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Untangling dissipative and Hamiltonian effects in bulk and boundary driven systems

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Abstract

Using the theory of large deviations, macroscopic fluctuation theory provides a framework to understand the behaviour of non-equilibrium dynamics and steady states in *diffusive* systems. We extend this framework to a minimal model of non-equilibrium *non-diffusive* system, specifically an open linear network on a finite graph. We explicitly calculate the dissipative bulk and boundary forces that drive the system towards the steady state, and non-dissipative bulk and boundary forces that drives the system in orbits around the steady state. Using the fact that these forces are orthogonal in a certain sense, we provide a decomposition of the large-deviation cost into dissipative and non-dissipative terms. We establish that the purely non-dissipative force turns the dynamics into a Hamiltonian system. These theoretical findings are illustrated by numerical examples.

1 Introduction

It is well known that if a microscopic stochastic particle system is in detailed balance, then large fluctuations around the macroscopic dynamics (large-deviations theory) induce a gradient flow of the free energy. This principle was first discovered by Onsager and Machlup in their groundbreaking paper [OM53] for a simple process with vanishing white noise, and their result may be identified with the more rigorous and general Freidlin-Wentzell theory [FW12]. However, as Onsager and Machlup stated in 1953:

> The proof of the reciprocal relations [...] was based on the hypothesis of microscopic reversibility, which we retain here. This excludes rotating systems (Coriolis forces) and systems with external magnetic fields. The assumption of Gaussian random variables is also restrictive: Our system must consist of many "sufficiently" independent particles, and equilibrium must be stable at least for times of the order of laboratory measuring times.

Regarding the Gaussian noise, extensions to different noise have been known for a long time, see for example [BDSG$^+$04]. What these models have in common is that, although on a microscopic level the noise is non-Gaussian, macroscopically these systems are diffusive, which corresponds to quadratic large deviations, i.e. the rate functional is of the form $\frac{1}{2}\int_0^T \|\dot\rho(t) - \frac{1}{2}\operatorname{grad}\mathcal{V}(\rho(t))\|^2_{\rho(t)}\,dt$ for some ρ-dependent norm, gradient corresponding to that norm, and free energy or quasipotential $\mathcal{V}$. A simple expanding-the-squares then yields the form predicted by Onsager and Machlup. Different, for example, Poissonian noise may lead to non-quadratic large deviations, but as discovered in [MPR14], the Onsager-Machlup principle still holds for systems in detailed balanced if one allows for *nonlinear* macroscopic response relation between the forces involved and the velocity.

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Regarding the ‘rotating systems’ mentioned by Onsager and Machlup, these generally correspond to a breaking of detailed balance at the microscopic scale, and a combination of dissipative and non-dissipative effects at the macroscopic scale. Although both effects are strongly intertwined, the field of macroscopic fluctuation theory (MFT) [BDSG+02, BDSG+04, BDSG+15] allows an orthogonal decomposition into dissipative and non-dissipative fluxes, albeit, for diffusive systems. For non-diffusive systems the large deviations are not quadratic and such decomposition becomes more subtle, but some progress has been made recently using a generalised orthogonality [KJZ18, RZ21].

In recent work [PRS21] it was discovered that for various non-quadratic large deviations, the resulting purely non-dissipative fluxes correspond to a Hamiltonian system with periodic orbit solutions. This precisely delineates the role of dissipative fluxes which drive the system to its steady state from non-dissipative fluxes which drive the system out of detailed balance precisely through a Hamiltonian flow. However all systems studied in that work are driven out of detailed balance by bulk effects. In the current work our aim is to precisely understand how bulk and boundary effects can jointly drive a system out of detailed balance, and we achieve this by studying a linear network with open boundaries. This minimal model is sufficiently rich to understand the role of bulk and boundary individually and provide guidelines to more complex nonlinear systems.

We avoid the terminology (non)equilibrium and (ir)reversibility and talk about (non)detailed balance instead.

2 Model

Throughout, $\mathcal{X}$ is a finite directed graph, with weights Q_{xy} on edges $(x,y) \in \mathcal{X}\times\mathcal{X}$, $x \neq y$. In addition, each node $x \in \mathcal{X}$ is equipped with weights $\lambda_{\mathrm{in}x}, \lambda_{\mathrm{out}x}$ modelling the in- and outflow of that node, see Figure 1 for an example (see Section 7 for numerical results for this example). We only assume (a) $Q_{xy} = 0 \iff Q_{yx} = 0$, (b) $\lambda_{\mathrm{in}x} = 0 \iff \lambda_{\mathrm{out}x} = 0$ and (c) that the graph with nonzero weights $Q_{xy} > 0$ is irreducible.

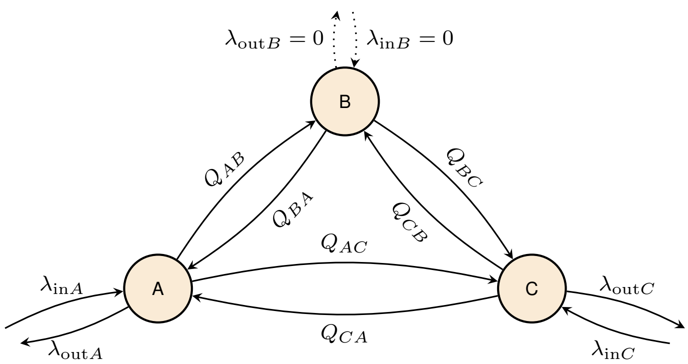

Figure 1: An example of a linear network with open boundaries.

Defining $Q_{xx} := -\sum_{y\in\mathcal{X}, y\neq x} Q_{xy}$ as usual, the macroscopic evolution of mass $\rho(t) \in \mathbb{R}^{\mathcal{X}}$ on the graph is

$$\dot\rho(t) = \big(Q - \mathrm{diag}(\lambda_{\mathrm{out}})\big)^{\mathsf{T}} \rho(t) + \lambda_{\mathrm{in}}. \tag{2.1}$$

In order to investigate non-dissipative effects we study *net* fluxes $j(t)$ in addition to the mass density $\rho(t)$. To this aim we equip the graph $\mathcal{X}$ with an (arbitrary) ordering, which defines the positive edges $\mathcal{E} := \{(x,y) : x,y \in \mathcal{X}, x < y\} \cup \{(\mathrm{in}x) : x \in \mathcal{X}\}$. The macroscopic *flux formulation* of (2.1) is

$$j_{xy}(t) = j^0_{xy}(\rho(t)), \qquad j_{\mathrm{in}x}(t) = j^0_{\mathrm{in}x}(\rho(t)), \qquad \dot\rho_x(t) = -\,\overline{\mathrm{div}}_x\, j(t), \tag{2.2}$$

where the traffic on the positive edges is $j^0_{xy}(\rho) := \rho_x Q_{xy} - \rho_y Q_{yx}$ and $j^0_{\mathrm{in}x}(\rho) := \lambda_{\mathrm{in}x} - \rho_x\lambda_{\mathrm{out}x}$, and the discrete divergence operator on fluxes $j \in \mathbb{R}^{\mathcal{E}}$ is defined as

$$\overline{\mathrm{div}}_x\, j := \sum_{y\in\mathcal{X}:y>x} j_{xy} - \sum_{y\in\mathcal{X}:y<x} j_{yx} - j_{\mathrm{in}x}. \tag{2.3}$$

This particular definition of the discrete divergence accounts for the net fluxes and arises from the following natural underlying (stochastic) microscopic particle system.

The large parameter n will be used to control the *order* of the total number of particles in the system, although this number is generally not conserved over time. At each node x, new particles are randomly created with rate $n\lambda_{\mathrm{in}x}$ and independently of all other particles, each particle either randomly jumps to node y with rate Q_{xy}, or is randomly destroyed with rate $\lambda_{\mathrm{out}x}$. We are interested in the random particle density $n\rho^{(n)}_x(t)$ which counts the number of particles at node x and time t, the cumulative net flux $nW^{(n)}_{xy}(t)$, which counts the number of jumps $x \to y$ minus the jumps $y \to x$ in time interval $(0,t]$, and the net flux $nW^{(n)}_{\mathrm{in}x}$, counting the number of particles created minus the number of particles destroyed at that node x in time interval $(0,t]$.

By Kurtz' Theorem [Kur70], the Markov process $(\rho^{(n)}(t), W^{(n)}(t))$ converges as $n\to\infty$ to the solution $(\rho(t), w(t))$ of (2.2), where we identify the derivative $\dot w(t)$ of the cumulative net flux with the net flux $j(t)$. We stress that for finite n, the continuity equation $\dot\rho = -\,\overline{\mathrm{div}}\, j$ holds almost surely, but random fluctuations occur in the fluxes.

On an exponential scale, these fluctuations satisfy a large-deviation principle [SW95, Ren18, PR19][1]

$$\mathrm{Prob}\big((\rho^{(n)}, W^{(n)}) \approx (\rho, w)\big) \overset{n\to\infty}{\sim} \exp\big(-n\textstyle\int_0^T \mathcal{L}\big(\rho(t), \dot w(t)\big)\,dt\big), \tag{2.4}$$

where we implicitly set the exponent to $-\infty$ if the continuity equation $\dot\rho(t) \equiv -\,\overline{\mathrm{div}}\, j(t)$ is violated, and

$$\begin{aligned}\mathcal{L}(\rho, j) := \sum\sum_{\substack{x,y\in\mathcal{X}\\x<y}} \inf_{j^+_{xy}\ge 0} \big[s(j^+_{xy} \mid \rho_x Q_{xy}) + s(j^+_{xy} - j_{xy} \mid \rho_y Q_{yx})\big]\\ + \sum_{x\in\mathcal{X}} \inf_{j^+_{\mathrm{in}x}\ge 0} \big[s(j^+_{\mathrm{in}x} \mid \lambda_{\mathrm{in}x}) + s(j^+_{\mathrm{in}x} - j_{\mathrm{in}x} \mid \rho_x\lambda_{\mathrm{out}x})\big],\end{aligned} \tag{2.5}$$

using the usual (non-negative and convex) relative entropy function $s(a \mid b) := a\log\frac{a}{b} - a + b$. The infima in the definition of $\mathcal{L}$ contracts the large-deviation principle of the one-way fluxes to the large-deviation principle of the net fluxes [DZ09, Thm. 4.2.1]. It is easily checked that $\mathcal{L}$ is non-negative and satisfies $\mathcal{L}(\rho, j^0) = 0$, i.e. j^0 is the zero-cost flux.

