arXiv:2103.14384v1 [math-ph] 26 Mar 2021

Variational structures beyond gradient flows: a macroscopic fluctuation-theory perspective

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March 29, 2021

Abstract

Macroscopic equations arising out of stochastic particle systems in detailed balance (called dissipative systems or gradient flows) have a natural variational structure, which can be derived from the large-deviation rate functional for the density of the particle system. While large deviations can be studied in considerable generality, these variational structures are often restricted to systems in detailed balance. Using insights from macroscopic fluctuation theory, in this work we aim to generalise this variational connection beyond dissipative systems by augmenting densities with fluxes, which encode non-dissipative effects. Our main contribution is an abstract framework, which for a given flux-density cost and a quasipotential, provides a decomposition into dissipative and non-dissipative components and a generalised orthogonality relation between them. We then apply this abstract theory to various stochastic particle systems – independent copies of jump processes, zero-range processes, chemical-reaction networks in complex balance and lattice-gas models.

1 Introduction

When studying an evolution equation, it is often helpful to know if it has an associated variational structure, in order to obtain physical insight and tools for mathematical analysis. An important example of such a structure is a gradient flow or dissipative system; in this case the structure consists of an energy functional and a dissipation mechanism, and the evolution equation is completely characterised by a corresponding minimisation problem involving these two objects. From a thermodynamic point of view, such a variational structure is often related to random fluctuations of an underlying microscopic particle system via a large-deviation principle — examples include the Boltzmann–Gibbs–Helmholtz free energy and the Onsager–Machlup theory.

It has recently become clear that macroscopic equations are always dissipative if the underlying microscopic stochastic system is in detailed balance. The energy functional and the dissipation mechanism for such macroscopic equations are then uniquely derived by an appropriate decomposition of the large-deviation rate functional associated to the microscopic systems [ADPZ11, ADPZ13, MPR14, PRV14]. These observations have provided a canonical approach to constructing a variational structure for such macroscopic equations. In addition to having a clear physical interpretation, these variational structures have been used to isolate interesting features of the macroscopic equations and study singular-limit problems arising therein.

So far, this approach has largely been limited to particle systems in detailed balance and corresponding macroscopic dissipative systems. Since a large deviation study is possible far beyond detailed balance, this leads to the following natural question.

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Do the large deviations of the underlying particle systems provide a variational structure beyond detailed balance?

While this is a hard question to answer in general, considerable progress has been made in the case of some specific systems in two seemingly independent directions.

One direction that is tailored to allow for non-dissipative effects is the study of so-called *FIR inequalities*, first introduced for the many-particle limit of Vlasov-type nonlinear diffusions [DLPS17], independent particles on a graph [HPST20] and chemical reactions [RZ21, Sec. 5]. These inequalities bound the free-energy difference and Fisher information by the large-deviation rate functional, providing a useful tool to study singular-limit problems and to derive error estimates [DLP+18, PR20]. Strictly speaking, these inequalities are not variational structures in the sense that they do not fully determine the macroscopic dynamics. However, in this paper we will construct a variational structure which generalises these inequalities and completely characterises the macroscopic dynamics.

Another direction of generalising dissipative systems is by using Macroscopic Fluctuation Theory (MFT) [BDSG+15]. The main idea here is to consider, in addition to the usual density of the particle system, the particle fluxes at the microscopic level, and to study the large deviations of these fluxes. Consequently using time-reversal arguments, MFT explicitly captures the dissipative and non-dissipative effects in the system. However, most MFT literature has been devoted to diffusive scaling of particle systems and corresponding quadratic rate functions. Such rate functions define a Hilbert space with a natural orthogonal decomposition into dissipative and non-dissipative components. Recently non-quadratic rate functions and connections to MFT have been explored in the case of independent particles on a graph [KJZ18] and chemical reaction networks [RZ21], but a general MFT for non-quadratic rate functions is largely open.

