\omega)(n_{\mathrm{L}}\bar{n}_{\mathrm{R}} - \bar{n}_{\mathrm{L}}n_{\mathrm{R}})} \leq \frac{\int \frac{\mathrm{d}\omega}{2\pi}\mathbb{T}(\omega)(n_{\mathrm{L}}\bar{n}_{\mathrm{R}} + \bar{n}_{\mathrm{L}}n_{\mathrm{R}})}{\int \frac{\mathrm{d}\omega}{2\pi}\mathbb{T}(\omega)(n_{\mathrm{L}}\bar{n}_{\mathrm{R}} - \bar{n}_{\mathrm{L}}n_{\mathrm{R}})},$$

where $n_{\mathrm{L}}\bar{n}_{\mathrm{R}} \geq \bar{n}_{\mathrm{L}}n_{\mathrm{R}}$ is assumed. The last term can be simplified,

$$\text{last term} = \frac{\int \frac{\mathrm{d}\omega}{2\pi}\mathbb{T}(\omega)\bar{n}_{\mathrm{L}}n_{\mathrm{R}}(\mathrm{e}^{A} + 1)}{\int \frac{\mathrm{d}\omega}{2\pi}\mathbb{T}(\omega)\bar{n}_{\mathrm{L}}n_{\mathrm{R}}(\mathrm{e}^{A} - 1)} = \coth(A/2),$$

where the relation for the affinity

$$A = \ln \frac{n_{\mathrm{L}}\bar{n}_{\mathrm{R}}}{\bar{n}_{\mathrm{L}}n_{\mathrm{R}}} = \beta\,(\mu_{\mathrm{L}} - \mu_{\mathrm{R}})$$

is used.

$$\boxed{\frac{2D}{J} \leq \coth(A/2)}$$

Symmetric Simple Exclusion Process (SSEP)

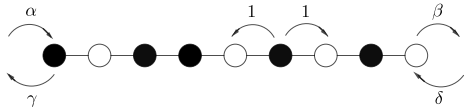

Figure 5: The symmetric simple exclusion process. The black (white) circles denote occupied (vacant) sites.

Dynamics:

- particles hop to a vacant neighboring site at a rate of 1 in the bulk.
- particles enter (exit) at the left and right boundries at rates α (γ) and δ (β).

For this system, we have

$$\rho_{\mathrm{L}} = \frac{\alpha}{\alpha+\gamma}, \qquad a = \frac{1}{\alpha+\gamma},$$
$$\rho_{\mathrm{R}} = \frac{\delta}{\beta+\delta}, \qquad b = \frac{1}{\beta+\delta},$$

where ρ_{L} and ρ_{R} are identified as the densities of the left and right reservoirs.

Symmetric Simple Exclusion Process (SSEP)

The mean current and the diffusivity are given by

$$J = (\rho_{\mathrm{L}} - \rho_{\mathrm{R}})/\tilde{L},$$

$$D = \frac{1}{2\tilde{L}}(\rho_{\mathrm{L}} + \rho_{\mathrm{R}} - 2\rho_{\mathrm{L}}\rho_{\mathrm{R}}) + \frac{a(a-1)(2a-1) + b(b-1)(2b-1) - \tilde{L}(\tilde{L}-1)(2\tilde{L}-1)}{6\tilde{L}^3(\tilde{L}-1)}(\rho_{\mathrm{L}} - \rho_{\mathrm{R}})^2,$$

where $\tilde{L} \equiv L + a + b - 1$ and L denotes the number of sites.

The affinity can be evaluated,

$$A = \ln \frac{\rho_{\mathrm{L}}\bar{\rho}_{\mathrm{R}}}{\bar{\rho}_{\mathrm{L}}\rho_{\mathrm{R}}} = \ln \frac{\alpha\beta}{\gamma\delta},$$

where $\bar{\rho}_{\mathrm{L}} \equiv 1 - \rho_{\mathrm{L}}$ and $\bar{\rho}_{\mathrm{R}} \equiv 1 - \rho_{\mathrm{R}}$.