It will often be convenient to work with the convex (bi-)dual of $\mathcal{L}(\rho,\cdot)$, defined for forces $\zeta \in \mathbb{R}^{\mathcal{E}}$ acting on net fluxes

$$\begin{aligned}\mathcal{H}(\rho,\zeta) := \sup_{j\in\mathbb{R}^{\mathcal{E}}} \zeta\cdot j - \mathcal{L}(\rho, j) = \sum\sum_{\substack{x,y\in\mathcal{X}\\x<y}} \big[\rho_x Q_{xy}\left(e^{\zeta_{xy}} - 1\right) + \rho_y Q_{yx}\left(e^{-\zeta_{xy}} - 1\right)\big]\\ + \sum_{x\in\mathcal{X}} \big[\lambda_{\mathrm{in}x}\left(e^{\zeta_{\mathrm{in}x}} - 1\right) + \rho_x\lambda_{\mathrm{out}x}\left(e^{-\zeta_{\mathrm{in}x}} - 1\right)\big].\end{aligned}$$

As $j^0(\rho)$ from (2.2) is the zero-cost flux, we can write $j^0(\rho) = \nabla_\zeta \mathcal{H}(\rho, 0)$.

[1] We ignore possible contributions from random initial fluctuations since they they play no role in our paper whatsoever.

3 Invariant measure, quasipotential and time reversal

The macroscopic equation (2.1) has a unique, coordinate-wise positive steady state $\pi \in \mathbb{R}^{\mathcal{X}}$ (see Appendix A.1). Moreover, for fixed n, the random process $\rho^{(n)}(t)$ has the unique invariant measure $\Pi^{(n)} \in \mathcal{P}(\mathbb{R}^{\mathcal{X}})$ of product-Poisson form

$$\Pi^{(n)}(\rho) := \begin{cases} \prod_{x\in\mathcal{X}} \frac{(n\pi_x)^{n\rho_x} e^{-n\pi_x}}{(n\rho_x)!} & \rho \in (\frac{1}{n}\mathbb{N}_0)^{\mathcal{X}}, \\ 0, & \text{otherwise}, \end{cases} \tag{3.1}$$

see Appendix A.1. By Stirling's formula one obtains that the invariant measure satisfies a large deviation principle $\Pi^{(n)}(\rho) \sim e^{-n\mathcal{V}(\rho)}$ with quasipotential

$$\mathcal{V}(\rho) := \sum_{x\in\mathcal{X}} s(\rho_x|\pi_x), \tag{3.2}$$

which can also be interpreted as $(k_B T)^{-1}\times$ the Helmholtz free energy if $\pi_x = e^{-E_x/k_B T}$ for some energy function E_x, Boltzmann constant k_B and temperature T. Let the discrete gradient $\overline{\nabla}$ be the adjoint of $-\overline{\operatorname{div}}$ from (2.3), i.e. $\overline{\nabla}_{xy}\,\xi := \xi_y - \xi_x$, $\overline{\nabla}_{\mathrm{in}x}\,\xi := \xi_x$. With this notation the quasipotential (3.2) is related to the dynamic large deviations through the Hamilton-Jacobi-Bellman equation $\mathcal{H}(\rho, \overline{\nabla}\,\nabla\,\mathcal{V}(\rho)) = 0$; this can be calculated explicitly but also follows abstractly from the large-deviation principle for the invariant measure, see for example [BDSG+02, Eq. (2.7)] or [PRS21, Thm. 3.6].

Without further assumptions, the quasipotential $\mathcal{V}$ is indeed a Lyapunov functional along the macroscopic dynamics (2.1), which can be calculated explicitly

$$\begin{aligned} &-\frac{1}{2}\frac{d}{dt}\mathcal{V}\big(\rho(t)\big) \\ &= \underbrace{\sum_{\substack{x,y\in\mathcal{X}\\x\neq y}} s\Big(\rho_x Q_{xy} \mid \sqrt{\rho_x\rho_y\tfrac{\pi_x}{\pi_y}}Q_{xy}\Big) + \sum_{x\in\mathcal{X}}\Big[s\Big(\lambda_{\mathrm{in}x} \mid \sqrt{\frac{\rho_x}{\pi_x}}\lambda_{\mathrm{in}x}\Big) + s\Big(\rho_x\lambda_{\mathrm{out}x} \mid \sqrt{\rho_x\pi_x}\lambda_{\mathrm{out}x}\Big)\Big]}_{=\mathcal{L}^{\mathrm{asym}}(\rho,j^0(\rho))\geq 0} \\ &\underbrace{+\frac{1}{2}\sum_{\substack{x,y\in\mathcal{X}\\x\neq y}}\Big(\sqrt{\rho_x Q_{xy}} - \sqrt{\rho_y Q_{xy}\frac{\pi_x}{\pi_y}}\Big)^2 + \frac{1}{2}\sum_{x\in\mathcal{X}}\Big[\Big(\sqrt{\lambda_{\mathrm{in}x}} - \sqrt{\frac{\rho_x}{\pi_x}\lambda_{\mathrm{in}x}}\Big)^2 + \Big(\sqrt{\rho_x\lambda_{\mathrm{out}x}} - \sqrt{\pi_x\lambda_{\mathrm{out}x}}\Big)^2\Big]}_{=\Psi^*_{F^{\mathrm{asym}}}(\rho,F^{\mathrm{sym}}(\rho))\geq 0}. \end{aligned} \tag{3.3}$$

In Section 5 we introduce $\mathcal{L}^{\mathrm{asym}}(\rho, j^0(\rho))$ and see that it forms the cost of the macroscopic dynamics (2.2) if the underlying particle system is modified to a "purely non-dissipative" system; in the same section we introduce what we call the "modified Fisher information" $\Psi^*_{F^{\mathrm{asym}}}(\rho, F^{\mathrm{sym}}(\rho))$.

Before discussing the general setting, let us first discuss the detailed balance (equilibrium) case. The Markov process $\rho^{(n)}(t)$ is in *microscopic detailed balance* with respect to $\Pi^{(n)}$ if the random path $t \mapsto (\rho^{(n)}(t), W^{(n)}(t))$ starting from $\rho^{(n)}(0) \sim \Pi^{(n)}$, $W^{(n)}(0) = 0$ has the same probability as the time-reversed path $t \mapsto (\rho^{(n)}(T-t), W^{(n)}(T) - W^{(n)}(T-t))$ [Ren18, Sec. 4.1]. For our simple setting, this notion of microscopic detailed balance is equivalent to what may be called *macroscopic detailed balance* [2]:

$$\pi_x Q_{xy} = \pi_y Q_{yx} \qquad \text{and} \qquad \lambda_{\mathrm{in}x} = \pi_x \lambda_{\mathrm{out}x}. \tag{3.4}$$

[2] For more involved systems, for instance, chemical reaction networks, microscopic and macroscopic detailed balance need not be the same [ACK10].

It is easily calculated that on the large-deviation scale, (micro and macroscopic) detailed balance is equivalent to $\mathcal{L}(\rho,j) = \mathcal{L}(\rho,-j) + \langle \overline{\nabla}\, \nabla\, \mathcal{V}(\rho), j\rangle$, which is in turn equivalent to $\mathcal{H}(\rho,\zeta) = \mathcal{H}(\rho, \overline{\nabla}\, \nabla\, \mathcal{V}(\rho) - \zeta)$ by convex duality.

By contrast, if detailed balance does *not* hold, then, starting from $\rho^{(n)}(0), \rho^{(n)}(T) \sim \Pi^{(n)}(T)$, $W^{(n)}(0) = 0$, we obtain after time reversal that $\overleftarrow{\rho}^{(n)}(t) := \rho^{(n)}(T-t)$, and $\overleftarrow{W}^{(n)}(t) := W^{(n)}(T) - W^{(n)}(T-t)$ are the normalised particle density and cumulative net flux of a *different* particle system, where at each node x, new particles are created with rate $n\pi_x\lambda_{\mathrm{out}x}$, each particle independently jumps to node y with rate $\mathcal{Q}_{yx}\pi_y/\pi_x$ and is destroyed with rate $\lambda_{\mathrm{in}x}/\pi_x$, see again [Ren18, Sec. 4.1]. Analogous to (2.4), $(\overleftarrow{\rho}^{(n)}(t), \overleftarrow{W}^{(n)}(t))$ satisfies a large-deviation principle with rate functional $\int_0^T \overleftarrow{\mathcal{L}}\big(\rho(t), \dot{w}(t)\big)\, dt$, which is related to the original rate functional through the relation $\overleftarrow{\mathcal{L}}(\rho,j) = \mathcal{L}(\rho,-j) + \langle \overline{\nabla}\, \nabla\, \mathcal{V}(\rho), j\rangle$, and by convex duality $\overleftarrow{\mathcal{H}}(\rho,\zeta) = \mathcal{H}(\rho, \overline{\nabla}\, \nabla\, \mathcal{V}(\rho) - \zeta)$, see for example [BDSG+02, Sec. 2.7],[Ren18, Sec. 4.2].

4 Force-dissipation decomposition and connections to Onsager-Machlup relation

Our aim is now to decompose the large-deviation cost function (2.5) as a power balance

$$\mathcal{L}(\rho,j) = \Psi(\rho,j) + \Psi^*\big(\rho, F(\rho)\big) - F(\rho)\cdot j, \tag{4.1}$$

for some force field $F(\rho) \in \mathbb{R}^{\mathcal{E}}$ and convex dual (in the second argument) non-negative dissipation potentials Ψ, Ψ^*. By convex duality, their non-negativity implies that $\Psi(\rho,0) \equiv 0 \equiv \Psi^*(\rho,0)$, reflecting the physical principle: *there is no dissipation in the absence of fluxes and forces*. Recall that $\mathcal{L} = 0$ for the macroscopic flow (2.2), which turns (4.1) into a power balance. This is equivalent to the nonlinear response relation $j^0(\rho) = \nabla_\zeta\, \Psi^*\big(\rho, F(\rho)\big)$ between forces and fluxes.