Spurred on by these exciting new developments, we provide a partial but affirmative answer to the question posed above. The basis of our analysis is an abstract action functional $(\rho, j) \mapsto \int_0^T \mathcal{L}(\rho(t), j(t))\,dt$. This functional will correspond to the large deviations of random particle systems, but this identification is not necessary for our analysis; in this sense our approach is purely macroscopic. Inspired by FIR-inequalities and MFT, we set up an abstract framework whose central outcome will be a series of decompositions of the integrand $\mathcal{L}$ into distinct dissipative and non-dissipative components. These decompositions generalise: (1) the connection between large deviations and dissipative systems from [MPR14] to include non-dissipative effects, (2) the known cases of FIR inequalities [HPST20] to a general setting, and (3) MFT to non-quadratic action functions.

Finally we illustrate our abstract framework by applying it to various examples.

1.1 Summary of results

Abstract results. Consider the macroscopic densities and fluxes $[0, T] \ni t \mapsto (\rho(t), j(t))$ that are evolving according to a coupled system of evolution equations:

$$\dot\rho(t) = -\operatorname{div} j(t), \tag{1.1a}$$

$$j(t) = j^0(\rho(t)), \tag{1.1b}$$

with an associated action functional

$$(\rho, j) \mapsto \int_0^T \mathcal{L}(\rho(t), j(t))\,dt, \tag{1.2}$$

where the non-negative cost function $\mathcal{L}$ has the crucial property that for any (ρ, j),

$$j = j^0(\rho) \iff \mathcal{L}\big(\rho, j\big) = 0,$$

and hence the action (1.2) is minimised by the trajectory (1.1b). We will interpret equation (1.1a) as a continuity equation and call $j^0(\rho)$ the *zero-cost flux* associated to $\mathcal{L}$. Equation (1.1) often describes the macroscopic dynamics arising from a microscopic stochastic particle system and (1.2) is typically the corresponding large-deviation rate functional.

Although writing the flux explicitly in (1.1b) instead of directly studying $\dot\rho(t) = -\operatorname{div} j^0(\rho(t))$ might seem superfluous at first sight, it is motivated by the fact that fluxes can encode information on non-dissipative, for instance divergence-free, effects in the system. Consequently, while studying densities is usually sufficient for dissipative systems [Ons31a, Ons31b, OM53, MPR14, MPPR17] (see Section 1.2 below for more details), the inclusion of fluxes is better suited to describe non-dissipative effects at the macroscopic level [BDSG$^+$15, Mae18].

Our abstract framework assumes the existence of three objects: a sufficiently regular density-flux cost function $\mathcal{L}(\rho, j)$, an operator that will play the role of divergence and as such defines the continuity equation (1.1a) and a non-negative *quasipotential* $\mathcal{V}$ associated to $\mathcal{L}$. The basis of our approach will be the unique decomposition $\mathcal{L}(\rho, j) = \Phi(\rho, j) + \Phi^*(\rho, F(\rho)) - \langle F(\rho), j\rangle$, for some corresponding *driving force* $F(\rho) := -d\mathcal{L}(\rho, 0)$ and *dissipation potential* Φ with convex dual Φ^* (see Theorem 2.7 for details). Borrowing ideas from MFT, we uniquely decompose this driving force into a *symmetric* and *antisymmetric* part

$$F(\rho) = F^{\mathrm{sym}}(\rho) + F^{\mathrm{asym}}(\rho).$$

In the context of MFT and large deviations of microscopic systems, the symmetry refers to a time-reversal argument. In particular, if the microscopic system is in detailed balance, then $F(\rho) = F^{\mathrm{sym}}(\rho)$ and the (macroscopic) dynamics is purely dissipative, i.e. described by a gradient flow of $\mathcal{V}$ [MPR14]. As such one can think of $F^{\mathrm{sym}}(\rho)$ as the dissipative part of the force. More generally, from a physical point of view, a purely dissipative system is thermodynamically closed, so that the work done is related to the free energy or quasipotential via

$$\int_0^T \big\langle F^{\mathrm{sym}}(\rho(t)), j(t)\big\rangle\, dt = -\frac{1}{2}\mathcal{V}(\rho(T)) + \frac{1}{2}\mathcal{V}(\rho(0)),$$

or formulated locally in time for the power

$$\big\langle F^{\mathrm{sym}}(\rho(t)), j(t)\big\rangle = -\frac{1}{2}\frac{d}{dt}\mathcal{V}(\rho(t)). \tag{1.3}$$