We obtain

$$\frac{2D}{J} = \frac{\rho_{\mathrm{L}} + \rho_{\mathrm{R}} - 2\rho_{\mathrm{L}}\rho_{\mathrm{R}}}{\rho_{\mathrm{L}} - \rho_{\mathrm{R}}} + \frac{a(a-1)(2a-1) + b(b-1)(2b-1) - \tilde{L}(\tilde{L}-1)(2\tilde{L}-1)}{3\tilde{L}^2(\tilde{L}-1)}(\rho_{\mathrm{L}} - \rho_{\mathrm{R}}).$$

The first term on the right-hand side can be further simplified as

$$\frac{\rho_{\mathrm{L}} + \rho_{\mathrm{R}} - 2\rho_{\mathrm{L}}\rho_{\mathrm{R}}}{\rho_{\mathrm{L}} - \rho_{\mathrm{R}}} = \frac{\rho_{\mathrm{L}}\bar{\rho}_{\mathrm{R}} + \rho_{\mathrm{R}}\bar{\rho}_{\mathrm{L}}}{\rho_{\mathrm{L}}\bar{\rho}_{\mathrm{R}} - \rho_{\mathrm{R}}\bar{\rho}_{\mathrm{L}}} = \frac{\alpha\beta + \delta\gamma}{\alpha\beta - \delta\gamma} = \frac{\mathrm{e}^{A} + 1}{\mathrm{e}^{A} - 1} = \coth(A/2),$$

giving what we expect. The second term can be shown that it is negative (details omitted here).

$$\boxed{\frac{2D}{J} \leq \coth(A/2)}$$

Symmetric Simple Exclusion Process (SSEP)

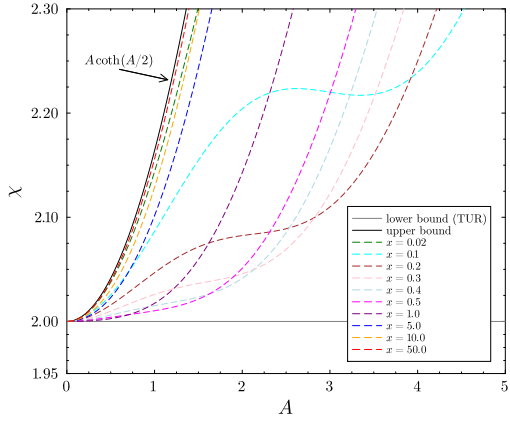

Figure 6: The behavior of $\chi \equiv 2DA/J$ as a function of A with different particle densities (controlled by a parameter $x \equiv \gamma/\alpha$ with small value for high density and large value for low density) for SSEP. The parameter values are $\gamma = \beta = 1$ and $L = 10$. The condition $y = \mathrm{e}^{A}x$ with $y \equiv \beta/\delta$ is also imposed.

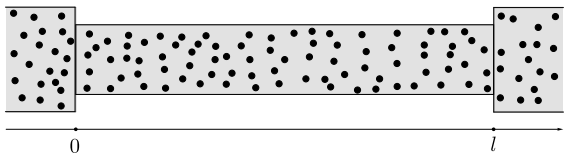

Figure 7: Schematic representation of a system in contact with 2 particle reservoirs.

$$\bar{N}_{\mathrm{L}} \underset{W_0^{(-)}}{\overset{W_0^{(+)}}{\rightleftharpoons}} N_1 \underset{W_1^{(-)}}{\overset{W_1^{(+)}}{\rightleftharpoons}} N_2 \underset{W_2^{(-)}}{\overset{W_2^{(+)}}{\rightleftharpoons}} \cdots \underset{W_{i-1}^{(-)}}{\overset{W_{i-1}^{(+)}}{\rightleftharpoons}} N_i \underset{W_i^{(-)}}{\overset{W_i^{(+)}}{\rightleftharpoons}} \cdots \underset{W_{L-2}^{(-)}}{\overset{W_{L-2}^{(+)}}{\rightleftharpoons}} N_{L-1} \underset{W_{L-1}^{(-)}}{\overset{W_{L-1}^{(+)}}{\rightleftharpoons}} N_I \underset{W_L^{(-)}}{\overset{W_L^{(+)}}{\rightleftharpoons}} \bar{N}_{\mathrm{R}}$$