The decomposition (4.1) exists uniquely [MPR14], where the force and dual dissipation potential are explicitly given by

$$F_{xy}(\rho) := -\nabla_{j_{xy}} \mathcal{L}(\rho,0) = \frac{1}{2}\log\frac{\rho_x Q_{xy}}{\rho_y Q_{yx}} \quad \text{and} \quad F_{\mathrm{in}x}(\rho) := -\nabla_{j_{\mathrm{in}x}} \mathcal{L}(\rho,0) = \frac{1}{2}\log\frac{\lambda_{\mathrm{in}x}}{\rho_x\lambda_{\mathrm{out}x}}, \tag{4.2}$$

$$\begin{aligned}\Psi^*(\rho,\zeta) &:= \mathcal{H}\big(\rho, \zeta - F(\rho)\big) - \mathcal{H}\big(\rho, -F(\rho)\big)\\ &= 2\sum_{\substack{x,y\in\mathcal{X}\\ x<y}} \sqrt{\rho_x Q_{xy}\rho_y Q_{yx}}\big(\cosh(\zeta_{xy}) - 1\big) + 2\sum_{x\in\mathcal{X}} \sqrt{\lambda_{\mathrm{in}x}\rho_x\lambda_{\mathrm{out}x}}\big(\cosh(\zeta_{\mathrm{in}x}) - 1\big).\end{aligned} \tag{4.3}$$

The middle term

$$\Psi^*(\rho, F(\rho)) = \frac{1}{2}\sum\sum_{x\neq y}\big(\sqrt{\rho_x Q_{xy}} - \sqrt{\rho_y Q_{yx}}\big)^2 + \sum_x\big(\sqrt{\lambda_{\mathrm{in}x}} - \sqrt{\rho_x\lambda_{\mathrm{out}x}}\big)^2 \tag{4.4}$$

is often called the *Fisher information*; it quantifies the energy needed to shut down all fluxes under force F, and also controls the long-time behaviour of the ergodic average $T^{-1}\int_0^T \rho(t)\, dt$ [NR21].

If detailed balance holds, the force is related to the quasipotential through $F(\rho) = -\frac{1}{2}\overline{\nabla}\, \nabla\, \mathcal{V}(\rho)$, which reflects the classical principle that systems in (macroscopic) detailed balance are completely driven by the free energy. This can be checked explicitly, but is also known to hold more generally [MPR14], since in that case the decomposition (4.1) can be interpreted as a generalised Onsager-Machlup relation. In particular, under detailed balance, the work done by the force along a trajectory equals the free-energy loss as

$$F\big(\rho(t)\big)\cdot j(t) = -\frac{1}{2}\,\overline{\nabla}\,\nabla\,\mathcal{V}\big(\rho(t)\big)\cdot j(t) = \frac{1}{2}\,\nabla\,\mathcal{V}(\rho(t))\cdot\overline{\mathrm{div}}\,j(t) \\ = -\frac{1}{2}\,\nabla\,\mathcal{V}(\rho(t))\cdot\dot\rho(t) = -\frac{1}{2}\frac{d}{dt}\,\mathcal{V}(\rho(t)). \tag{4.5}$$

More generally without detailed balance, the cost function $\overleftarrow{\mathcal{L}}(\rho, j)$ of the time-reversed dynamics admits a similar decomposition as in (4.1), with the same dissipation potential (4.3) and driving force $\overleftarrow{F}_{xy}(\rho) = \frac{1}{2}\log\frac{\rho_x Q_{yx}\pi_y/\pi_x}{\rho_y Q_{xy}\pi_x/\pi_y}$ and $\overleftarrow{F}_{\mathrm{in}x}(\rho) = \frac{1}{2}\log\frac{\pi_x\lambda_{\mathrm{out}x}}{\rho_x\lambda_{\mathrm{in}x}/\pi_x}$. This allows to naturally define symmetric and antisymmetric forces with respect to time-reversal [BDSG+15, RZ21, PRS21], which leads to the symmetric force $F^{\mathrm{sym}}(\rho) = -\frac{1}{2}\,\overline{\nabla}\,\nabla\mathcal{V}(\rho)$ that coincides with the case of detailed balance (4.5) and a constant antisymmetric force

$$F^{\mathrm{asym}}_{xy} := \frac{1}{2}[F_{xy}(\rho) - \overleftarrow{F}_{xy}(\rho)] = \frac{1}{2}\log\frac{\pi_x Q_{xy}}{\pi_y Q_{yx}}, \quad F^{\mathrm{asym}}_{\mathrm{in}x} := \frac{1}{2}[F_{\mathrm{in}x}(\rho) - \overleftarrow{F}_{\mathrm{in}x}(\rho)] = \frac{1}{2}\log\frac{\lambda_{\mathrm{in}x}}{\pi_x\lambda_{\mathrm{out}x}}. \tag{4.6}$$

The antisymmetric force $F^{\mathrm{asym}} = 0$ precisely if macroscopic detailed balance (3.4) holds. So F^{asym}_{xy} and $F^{\mathrm{asym}}_{\mathrm{in}x}$ are exactly the bulk and boundary forces that drive the system out of detailed balance. While it may seem surprising that F^{asym} is independent of ρ, it should be noted that this happens for various other systems as well [PRS21, Sec. 5].

5 Dissipative–non-dissipative decomposition of the cost

We now use the notion of generalised orthogonality [KJZ18, RZ21, PRS21] to further decompose the dual dissipation Ψ^* in (4.1) into purely dissipative and non-dissipative terms. As a generalisation of quadratic expansions, one writes

$$\begin{aligned}\Psi^*\big(\rho, F(\rho)\big) &= \Psi^*\big(\rho, F^{\mathrm{sym}}(\rho) + F^{\mathrm{asym}}\big)\\ &= \Psi^*\big(\rho, F^{\mathrm{asym}}\big) + \underbrace{\theta_\rho\big(F^{\mathrm{sym}}(\rho), F^{\mathrm{asym}}\big)}_{=0} + \Psi^*_{F^{\mathrm{asym}}}\big(\rho, F^{\mathrm{sym}}(\rho)\big)\\ &= \Psi^*\big(\rho, F^{\mathrm{sym}}(\rho)\big) + \underbrace{\theta_\rho\big(F^{\mathrm{sym}}(\rho), F^{\mathrm{asym}}\big)}_{=0} + \Psi^*_{F^{\mathrm{sym}}}\big(\rho, F^{\mathrm{asym}}\big),\end{aligned}$$

see Appendix A.3 for the construction and explicit definitions of the objects in this calculation. These expansions are not quite the same as in the quadratic case – one of the potentials needs to be modified. This yields the *modified Fisher informations*, cf. (4.4),

$$
\begin{aligned}
\Psi^*_{F^{\mathrm{asym}}}\big(\rho, F^{\mathrm{sym}}(\rho)\big) &= \frac{1}{2}\sum_{\substack{x,y\in\mathcal{X}\\x\neq y}}\Big(\sqrt{\rho_x Q_{xy}} - \sqrt{\rho_y \frac{\pi_x}{\pi_y} Q_{xy}}\Big)^2 \\
&\quad + \frac{1}{2}\sum_{x\in\mathcal{X}}\Big(\sqrt{\lambda_{\mathrm{in}x}} - \sqrt{\frac{\rho_x}{\pi_x}\lambda_{\mathrm{in}x}}\Big)^2 + \frac{1}{2}\sum_{x\in\mathcal{X}}\Big(\sqrt{\rho_x\lambda_{\mathrm{out}x}} - \sqrt{\pi_x\lambda_{\mathrm{out}x}}\Big)^2, \\
\Psi^*_{F^{\mathrm{sym}}}\big(\rho, F^{\mathrm{asym}}\big) &= \frac{1}{2}\sum_{\substack{x,y\in\mathcal{X}\\x\neq y}}\Big(\sqrt{\rho_x Q_{xy}} - \sqrt{\rho_x \frac{\pi_y}{\pi_x} Q_{yx}}\Big)^2 \\
&\quad + \frac{1}{2}\sum_{x\in\mathcal{X}}\Big(\sqrt{\lambda_{\mathrm{in}x}} - \sqrt{\pi_x\lambda_{\mathrm{out}x}}\Big)^2 + \frac{1}{2}\sum_{x\in\mathcal{X}}\Big(\sqrt{\rho_x\frac{\lambda_{\mathrm{in}x}}{\pi_x}} - \sqrt{\rho_x\lambda_{\mathrm{out}x}}\Big)^2.
\end{aligned}
$$

The fact that the generalised cross term $\theta\big(F^{\mathrm{sym}}, F^{\mathrm{asym}}\big)$ vanishes reflects an orthogonality of the symmetric and antisymmetric forces in a generalised sense [RZ21, Prop. 4.2], [PRS21, Prop. 2.24]. This orthogonality also means that the quasipotential $\mathcal{V}$ and steady state π are unaltered by turning F^{asym} on or off (see again Appendix A.3), which is also observed in the numerical examples in Section 7.

Applying this expansion of dissipation potentials to (4.1) leads to two distinct and physically relevant decompositions

$$
\begin{aligned}
\mathcal{L}(\rho,j) &= \underbrace{\Psi(\rho,j) + \Psi^*(\rho,F^{\mathrm{asym}}) - F^{\mathrm{asym}}\cdot j}_{=:\mathcal{L}^{\mathrm{asym}}(\rho,j)} + \Psi^*_{F^{\mathrm{asym}}}\big(F^{\mathrm{sym}}(\rho)\big) - F^{\mathrm{sym}}(\rho)\cdot j, \qquad (5.1a)\\
&= \underbrace{\Psi(\rho,j) + \Psi^*\big(\rho,F^{\mathrm{sym}}(\rho)\big) - F^{\mathrm{sym}}\cdot j}_{=:\mathcal{L}^{\mathrm{sym}}(\rho,j)} + \Psi^*_{F^{\mathrm{sym}}}(F^{\mathrm{asym}}) - F^{\mathrm{asym}}\cdot j. \qquad (5.1b)
\end{aligned}
$$

The two "modified cost functions" $\mathcal{L}^{\mathrm{sym}}, \mathcal{L}^{\mathrm{asym}}$ are non-negative by convex duality, and are in fact themselves large-deviation cost functions of particle system with modified jump rates, see Appendix A.2. Since $F^{\mathrm{sym}} = -\frac{1}{2}\overline{\nabla}\,\nabla\,\mathcal{V}$, the symmetric cost $\mathcal{L}^{\mathrm{sym}}$ encodes the (non-quadratic) Onsager-Machlup dissipative (gradient-flow) part of the dynamics, even without assuming detailed balance. By analogy, $\mathcal{L}^{\mathrm{asym}}$ encodes a *non-dissipative* dynamics that is in some sense the time-antisymmetric counterpart of a gradient flow; this will be explored in Section 6. Both expressions (5.1) decompose the cost function $\mathcal{L}$ into terms corresponding to the dissipative and non-dissipative dynamics, but because Ψ^* is non-quadratic, there are two distinct ways to do so[3].