Thus for non-closed systems one can think of $F^{\mathrm{sym}}(\rho)$ as an internally generated force and the remainder, $F^{\mathrm{asym}}(\rho)$, as the force exerted by the system upon the environment. While

$$\big\langle F^{\mathrm{asym}}(\rho(t)), j(t)\big\rangle \quad \text{and} \quad \big\langle F(\rho(t)), j(t)\big\rangle \tag{1.4}$$

can be understood as expressions of power or rates of work, they are generally *not* exact differentials.

In our main result, Theorem 2.27, we relate the cost function $\mathcal{L}$ to the three powers from (1.3) and (1.4). Specifically, for any $\lambda \in [0, 1]$, the cost function $\mathcal{L}$ admits the following decompositions

$$\mathcal{L}(\rho, j) = \mathcal{L}_{(1-2\lambda)F}(\rho, j) + \mathcal{R}^\lambda_F(\rho) - 2\lambda\langle F(\rho), j\rangle, \qquad \text{with } \mathcal{R}^\lambda_F(\rho) \geq 0, \tag{1.5a}$$

$$\mathcal{L}(\rho, j) = \mathcal{L}_{F-2\lambda F^{\mathrm{sym}}}(\rho, j) + \mathcal{R}^\lambda_{F^{\mathrm{sym}}}(\rho) - 2\lambda\langle F^{\mathrm{sym}}(\rho), j\rangle, \qquad \text{with } \mathcal{R}^\lambda_{F^{\mathrm{sym}}}(\rho) \geq 0, \tag{1.5b}$$

$$\mathcal{L}(\rho, j) = \mathcal{L}_{F-2\lambda F^{\mathrm{asym}}}(\rho, j) + \mathcal{R}^\lambda_{F^{\mathrm{asym}}}(\rho) - 2\lambda\langle F^{\mathrm{asym}}(\rho), j\rangle, \qquad \text{with } \mathcal{R}^\lambda_{F^{\mathrm{asym}}}(\rho) \geq 0. \tag{1.5c}$$

The parameter λ can be used to switch between different forces and the non-negative terms $\mathcal{L}_G(\rho, j)$ are modified versions of $\mathcal{L}$ where the driving force $F(\rho)$ is replaced by a different covector field $G(\rho)$. Consequently, the zero-cost flux of $\mathcal{L}_G$ will be a modified dynamics, different from (1.1b). Of particular interest is the case $\lambda = \frac{1}{2}$, where the decompositions (1.5b) and (1.5c) can be seen as two different ways to split $\mathcal{L}$ into *purely dissipative* and *purely non-dissipative* components. Indeed, the modified cost $\mathcal{L}_{F^{\mathrm{sym}}}$ is related to a purely dissipative system that can be formalised as a gradient flow (see Section 1.2.1). By contrast, we interpret the zero-cost flux of $\mathcal{L}_{F^{\mathrm{asym}}}$ as purely non-dissipative. Although the variational structure and physical interpretation of $\mathcal{L}_{F^{\mathrm{asym}}}$ remains an open question (see discussion in Section 6), we show for certain examples that its zero-cost behaviour corresponds to a purely Hamiltonian macroscopic evolution. This idea is clearly illustrated by Figure 1, where we plot the phase digram for the zero-cost flux associated with $\mathcal{L}_F$, $\mathcal{L}_{F^{\mathrm{sym}}}$ and $\mathcal{L}_{F^{\mathrm{asym}}}$ in the case of independent Markov jump particles on a three-point state space. For details on this example see Section 2.6 and 4.