Transport of Charged Particles

The transition rates are

$$W_i^{(+)} = \frac{\mathcal{D}}{\Delta x^2}\psi(\Delta U_{i,i+1})N_i$$
$$W_i^{(-)} = \frac{\mathcal{D}}{\Delta x^2}\psi(\Delta U_{i+1,i})N_{i+1}$$

The intrinsic energy change

$$\Delta U_{i,i+1} = e(\Phi_{i+1} - \Phi_i) + \frac{e^2 L \Delta x^2}{2(L+1)\epsilon\Omega}$$

The function

$$\psi(\Delta U) = \frac{\beta\Delta U}{\exp(\beta\Delta U) - 1} \qquad \text{and} \qquad \psi(\Delta U) = \psi(-\Delta U)\exp(-\beta\Delta U)$$

The (theoretical) affinity

$$A^{(\mathrm{t})} = \beta e(\Phi_{\mathrm{L}} - \Phi_{\mathrm{R}})$$

Transport of Charged Particles

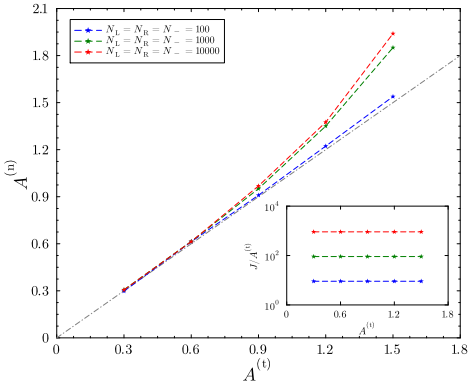

Figure 8: The comparison between numerical affinities and theoretical affinities. The asterisks are numerical points with dashed lines joining them. It is set that $\bar{N}_L = \bar{N}_R = N_-$, and takes different values in three cases. The parameter values are $\beta = e = 1.0$, $D = \epsilon = 0.01$, $\Omega = 10000$, $\Delta x = 0.1$, $L = 10$.

$$A^{(n)} = \ln \frac{2D + J}{2D - J} \geq A^{(t)}$$

$$\Downarrow$$

$$\frac{2D}{J} \leq \coth(A/2)$$

Transport of Charged Particles

In the low-density limit, the cumulant generating function can be exactly solved,

$$Q(\lambda) = W_+ \left(1 - \mathrm{e}^{-\lambda}\right) + W_- \left(1 - \mathrm{e}^{+\lambda}\right),$$

where the global transition rates are

$$W_+ = \frac{\mathcal{D}\bar{N}}{\Delta x^2 (L+1)} \frac{\beta e(\Phi_\mathrm{R} - \Phi_\mathrm{L})}{\exp\left[\beta e(\Phi_\mathrm{R} - \Phi_\mathrm{L})\right] - 1}, \qquad W_- = \frac{\mathcal{D}\bar{N}}{\Delta x^2 (L+1)} \frac{\beta e(\Phi_\mathrm{L} - \Phi_\mathrm{R})}{\exp\left[\beta e(\Phi_\mathrm{L} - \Phi_\mathrm{R})\right] - 1}.$$

In this case,

$$J = W_+ - W_-, \qquad D = \frac{W_+ + W_-}{2}, \qquad A = \ln \frac{W_+}{W_-} = \beta e(\Phi_\mathrm{L} - \Phi_\mathrm{R}).$$

$$\Downarrow$$

$$\boxed{\frac{2D}{J} = \coth(A/2)}$$

Conclusion

We have conjectured an inequality bounding from above the current fluctuation in one-dimensional transport systems

$$\boxed{\frac{2D}{J} \leq \coth(A/2)}$$

Our conjectured inequality is shown to hold case-by-case in several systems for classical diffusive transport and quantum ballistic transport.

For quantum ballistic systems, the transmission function encoding the detailed dynamics is irrelevant in the above proof, manifesting that the proof applies to a broad class of dfferent quantum systems.

The equality sign holds under certain conditions, showing that our inequality is tightest.

Thank You!