Of particular interest are the decompositions (5.1) along the zero-cost traffic $j^0(\rho)$. The work done by the symmetric force is $F^{\mathrm{sym}}\cdot j^0 = -\frac{1}{2}\frac{d}{dt}\overline{\nabla}\,\nabla\mathcal{V}$, so that we retrieve the free-energy loss (3.3) from (5.1a), with the explicit expression for $\mathcal{L}^{\mathrm{asym}}(\rho, j^0)$ given by the $s(\cdot|\cdot)$ terms in (3.3). Analogously, inserting j^0 into (5.1b), we find an explicit expression for the work done by the antisymmetric force

$$
\int_0^T F^{\mathrm{asym}}\cdot j^0\big(\rho(t)\big)\,dt = -\int_0^T \Big[\mathcal{L}^{\mathrm{sym}}\big(\rho(t), j^0(t)\big) + \Psi^*_{F^{\mathrm{asym}}}\big(\rho(t), F^{\mathrm{sym}}(\rho(t))\big)\Big]\,dt \le 0 \qquad (5.2)
$$

[3](5.1a) is related to "FIR inequalities" that have been used to study singular limits and prove errors estimates [DLPS17, DLP+18, PR21]; the cost $\mathcal{L}^{\mathrm{asym}}$ quantifies the gap in the inequality.

with

$$\begin{aligned}\mathcal{L}^{\mathrm{sym}}\big(\rho, j^0(\rho)\big) &= \sum\sum_{\substack{x,y\in\mathcal{X}\\ x\neq y}} s\Big(\rho_x Q_{xy} \mid \rho_x \sqrt{\tfrac{\pi_x}{\pi_y} Q_{xy} Q_{yx}}\Big) \\ &\quad + \sum_{x\in\mathcal{X}} \Big[s\big(\lambda_{\mathrm{in}x} \mid \sqrt{\pi_x \lambda_{\mathrm{in}x}\lambda_{\mathrm{out}x}}\big) + s\Big(\rho_x\lambda_{\mathrm{out}x} \mid \rho_x \sqrt{\tfrac{\lambda_{\mathrm{in}x}\lambda_{\mathrm{out}x}}{\pi_x}}\Big)\Big].\end{aligned} \tag{5.3}$$

While, a priori, both $\mathcal{L}^{\mathrm{sym}}(\rho, j)$ and $\mathcal{L}^{\mathrm{asym}}(\rho, j)$ appear as a minimisation over one-way fluxes as in (2.5) (see Appendix A.2), for $j = j^0(\rho)$, the minimising one-way flux is exactly $j^+_{xy} = \rho_x Q_{xy}$, $j^+_{\mathrm{in}x} = \lambda_{\mathrm{in}x}$ which considerably simplifies the expressions.

6 Dissipative and non-dissipative zero-cost dynamics

Recall from Section (4) that $\mathcal{L} = 0$ for the full macroscopic dynamics and so $\dot\rho = -\overline{\mathrm{div}}\,\nabla_\zeta\,\Psi^*(\rho, F^{\mathrm{sym}}(\rho) + F^{\mathrm{asym}})$. Similarly $\mathcal{L}^{\mathrm{sym}} = 0$ yields the nonlinear *gradient flow* $\dot\rho = -\overline{\mathrm{div}}\,\nabla_\zeta\,\Psi^*(\rho, -\frac{1}{2}\,\overline{\nabla}\,\nabla\,\mathcal{V}(\rho))$ driven by the free energy $\mathcal{V}$. How can the zero-cost dynamics of $\mathcal{L}^{\mathrm{asym}}$ be given a physical interpretation? The ODE describing this dynamics is

$$\begin{aligned}\dot\rho_x(t) &= -\,\overline{\mathrm{div}}_x\,\nabla_\zeta\,\Psi^*(\rho, F^{\mathrm{asym}}) \\ &= \sum\sum_{\substack{x,y\in\mathcal{X}\\ x\neq y}} \sqrt{\rho_x(t)\rho_y(t)}\Big(Q_{yx}\sqrt{\tfrac{\pi_y}{\pi_x}} - Q_{xy}\sqrt{\tfrac{\pi_x}{\pi_y}}\Big) + \sqrt{\rho_x}\Big(\lambda_{\mathrm{in}x}\tfrac{1}{\sqrt{\pi_x}} - \lambda_{\mathrm{out}x}\sqrt{\pi_x}\Big).\end{aligned} \tag{6.1}$$

Our novel and maybe surprising result is that this equation in fact has a Hamiltonian structure $\dot\rho = \mathbb{J}(\rho)\,\nabla\,\mathcal{U}(\rho)$ with energy and Poisson structure given by

$$\mathcal{U}(\rho) = \sum_{x\in\mathcal{X}} (\sqrt{\pi_x} - \sqrt{\rho_x})^2, \tag{6.2}$$

$$\begin{aligned}\mathbb{J}_{xy}(\rho) =& 2\sum_{z\in\mathcal{X}} \sqrt{\rho_x\rho_y\rho_z}\Big[\sqrt{\frac{\pi_x\pi_z}{\pi_y}}Q_{zy} - \sqrt{\frac{\pi_x\pi_y}{\pi_z}}Q_{yz} - \sqrt{\frac{\pi_y\pi_z}{\pi_x}}Q_{zx} + \sqrt{\frac{\pi_x\pi_y}{\pi_z}}Q_{xz}\Big] \\ &+ 2\sqrt{\rho_x\rho_y}\Big[\sqrt{\frac{\pi_x}{\pi_y}}\lambda_{\mathrm{in}y} - \sqrt{\pi_x\pi_y}\lambda_{\mathrm{out}y} - \sqrt{\frac{\pi_y}{\pi_x}}\lambda_{\mathrm{in}x} + \sqrt{\pi_x\pi_y}\lambda_{\mathrm{out}x}\Big], \quad x, y\in\mathcal{X}, x\neq y.\end{aligned} \tag{6.3}$$

We include a brief derivation in Appendix A.4 and in Appendix A.5 verify that the corresponding Poisson bracket $[\mathscr{F}^1, \mathscr{F}^2]_\rho := \nabla\,\mathscr{F}^1(\rho)\cdot\mathbb{J}(\rho)\,\nabla\,\mathscr{F}^2(\rho)$ satisfies the Jacobi identity (requisite for a Hamiltonian system). The energy (6.2) is known as the Hellinger distance [Hel09], mostly used in statistics [Ber77] and recently also to describe certain reaction dynamics as gradient flows [LMS18].

The Hamiltonian structure $(\mathcal{U}, \mathbb{J})$ for the ODE (6.1) is generally not unique. In contrast to the gradient flow for $\mathcal{L}^{\mathrm{sym}}$, it is not clear to us whether $\mathcal{U}$ and $\mathbb{J}$ are somehow related to the variational structure provided by $\mathcal{L}^{\mathrm{asym}}$. A natural question is then whether – in the spirit of metriplectic systems [Mor86] or GENERIC [Ö05] – there could be a Hamiltonian structure for (6.1) so that the energy $\mathcal{U}$ is also conserved along the full dynamics $\mathcal{L} = 0$. The answer to this question is negative, because by (3.3) the full dynamics simultaneously dissipates free energy until the unique steady state is reached. Another fundamental difference with GENERIC is that here the full dynamics is retrieved by adding the forces $F = F^{\mathrm{sym}} + F^{\mathrm{asym}}$, whereas in GENERIC one retrieves the full dynamics by adding velocities or fluxes.

7 Insights from a simple system

Consider the simple example of Figure 1 with $\mathcal{X} = \{A, B, C\}$ and define the positive edges as $\mathcal{E} = \{(A,B),(A,C),(B,C)\} \cup \{\mathrm{in}A, \mathrm{in}C\}$ (with no in/out-flow at B). In what follows we use $j^0, j^{\mathrm{sym},0}, j^{\mathrm{asym},0}$ for the zero-cost flux for $\mathcal{L}, \mathcal{L}^{\mathrm{sym}}, \mathcal{L}^{\mathrm{asym}}$ respectively.

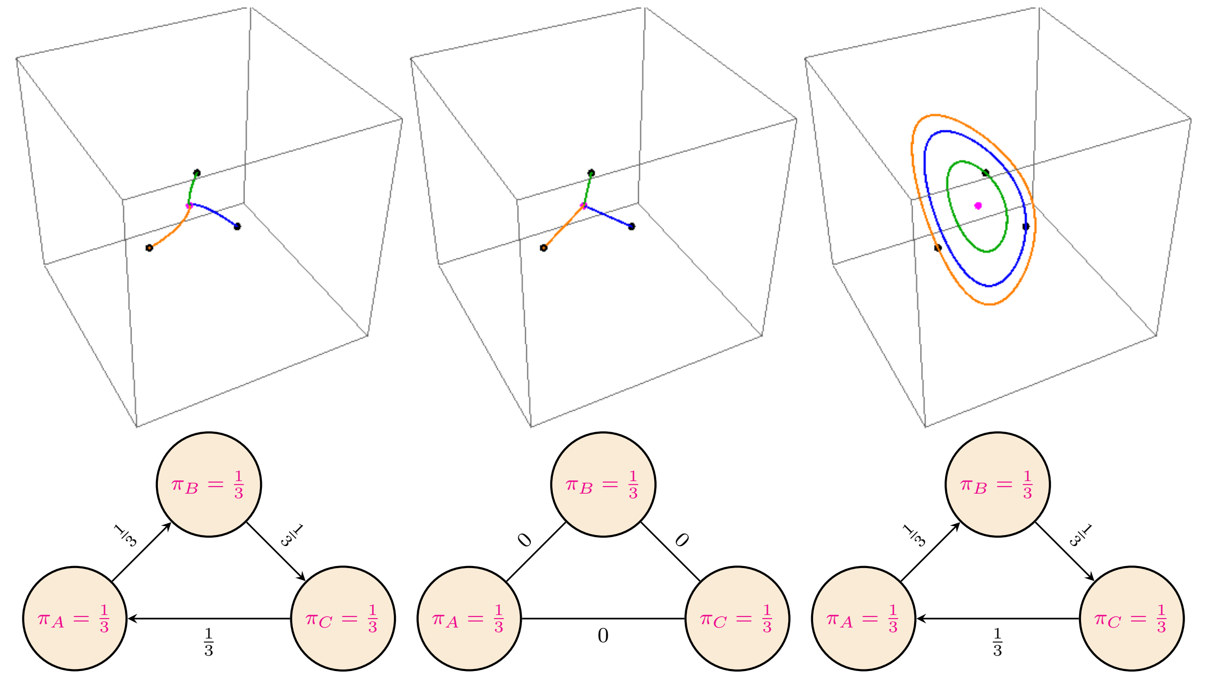

Figure 2: Case A: Pure bulk effects. Top row: Plots of the zero-cost trajectories $\rho(t)$ associated to j^0, $j^{0,\mathrm{sym}}$, $j^{0,\mathrm{asym}}$, starting from three different initial conditions (black dots) with the steady states depicted by the pink dots. Bottom row: The steady states π (in pink) and steady-state fluxes (magnitude indicated by values and direction by arrows) corresponding to j^0, $j^{0,\mathrm{sym}}$, $j^{0,\mathrm{asym}}$ respectively.