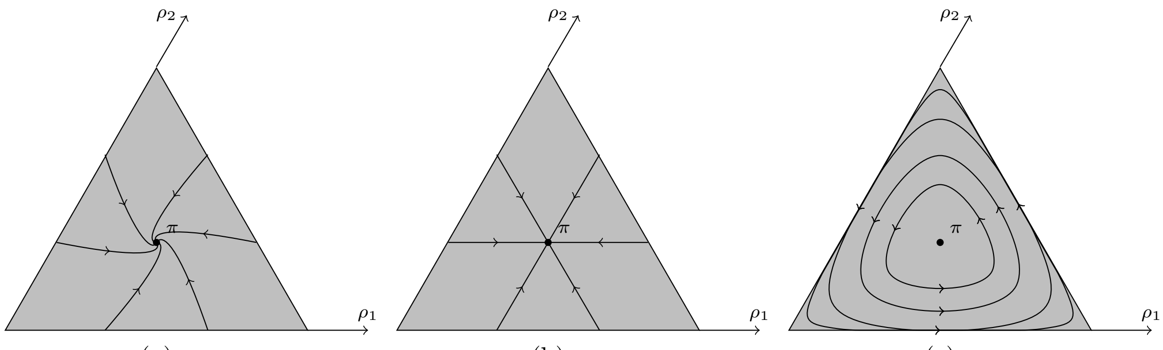

Figure 1: Consider the setting of independent and irreducible Markov jump particles on a three-point state space with invariant measure $\pi = (\frac{1}{3}, \frac{1}{3}, \frac{1}{3})$. Phase digram for the (zero-cost) trajectories $\rho(t)$ associated to (a) $\mathcal{L}(\rho(t), j(t)) = 0$; (b) $\mathcal{L}_{F^{\rm sym}}(\rho(t), j(t)) = 0$; (c) $\mathcal{L}_{F^{\rm asym}}(\rho(t), j(t)) = 0$. Here ρ_i is the mass at point i and we do not plot ρ_3 since $\sum_i \rho_i = 1$. The zero-cost trajectories for $\mathcal{L}_{F^{\rm sym}}$ and $\mathcal{L}_{F^{\rm asym}}$ follow a purely dissipative and Hamiltonian dynamics respectively.

The middle terms in the right hand side of (1.5) are inspired by [HPST20, Def. 1.5], [RZ21, Sec. 5], and are called *generalised Fisher informations*. For $\lambda \in [0, 1]$ and covector fields $G = F, F^{\rm sym}, F^{\rm asym}$, they are defined as

$$\mathcal{R}^\lambda_G(\rho) = -\mathcal{H}\big(\rho, -2\lambda G(\rho)\big), \tag{1.6}$$

where $\mathcal{H}$ is the convex dual of $\mathcal{L}$. The terminology is motivated by the fact that (see Proposition 2.16)

$$\lim_{\lambda\to 0} \frac{1}{\lambda} \mathcal{R}^\lambda_G(\rho) = \langle G(\rho), j^0(\rho)\rangle,$$

which in the case $G = F^{\rm sym}$ is the time derivative or dissipation rate of the quasipotential along the zero-cost path, i.e. in the limit $\lambda \to 0$, $\mathcal{R}^\lambda_{F^{\rm sym}}$ coincides with the classical Fisher information [HPST20]. The non-negativity of the generalised Fisher informations in (1.5) is essential, since it shows that the three powers in (1.3) and (1.4) are non-negative along the zero-cost flux, thus generalising the second law of thermodynamics.

From a physical point of view, all three decompositions (1.5) are in fact power balances. Mathematically, since the modified cost functions $\mathcal{L}_G$ are non-negative, the decompositions (1.5) can be exploited to estimate the three powers and Fisher informations by the action, thus generalising FIR inequalities as we explain below.

Applications. Above we discussed the abstract framework and results derived from it – and this is purely macroscopic in that we do not require any connection to particle systems and large deviations. In the latter part of this paper we apply this abstract theory to several microscopic particle systems.