Case A: Pure bulk effects. We assume that the forward transition rates $Q_{AB} = Q_{BC} = Q_{CA} = 2$ and backward transition rates $Q_{AB} = Q_{BC} = Q_{CA} = 1$ and $\lambda_{\mathrm{in}x} = \lambda_{\mathrm{out}x} = 0$ for $x = A, B$. This corresponds to a closed system being driven out of detailed balance purely by the bulk force, which is encoded in the different forward and backward transition rates (no detailed balance). Since there is no in and outflow, the total mass of the system is preserved at all times (and equal to the mass at $t = 0$) with the steady state $\pi = (\frac{1}{3}, \frac{1}{3}, \frac{1}{3})$. The zero-cost trajectories and corresponding steady states are plotted in Figure 2.

There are three interesting observations about the trajectories. First, in line with preceding discussions, both the full and symmetric zero-cost trajectories (top row, left & middle) converge to the steady state π whereas the antisymmetric zero-cost trajectory (top row, right) orbits around the steady state. Second, that all the trajectories are confined to a plane which corresponds to the conservation of total mass ($\sum_x \rho_x(t) = 1$). Third, the symmetric zero-cost trajectories are straight lines since the purely dissipative dynamics is a gradient flow of a linear system (since there is no in/out flow).

From the steady states we see that, as expected, the symmetric zero-cost dynamics has an equilibrium/detailed balanced steady state (bottom row, middle), and the full system (bottom row, left) has a non-equilibrium steady state. Surprisingly, the (static) steady state π of the antisymmetric dynamics (bottom row, right) leaves the steady state and even the corresponding flux of the full system unchanged. This is in line with the observation that the forces orthogonal to the symmetric force are precisely the ones that leave the quasipotential unchanged (see discussion at the end of Appendix A.3).

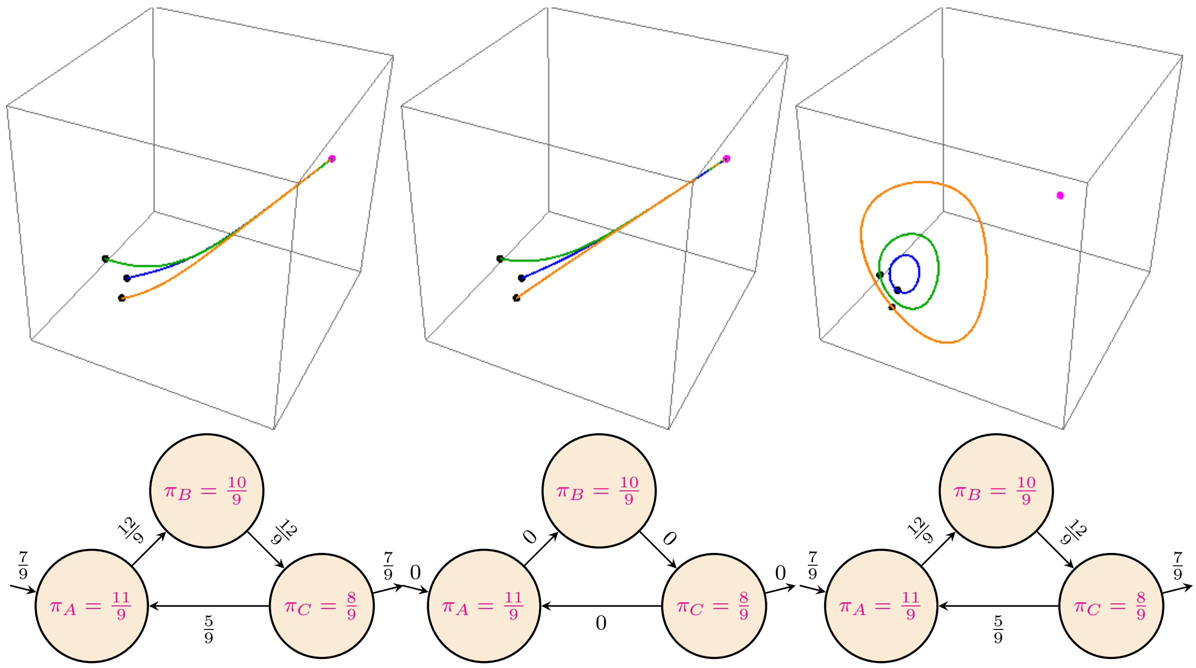

Figure 3: Case B: bulk and boundary effects. Top row: Plots of the zero-cost trajectories $\rho(t)$ associated to j^0, $j^{0,\mathrm{sym}}$, $j^{0,\mathrm{asym}}$, starting from three initial conditions (black dotes) with the steady states denotes by the pink dots. The initial conditions are the same as in Figure 2. Bottom row: The steady states π (in pink) and steady-state fluxes (magnitude indicated by values and direction by arrows) corresponding to to j^0, $j^{0,\mathrm{sym}}$, $j^{0,\mathrm{asym}}$ respectively.

Case B: Bulk and boundary effects. As in Case A we assume that $Q_{AB} = Q_{BC} = Q_{CA} = 2$ and $Q_{AB} = Q_{BC} = Q_{CA} = 1$. For the boundary we assume that $\lambda_{\mathrm{in}A} = \lambda_{\mathrm{out}C} = 2$ and $\lambda_{\mathrm{out}A} = \lambda_{\mathrm{in}C} = 1$. This case corresponds to the system being driven out of detailed balance by both bulk and boundary effects. Regardless of initial condition, the steady state $\pi = (\frac{11}{9}, \frac{10}{9}, \frac{8}{9})$ is unique and positive but no longer a probability density, see Appendix A.1. The zero-cost trajectories and corresponding steady states are plotted in Figure 3.

As in the previous case, both the full and symmetric zero-cost trajectories (top row, left & middle) converge to the steady state π while the antisymmetric zero-cost trajectory orbits around the static steady state (top row, right), however, with the crucial difference that the trajectories are no longer confined to a plane since the mass is not conserved due to in/out flow at the nodes. We point out that the trajectories of the full and symmetric system are different even though they appear to be the quite close from the figures (compare in particular the orange trajectory in the top row of Figure 3).

A natural next step is to study the behaviour of the system under varying combinations of symmetric and antisymmetric bulk and boundary forces. Consider for example the system of case B, where the force is replaced by $\tilde{F}_{xy} := F^{\mathrm{sym}}_{xy}$ and $\tilde{F}_{\mathrm{in}x} := F^{\mathrm{asym}}_{\mathrm{in}x}$, i.e. purely symmetric bulk force and antisymmetric boundary force. This altered system will also have an altered steady state $\tilde{\pi}$, and as a consequence, the decomposition into symmetric and antisymmetric forces will be different, that is, in general $\tilde{F}^{\mathrm{sym}} \neq F^{\mathrm{sym}}$, $\tilde{F}^{\mathrm{asym}} \neq F^{\mathrm{asym}}$. In fact, it is impossible to construct a system where the bulk is in detailed balance ($F_{xy} = F^{\mathrm{sym}}_{xy}$) but the boundaries are not ($F_{\mathrm{in}x} \neq F^{\mathrm{sym}}_{\mathrm{in}x}$). Indeed, the steady state corresponding to such system would have some nodes with non-trivial in and outflow, but since the bulk has zero net fluxes, mass cannot be transported from the inflow to the outflow nodes. By contrast, take the system of case A with the family of uniform steady states $\pi = (a, a, a), a > 0$. If one now adds boundary forces such that $\lambda_{\mathrm{in}x}/\lambda_{\mathrm{out}x} = \pi_x = a$ for some $a > 0$, then the steady state of the altered system is still $\pi = (a, a, a)$. One can thus construct a system where the bulk is not in detailed balance ($F_{xy} \neq F^{\mathrm{sym}}_{xy}$) but the boundaries are ($F_{\mathrm{in}x} = F^{\mathrm{sym}}_{\mathrm{in}x}$).

8 Discussion

As pioneered by Onsager and Machlup, microscopic fluctuations on the large-deviation scale provide a free energy balance for the macroscopic dynamics. By taking fluxes into account, macroscopic fluctuation theory extends this principle to non-equilibrium systems to obtain explicit balances (4.1), (3.3) and (5.2) in terms of the work done by the full, symmetric and antisymmetric forces $F, F^{\mathrm{sym}}, F^{\mathrm{asym}}$ respectively.

With the aim of understanding the role of bulk and boundary effects in non-equilibrium non-diffusive systems, we study an open linear system on a graph. The derivation of the three energy balances poses a number of challenges. First, we derive the explicit quasipotential (3.2) (free energy) as the large-deviation rate of the microscopic invariant measure. Second, since the microscopic fluctuations are Poissonian rather than white noise, the large-deviation cost $\mathcal{L}$ cost is non-quadratic and therefore requires a generalised notion of orthogonality of forces. Whereas the modified system $\mathcal{L}^{\mathrm{sym}} = 0$ is purely driven by the dissipation of free energy, the third challenge is to understand the system $\mathcal{L}^{\mathrm{asym}} = 0$. As observed for closed linear systems in [PRS21], it turns out that with open boundaries, this dynamics is indeed a Hamiltonian system – even satisfying the Jacobi identity. Our work thus allows to distinguish between dissipative (symmetric) and non-dissipative (antisymmetric/Hamiltonian) boundary and bulk mechanisms. We expect that these ideas will apply to more general nonlinear networks, for instance open networks with zero-range interactions (and related agent-based models in social sciences) and chemical-reaction networks attached to reservoirs.

A few intriguing questions emerge from our analysis in regards to the role of antisymmetric forces. It turns out the antisymmetric forces are the exactly the ones that leave the quasipotential and steady state invariant, see Appendix (A.3). This leads to the natural question if one can optimise these forces in a systematic manner to speed up convergence to equilibrium; this is a important challenge in sampling of free-energy in computational statistical mechanics. Finally, it may be intuitively clear that the antisymmetric flow, as the opposite of a dissipative dynamics, should be non-dissipative, the appearance of a full Hamiltonian system with the Hellinger distance as conserved energy seems rather surprising and it is not well understood how and why this structure emerges.

A Appendix

A.1 Invariant measure and steady state

Product-Poisson form of $\Pi^{(n)}$. We show that the invariant measure $\Pi^{(n)}$ for the (underlying) random process $\rho^{(n)}(t)$ (described in Section 2) indeed has the explicit expression (3.1), i.e. it satisfies the backward equation

$$\sum_{\rho\in(\frac{1}{n}\mathbb{N}_0)^{\mathcal{X}}} \Pi^{(n)}(\rho)(\mathcal{Q}^{(n)}f)(\rho) = 0, \tag{A.1}$$

for all bounded functions f on $\frac{1}{n}\mathbb{N}_0^{\mathcal{X}}$ where $\mathcal{Q}^{(n)}$ is the generator for $\rho^{(n)}(t)$. Using the product structure of $\Pi^{(n)}$ we have

$$\Pi^{(n)}(\rho+\tfrac{1}{n}\mathbb{1}_x)=\Pi^{(n)}(\rho)\tfrac{n\pi_x}{n\rho_x+1},\qquad \Pi^{(n)}(\rho-\tfrac{1}{n}\mathbb{1}_x)=\Pi^{(n)}(\rho)\tfrac{\rho_x}{\pi_x},$$
$$\Pi^{(n)}(\rho+\tfrac{1}{n}\mathbb{1}_x-\tfrac{1}{n}\mathbb{1}_y)=\Pi^{(n)}(\rho)(\tfrac{n\pi_x}{n\rho_x+1})(\tfrac{\rho_y}{\pi_y}). \tag{A.2}$$

Using this expression, and pulling out the function f, (A.1) is equivalent to the following expression for any ρ

$$\begin{aligned}
&\sum\sum_{\substack{x,y\in\mathcal{X}\\ x<y}}\Big[n(\rho_x+\tfrac{1}{n})Q_{xy}\Pi^{(n)}(\rho+\tfrac{1}{n}\mathbb{1}_x-\tfrac{1}{n}\mathbb{1}_y)-n\rho_xQ_{xy}\Pi^{(n)}(\rho)\Big]\\
&\quad+\sum_x\Big[n\lambda_{\mathrm{in}x}\Pi^{(n)}(\rho-\tfrac{1}{n}\mathbb{1}_x)-n\lambda_{\mathrm{in}x}\Pi^{(n)}(\rho)\Big]\\
&\quad+\sum_{x\in\mathcal{X}}\Big[n(\rho_x+\tfrac{1}{n})\lambda_{\mathrm{out}x}\Pi^{(n)}(\rho+\tfrac{1}{n}\mathbb{1}_x)-n\rho_x\lambda_{\mathrm{out}x}\Pi^{(n)}(\rho)\Big]\\
&\overset{(A.2)}{=} n\Pi^{(n)}(\rho)\sum_{x\in\mathcal{X}}\tfrac{\rho_x}{\pi_x}\underbrace{\Big[\sum_{\substack{y\in\mathcal{X}\\ y\neq x}}(\pi_yQ_{yx}-\pi_xQ_{xy})+\lambda_{\mathrm{in}x}-\pi_x\lambda_{\mathrm{out}x}\Big]}_{=0}+n\Pi^{(n)}(\rho)\underbrace{\sum_x(\pi_x\lambda_{\mathrm{out}x}-\lambda_{\mathrm{in}x})}_{=0},
\end{aligned}$$

where both sums are 0 since π is the steady state of (2.1).

Properties of macroscopic steady state. If the graph is closed, i.e. $\lambda_{\mathrm{in}},\lambda_{\mathrm{out}}=0$, then (2.1) is the Chapman-Kolmogorov equation for an irreducible Markov chain. Hence there is a coordinate-wise positive steady state, which is unique if the total mass $\sum_{x\in\mathcal{X}}\pi_x$ matches that of the initial condition $\rho(0)$ [Nor98, Thm. 3.5.2].

We now show that there exists a unique coordinate-wise positive steady state irregardless of the initial condition even when the graph is not closed, but satisfies the assumptions made in Section 2.

Since the graph is not closed and irreducible there exists at least one x such that $\lambda_{\mathrm{in}x},\lambda_{\mathrm{out}x}>0$. This implies that the matrix $(Q-\mathrm{diag}(\lambda_{\mathrm{out}}))$ is diagonally dominant with at least one strongly diagonally dominant row $|Q_{xx}-\lambda_{\mathrm{out}x}|>\sum_{y\neq x}|Q_{xy}|$. Furthermore, the matrix is irreducible since the graph is assumed to be irreducible. These properties imply that $(Q-\mathrm{diag}(\lambda_{\mathrm{out}}))$ is invertible [HJ90, Cor. 6.2.27] and so there exists a unique solution π of

$$(Q-\mathrm{diag}(\lambda_{\mathrm{out}}))^{\mathsf{T}}\pi=-\lambda_{\mathrm{in}}. \tag{A.3}$$

To study the sign of π, we decompose the graph $\mathcal{X}$ into $\mathcal{X}^+:=\{\pi_x\geq 0\}$ and $\mathcal{X}^-:=\{\pi_x<0\}$. If $\mathcal{X}^+=\emptyset$ then summing the stability equation (A.3) over all of $\mathcal{X}=\mathcal{X}^-$ leads to the contradiction

$$0=\sum_{x\in\mathcal{X}^-}(\pi_x\lambda_{\mathrm{out}x}-\lambda_{\mathrm{in}x})<0.$$

Similarly, if $\mathcal{X}^-,\mathcal{X}^+\neq\emptyset$, then summing the stability equation (A.3) over $\mathcal{X}^-$ gives the contradiction

$$0=\sum_{x\in\mathcal{X}^-}\sum_{y\in\mathcal{X}^+}(\pi_xQ_{xy}-\pi_yQ_{yx})+\sum_{x\in\mathcal{X}^-}(\pi_x\lambda_{\mathrm{out}x}-\lambda_{\mathrm{in}x})<0$$

since by irreducibility there is at least one pair $x \in \mathcal{X}^-$, $y \in \mathcal{X}^+$ for which $Q_{xy} > 0$, and all other terms are non-positive. We have thus shown that $\mathcal{X} = \mathcal{X}^+$.

Finally, to show that π is coordinate-wise positive, i.e. $\pi_x > 0$ for every x, assume by contradiction that there exists an $x \in \mathcal{X}$ for which $\pi_x = 0$. Since that node does not have any outflow, the stability equation in x reads

$$0 = \sum_{y \neq x} (\pi_x Q_{xy} - \pi_y Q_{yx}) + \pi_x \lambda_{\mathrm{out}x} - \lambda_{\mathrm{in}x} = -\sum_{y \neq x} \pi_y Q_{yx} - \lambda_{\mathrm{in}x},$$

and so $\lambda_{\mathrm{in}x} = 0$ and $\pi_y = 0$ whenever $Q_{yx} > 0$. By irreducibility and recursion, this would lead to the contradiction $\lambda_{\mathrm{in}} = 0$.

A.2 Expressions for modified cost functions

Equations (5.3), (3.3) give expressions for the symmetric and antisymmetric cost evaluated at j^0. The general expressions for these costs are

$$\begin{aligned}
\mathcal{L}^{\mathrm{sym}}(\rho, j) = &\sum\sum_{\substack{x,y \in \mathcal{X} \\ x<y}} \inf_{j^+_{xy} \geq 0} \Big[s\big(j^+_{xy} \mid \rho_x \sqrt{Q_{xy} Q_{yx} \tfrac{\pi_y}{\pi_x}}\big) + s\big(j^+_{xy} - j_{xy} \mid \rho_y \sqrt{Q_{xy} Q_{yx} \tfrac{\pi_x}{\pi_y}}\big) \Big] \\
&+ \sum_{x \in \mathcal{X}} \inf_{j^+_{\mathrm{in}x} \geq 0} \Big[s\big(j^+_{\mathrm{in}x} \mid \sqrt{\lambda_{\mathrm{in}x} \pi_x \lambda_{\mathrm{out}x}}\big) + s\big(j^+_{\mathrm{in}x} - j_{\mathrm{in}x} \mid \rho_x \sqrt{\tfrac{\lambda_{\mathrm{in}x} \lambda_{\mathrm{out}x}}{\pi_x}}\big) \Big], \\
\mathcal{L}^{\mathrm{asym}}(\rho, j) = &\sum\sum_{\substack{x,y \in \mathcal{X} \\ x<y}} \inf_{j^+_{xy} \geq 0} \Big[s\big(j^+_{xy} \mid \sqrt{\rho_x \rho_y} Q_{xy} \sqrt{\tfrac{\pi_x}{\pi_y}}\big) + s\big(j^+_{xy} - j_{xy} \mid \sqrt{\rho_x \rho_y} Q_{yx} \sqrt{\tfrac{\pi_y}{\pi_x}}\big) \Big] \\
&+ \sum_{x \in \mathcal{X}} \inf_{j^+_{\mathrm{in}x} \geq 0} \Big[s\big(j^+_{\mathrm{in}x} \mid \lambda_{\mathrm{in}x} \sqrt{\tfrac{\rho_x}{\pi_x}}\big) + s\big(j^+_{\mathrm{in}x} - j_{\mathrm{in}x} \mid \sqrt{\rho_x \pi_x \lambda_{\mathrm{out}x}}\big) \Big],
\end{aligned}$$

with the corresponding Hamiltonians

$$\begin{aligned}
\mathcal{H}^{\mathrm{sym}}(\rho, \zeta) = &\sum\sum_{\substack{x,y \in \mathcal{X} \\ x<y}} \Big[\rho_x \sqrt{Q_{xy} Q_{yx} \tfrac{\pi_y}{\pi_x}} \big(e^{\zeta_{xy}} - 1\big) + \rho_y \sqrt{Q_{xy} Q_{yx} \tfrac{\pi_x}{\pi_y}} \big(e^{-\zeta_{xy}} - 1\big) \Big] \\
&+ \sum_{x \in \mathcal{X}} \Big[\sqrt{\lambda_{\mathrm{in}x} \pi_x \lambda_{\mathrm{out}x}} \big(e^{\zeta_{\mathrm{in}x}} - 1\big) + \rho_x \sqrt{\tfrac{\lambda_{\mathrm{in}x} \lambda_{\mathrm{out}x}}{\pi_x}} \big(e^{-\zeta_{\mathrm{in}x}} - 1\big) \Big], \\
\mathcal{H}^{\mathrm{asym}}(\rho, \zeta) = &\sum\sum_{\substack{x,y \in \mathcal{X} \\ x<y}} \Big[\sqrt{\rho_x \rho_y} Q_{xy} \sqrt{\tfrac{\pi_x}{\pi_y}} \big(e^{\zeta_{xy}} - 1\big) + \sqrt{\rho_x \rho_y} Q_{yx} \sqrt{\tfrac{\pi_y}{\pi_x}} \big(e^{-\zeta_{xy}} - 1\big) \Big] \\
&+ \sum_{x \in \mathcal{X}} \Big[\lambda_{\mathrm{in}x} \sqrt{\tfrac{\rho_x}{\pi_x}} \big(e^{\zeta_{\mathrm{in}x}} - 1\big) + \sqrt{\rho_x \pi_x \lambda_{\mathrm{out}x}} \big(e^{-\zeta_{\mathrm{in}x}} - 1\big) \Big].
\end{aligned}$$

The integral $\int_0^T \mathcal{L}^{\mathrm{sym}}(\rho(t), j(t))\, dt$ is the large-deviation rate functional for the particle density and flux of a modified system, where particles jump from x to y with jump rate $n\rho_x \sqrt{Q_{xy} Q_{yx} \pi_y / \pi_x}$, particles are created at x with rate $\sqrt{\lambda_{\mathrm{in}x} \pi_x \lambda_{\mathrm{out}x}}$ and destroyed with rate $n\rho_x \sqrt{\lambda_{\mathrm{in}x} \lambda_{\mathrm{out}x} / \pi_x}$. Similarly, $\int_0^T \mathcal{L}^{\mathrm{asym}}(\rho(t), j(t))\, dt$ corresponds to a system where particles jump from x to y with jump rate $n\sqrt{\rho_x \rho_y} Q_{xy} \sqrt{\pi_x / \pi_y}$, particles are created at x with rate $n\lambda_{\mathrm{in}x} \sqrt{\rho_x / \pi_x}$ and destroyed with rate

$n\sqrt{\rho_x\pi_x\lambda_{\mathrm{out}x}}$. Observe that the symmetrised system describes independent jumping and destruction and constant creation as in the original system, whereas the antisymmetrised system introduces a nonlinear interaction between the particles.

A.3 Generalised orthogonality of forces

We now outline the generalised orthogonality of the symmetric and antisymmetric forces and the decomposition of the dissipation potentials discussed at the start of Section 5, see [KJZ18, RZ21, PRS21]. The modified potential and generalised product are defined as

$$\begin{aligned}
\Psi^*_{\tilde\zeta}(\rho,\zeta) :=& 2\sum\sum_{\substack{x,y\in\mathcal{X}\\x<y}} \sqrt{\rho_xQ_{xy}\rho_yQ_{yx}}\cosh(\tilde\zeta_{xy})\big(\cosh(\zeta_{xy})-1\big)\\
&+2\sum_{x\in\mathcal{X}}\sqrt{\lambda_{\mathrm{in}x}\rho_x\lambda_{\mathrm{out}x}}\cosh(\tilde\zeta_{\mathrm{in}x})\big(\cosh(\zeta_{\mathrm{in}x})-1\big),\\
\theta_\rho(\zeta,\tilde\zeta) :=& 2\sum\sum_{\substack{x,y\in\mathcal{X}\\x<y}} \sqrt{\rho_xQ_{xy}\rho_yQ_{yx}}\sinh(\tilde\zeta_{xy})\sinh(\zeta_{xy})\\
&+2\sum_{x\in\mathcal{X}}\sqrt{\lambda_{\mathrm{in}x}\rho_x\lambda_{\mathrm{out}x}}\sinh(\tilde\zeta_{\mathrm{in}x})\sinh(\zeta_{\mathrm{in}x}).
\end{aligned}$$

Using the addition rule $\cosh(\zeta+\zeta)=\cosh(\zeta)\cosh(\zeta)+\sinh(\zeta)\sinh(\zeta)$, one finds that dual dissipation potential (4.3) can be expanded as $\Psi^*(\rho,\zeta+\tilde\zeta)=\Psi^*(\rho,\tilde\zeta)+\theta_\rho(\zeta,\tilde\zeta)+\Psi^*_{\tilde\zeta}(\rho,\zeta)$.

Of particular interest is the case where $\zeta=F^{\mathrm{sym}}(\rho),\tilde\zeta=F^{\mathrm{asym}}$. Using the explicit expression for the forces (4.6) and the definition of $\sinh$ in terms of exponential function we find

$$\begin{aligned}
\theta_\rho\big(F^{\mathrm{sym}}(\rho),F^{\mathrm{asym}}\big) &= 4\sum_{\substack{x,y\in\mathcal{X}\\x<y}}\sqrt{\rho_xQ_{xy}\rho_yQ_{yx}}\sinh(F^{\mathrm{sym}}_{xy})\sinh(F^{\mathrm{asym}}_{xy})\\
&\quad+4\sum_{x\in\mathcal{X}}\sqrt{\lambda_{\mathrm{in}x}\rho_x\lambda_{\mathrm{out}x}}\sinh(F^{\mathrm{sym}}_{\mathrm{in}x})\sinh(F^{\mathrm{asym}}_{\mathrm{in}x})\\
&=\sum_{x\in\mathcal{X}}\frac{\rho_x}{\pi_x}\underbrace{\Big[\sum_{\substack{y\in\mathcal{X},\\y\neq x}}(\pi_xQ_{xy}-\pi_yQ_{yx})+\pi_x\lambda_{\mathrm{out}x}-\lambda_{\mathrm{in}x}\Big]}_{=0}\\
&\quad+\underbrace{\sum_{x\in\mathcal{X}}(\lambda_{\mathrm{in}x}-\pi_x\lambda_{\mathrm{out}x})}_{=0}=0.
\end{aligned}$$

This orthogonality is also related to the quasipotential as follows. First, consider a system with free energy $\mathcal{V}$ and force $F=F^{\mathrm{sym}}+F^{\mathrm{asym}}$, $F^{\mathrm{sym}}=-\frac12\overline{\nabla}\nabla\mathcal{V}$. Then $\mathcal{V}$ is also the quasipotential for the modified system where the nondissipative force F^{asym} is replaced by zero, i.e.

$$\mathcal{H}^{\mathrm{sym}}\big(\rho,\overline{\nabla}\nabla\mathcal{V}(\rho)\big)=\theta_\rho\big(-F^{\mathrm{sym}}(\rho),0\big)=0.$$

Second, consider a system in detailed balance with quasipotential $\mathcal{V}$ and $F=F^{\mathrm{sym}}=-\frac12\overline{\nabla}\nabla\mathcal{V}$. If one would add an additional force ζ, the modified Hamilton-Jacobi equation reads

$$\begin{aligned}
\mathcal{H}^{\mathrm{sym},\zeta}\big(\rho,\overline{\nabla}\nabla\mathcal{V}(\rho)\big) &:=\Psi^*\big(\rho,\overline{\nabla}\nabla\mathcal{V}(\rho)+F^{\mathrm{sym}}+\zeta\big)-\Psi^*\big(\rho,F^{\mathrm{sym}}+\zeta\big)\\
&=\Psi^*\big(\rho,-F^{\mathrm{sym}}+\zeta\big)-\Psi^*\big(\rho,F^{\mathrm{sym}}+\zeta\big)=-2\theta_\rho(F^{\mathrm{sym}},\zeta).
\end{aligned}$$

Thus, the forces ζ orthogonal to F^{sym} are precisely those forces that leave the quasipotential invariant when added to a symmetric force.

A.4 Derivation of Hamiltonian structure

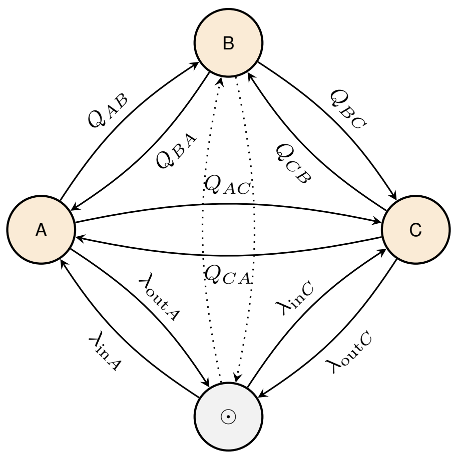

Figure 4: The graph from Figure 1 with an additional ghost node

We expand the graph with an additional ghost node $\tilde{\mathcal{X}} := \mathcal{X} \cup \{\odot\}$, where mass flowing in and out of the system is now extracted from respectively collected in $\odot$ instead, see Figure 4. This results in a dynamics that conserves the total mass $M := \sum_{x\in\mathcal{X}\cup\odot} \rho_x(0)$ (although $\rho_\odot(t)$ may become negative), and the rates of flowing out of a node x is either linear $\rho_x Q_{xy}$, $\rho_x \lambda_{\mathrm{out}x}$ or constant $\lambda_{\mathrm{in}x}$. The expanded system has the same, coordinate-wise positive steady state π on $\mathcal{X}$ as the original system, but with an additional coordinate $\pi_\odot$. By mass conservation, this coordinate satisfies $\pi_\odot = M - \sum_{x\in\mathcal{X}} \pi_x$, so if we initially place enough mass in the ghost node (which does not change the dynamics), then M will be sufficiently large so that $\pi_\odot > 0$.

We are then in the same setting as zero-range processes [PRS21, Prop. 5.3]. By results therein, the augmented antisymmetric zero-cost dynamics is a Hamiltonian flow and can be written as (abbreviating $\rho_{\mathcal{X}} := (\rho_x)_{x\in\mathcal{X}}$ defined in (6.1))

$$\begin{bmatrix} \dot\rho_{\mathcal{X}}(t) \\ \dot\rho_\odot(t) \end{bmatrix} = \tilde{\mathbb{J}}(\rho)\,\nabla\tilde{\mathcal{U}}(\rho) := \begin{bmatrix} \mathbb{J}(\rho) & \mathbb{J}_{\mathcal{X}\odot}(\rho) \\ -\,\mathbb{J}_{\mathcal{X}\odot}(\rho) & \mathbb{J}_{\odot\odot}(\rho) \end{bmatrix} \begin{bmatrix} \nabla_{\rho_{\mathcal{X}}}\tilde{\mathcal{U}}(\rho) \\ \nabla_{\rho_\odot}\tilde{\mathcal{U}}(\rho) \end{bmatrix}, \tag{A.4}$$

where $\tilde{\mathcal{U}}(\rho,\rho_\odot) = \mathcal{U}(\rho)$ and $\mathcal{U}, \mathbb{J}$ are given by (6.2),(6.3) and $\mathbb{J}_{\mathcal{X}\odot}, \mathbb{J}_{\odot\odot}$ are irrelevant by the following argument. Mass conservation implies that $\Lambda : (\rho_{\mathcal{X}}, \rho_\odot) \mapsto \rho_{\mathcal{X}}$ is a bijection with Jacobian $J_\Lambda = [I \mid 0]$. Applying the variable transformation Λ to (A.4) yields $\dot\rho_{\mathcal{X}}(t) = J_\Lambda \tilde{\mathbb{J}}(\rho) J_\Lambda^{\mathsf{T}}\,\nabla_{\rho_{\mathcal{X}}}\mathcal{U}(\rho) = \mathbb{J}(\rho)\,\nabla_{\rho_{\mathcal{X}}}\mathcal{U}(\rho)$ as claimed.

A.5 Jacobi identity

We verify that the bracket $[\mathscr{F}^1, \mathscr{F}^2]_\rho = \nabla\mathscr{F}^1(\rho)\cdot\mathbb{J}(\rho)\,\nabla\mathscr{F}^2(\rho)$ defined by the Poisson structure (6.3) indeed satisfies the Jacobi identity $[[\mathscr{F}^1,\mathscr{F}^2],\mathscr{F}^3]_\rho + [[\mathscr{F}^2,\mathscr{F}^3],\mathscr{F}^1]_\rho + [[\mathscr{F}^3,\mathscr{F}^1],\mathscr{F}^2]_\rho = 0$ for all sufficiently smooth functions $\mathscr{F}^i$ and all $\rho \in \mathbb{R}^{\mathcal{X}}$. Omitting ρ-dependencies to shorten notation, this identity is equivalent to the following tensor relation [PRS21, Lem A.1], for all $\rho \in \mathbb{R}^{\mathcal{X}}$ and $x, y, z \in \mathcal{X}$,

$$R^y_{xz} + R^z_{yx} + R^x_{zy} \equiv 0, \qquad R^z_{xy} := \sum_{a \neq z} \mathbb{J}_{az}\, \partial_a\, \mathbb{J}_{xy}\,. \tag{A.5}$$

We first calculate the derivative for $x \neq y$ (clearly $\mathbb{J}_{xx} \equiv 0$),

$$\partial_a\, \mathbb{J}_{xy} = \begin{cases} \sqrt{\frac{\rho_x \rho_y}{\rho_a}} B^a_{xy}, & a \neq x, y \\ \sum_{z \neq x} \sqrt{\frac{\rho_y \rho_z}{\rho_x}} B^z_{xy} + 2\sqrt{\rho_y} B^x_{xy} + \sqrt{\frac{\rho_y}{\rho_x}} B^{\odot}_{xy}, & a = x, \\ \sum_{z \neq y} \sqrt{\frac{\rho_x \rho_z}{\rho_y}} B^z_{xy} + 2\sqrt{\rho_x} B^y_{xy} + \sqrt{\frac{\rho_x}{\rho_y}} B^{\odot}_{xy}, & a = y, \end{cases}$$

$$B^z_{xy} := \sqrt{\frac{\pi_x \pi_z}{\pi_y}} Q_{zy} - \sqrt{\frac{\pi_x \pi_y}{\pi_z}} Q_{yz} - \sqrt{\frac{\pi_y \pi_z}{\pi_x}} Q_{zx} + \sqrt{\frac{\pi_x \pi_y}{\pi_z}} Q_{xz},$$

$$B^{\odot}_{xy} := \sqrt{\frac{\pi_x}{\pi_y}} \lambda_{\mathrm{in}y} - \sqrt{\pi_x \pi_y} \lambda_{\mathrm{out}y} - \sqrt{\frac{\pi_y}{\pi_x}} \lambda_{\mathrm{in}x} + \sqrt{\pi_x \pi_y} \lambda_{\mathrm{out}x}.$$

The tensor then decomposes into terms of different orders $R^z_{xy} = {}^2R^z_{xy} + {}^3R^z_{xy} + {}^4R^z_{xy}$ of $\sqrt{\rho}$, where

$${}^2R^z_{xy} := 2\big[\sqrt{\rho_x \rho_z} B^{\odot}_{xy} B^{\odot}_{yz} + \sqrt{\rho_y \rho_z} B^{\odot}_{xy} B^{\odot}_{xz}\big],$$

$${}^3R^z_{xy} := 2 \sum_a \big[\sqrt{\rho_x \rho_y \rho_z} B^a_{xy} B^{\odot}_{az} + \sqrt{\rho_a \rho_y \rho_z}(B^a_{xy} B^{\odot}_{xz} + B^{\odot}_{xy} B^a_{xz}) + \sqrt{\rho_a \rho_x \rho_z}(B^a_{xy} B^{\odot}_{yz} + B^{\odot}_{xy} B^a_{yz})\big],$$

$${}^4R^z_{xy} := 2 \sum_{a,b}\sum \big[\sqrt{\rho_b \rho_x \rho_y \rho_z} B^a_{xy} B^b_{az} + \sqrt{\rho_a \rho_b \rho_y \rho_z} B^a_{xy} B^b_{xz} + \sqrt{\rho_a \rho_b \rho_x \rho_z} B^a_{xy} B^b_{yz}\big].$$

Since (A.5) needs to hold for all $\rho \in \mathbb{R}^{\mathcal{X}}$, we may check it for each order separately. Using the skew-symmetry of $(B^{\odot}_{xy})_{xy}$, for the second-order terms we have

$$\begin{aligned} &{}^2R^y_{xz} + {}^2R^z_{yx} + {}^2R^x_{zy} \\ &\quad = 2\sqrt{\rho_x \rho_y} B^{\odot}_{zy}\big[B^{\odot}_{xz} + B^{\odot}_{zx}\big] + 2\sqrt{\rho_x \rho_z} B^{\odot}_{yx}\big[B^{\odot}_{yz} + B^{\odot}_{zy}\big] + 2\sqrt{\rho_y \rho_z} B^{\odot}_{xz}\big[B^{\odot}_{xy} + B^{\odot}_{yx}\big] \equiv 0 \end{aligned}$$

Using the skew-symmetry of $(B^z_{xy})_{xy}$ and $(B^{\odot}_{xy})_{xy}$, for the third order terms we find

$$\begin{aligned} {}^3R^y_{xz} + {}^3R^z_{yx} + {}^3R^x_{zy} = 2 \textstyle\sum_a \big[&\sqrt{\rho_x \rho_y \rho_z}\big(B^a_{xz} B^{\odot}_{ay} + B^a_{yx} B^{\odot}_{az} + B^a_{zy} B^{\odot}_{ax}\big) \\ &+ \sqrt{\rho_a \rho_x \rho_y}\big(B^a_{xz} B^{\odot}_{zy} + B^a_{zx} B^{\odot}_{zy} + B^a_{zy} B^{\odot}_{xz} + B^a_{zy} B^{\odot}_{zx}\big) \\ &+ \sqrt{\rho_a \rho_x \rho_z}\big(B^a_{yx} B^{\odot}_{yz} + B^a_{yx} B^{\odot}_{zy} + B^a_{yz} B^{\odot}_{yx} + B^a_{zy} B^{\odot}_{yx}\big) \\ &+ \sqrt{\rho_a \rho_y \rho_z}\big(B^a_{xz} B^{\odot}_{xy} + B^a_{xz} B^{\odot}_{yx} + B^a_{xy} B^{\odot}_{xz} + B^a_{yx} B^{\odot}_{xz}\big)\big] \\ = 2\sqrt{\rho_x \rho_y \rho_z} \sum_a &\big(B^a_{xz} B^{\odot}_{ay} + B^a_{yx} B^{\odot}_{az} + B^a_{zy} B^{\odot}_{ax}\big). \end{aligned}$$

Hence the sum over the constants needs to be zero. After a lengthy calculation we find

$$\begin{aligned} &\sum_a \big(B^a_{xz} B^{\odot}_{ay} + B^a_{yx} B^{\odot}_{az} + B^a_{zy} B^{\odot}_{ax}\big) \\ &= \frac{1}{\sqrt{\pi_z}}\Big(\sqrt{\frac{\pi_x}{\pi_y}} \lambda_{\mathrm{in}y} - \sqrt{\pi_x \pi_y} \lambda_{\mathrm{out}y} - \sqrt{\frac{\pi_y}{\pi_x}} \lambda_{\mathrm{in}x} + \sqrt{\pi_x \pi_y} \lambda_{\mathrm{out}x}\Big) \sum_{a \neq z} \big(\pi_a Q_{az} - \pi_z Q_{za}\big) \\ &\quad + \frac{1}{\sqrt{\pi_x}}\Big(\sqrt{\frac{\pi_y}{\pi_z}} \lambda_{\mathrm{in}z} - \sqrt{\pi_y \pi_z} \lambda_{\mathrm{out}z} - \sqrt{\frac{\pi_z}{\pi_y}} \lambda_{\mathrm{in}y} + \sqrt{\pi_y \pi_z} \lambda_{\mathrm{out}y}\Big) \sum_{a \neq z} \big(\pi_a Q_{ax} - \pi_x Q_{xa}\big) \\ &\quad + \frac{1}{\sqrt{\pi_y}}\Big(\sqrt{\frac{\pi_z}{\pi_x}} \lambda_{\mathrm{in}x} - \sqrt{\pi_x \pi_z} \lambda_{\mathrm{out}x} - \sqrt{\frac{\pi_x}{\pi_z}} \lambda_{\mathrm{in}z} + \sqrt{\pi_x \pi_z} \lambda_{\mathrm{out}z}\Big) \sum_{a \neq z} \big(\pi_a Q_{ay} - \pi_y Q_{ya}\big). \end{aligned}$$

Using the stability equation (A.3), the three sums on the right can be replaced by expressions depending on $\lambda_{\mathrm{in}}, \lambda_{\mathrm{out}}$ only. This yields twelve paired terms that cancel each other out, so that indeed ${}^3R^y_{xz} + {}^3R^z_{yx} + {}^3R^x_{zy} \equiv 0$.

Finally, for the fourth order terms, ${}^4R^y_{xz} + {}^4R^z_{yx} + {}^4R^x_{zy} \equiv 0$, because this describes the closed graph setting $\lambda_{\mathrm{in}}, \lambda_{\mathrm{out}} = 0$, which satisfies the Jacobi identity [PRS21, App. A].

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