First, we focus on independent Markov jump particles on a finite graph as a guiding example throughout this paper, and generalise the results of [KJZ18]. Second, we study zero-range processes in a scaling which leads to an ordinary differential equation (ODE) in the limit. Third, we study chemical reaction networks in complex balance [AK11] and generalise the results in [RZ21]. In all these three examples the macroscopic dynamics are ODEs and the large-deviation principle yields a exponential rate functional.

Finally, we focus on the setting of particles that hop on a lattice in a diffusive limit, which leads to convection-diffusion equation as the macroscopic evolution. These particles can either be independent random walkers or interact via exclusion. In this setting, the large-deviation principle yields a quadratic rate functional, and we recover the classical MFT results [BDSG+15].

Boundary issues and global-in-time decompositions. The decompositions (1.5) do not involve time, and therefore when considering trajectories $t \mapsto (\rho(t), j(t))$, they should be considered as local-in-time or instantaneous decompositions of $\mathcal{L}(\rho(t), j(t))$ at time t. Naively, one would simply integrate in time to obtain global decompositions of the rate functional $\int_0^T \mathcal{L}(\rho(t), j(t))\, dt$ for arbitrary trajectories (ρ, j). This argument is formal since, strictly speaking, the decompositions (1.5) hold only for ρ, j for which the required terms are defined. More precisely, it turns out that the forces F, F^{sym} and F^{asym} are well-defined only on a proper subset of the domain of definition for the modified cost functions $\mathcal{L}_G$ and generalised Fisher informations $\mathcal{R}_G^\lambda$. This issue is often ignored in the MFT literature.

This issue becomes clear in the various examples we consider. For instance when dealing with independent jump processes on a finite lattice $\mathcal{X}$, the large-deviation cost is well defined for any trajectory in the space of probability measures i.e. $\rho(t) \in \mathcal{P}(\mathcal{X})$ (see Example 2.1), whereas the symmetric force is only well-defined for trajectories in the space of strictly positive probability measures, i.e. $\rho(t) \in \mathcal{P}_+(\mathcal{X})$ (see (2.27)). This difference in the domains arises due to the logarithm present in the definition of the symmetric force. Such issues are typically dealt by first extending the domains of definition of the forces involved by appropriately regularising them, second by proving the decompositions on these extended domains, and finally passing to the limit in the regularisations (see for instance the proof of [HPST20, Thm. 1.6]). Although we expect that similar arguments can be applied to (1.5) to arrive at global-in-time decompositions, in this first study we focus on local-in-time results.

1.2 Related work

As mentioned earlier, this work connects and generalises existing literature in various directions. Barring fairly recent works [KJZ18, Ren18b, RZ21] which deal with particular examples, the connections between MFT, dissipative systems and FIR inequalities have largely been unexplored in the literature. Not all of these works consider fluxes, and so we will also make use of a 'contracted' cost function,

$$\hat{\mathcal{L}}(\rho, u) := \inf\{\mathcal{L}(\rho, j) : u = -\operatorname{div} j\}, \tag{1.7}$$

where the *velocity* u is a placeholder for $\dot\rho(t)$ and $-\operatorname{div}$ is the abstract operator that maps fluxes to velocities as in (1.1a). This construction is consistent with the notion of contraction in large deviations (see Example 2.1). Since $\hat{\mathcal{L}}(\rho, -\operatorname{div} j^0(\rho)) = 0$, we refer to $u^0(\rho) := -\operatorname{div} j^0(\rho)$ as the *zero-cost velocity.*

1.2.1 Dissipative/Gradient systems

In the case of dissipative systems $F = F^{\mathrm{sym}}$ and $F^{\mathrm{asym}} = 0$, and therefore with $\lambda = \frac{1}{2}$ both (1.5a) and (1.5b) become

$$\begin{aligned} \mathcal{L}(\rho, j) &= \mathcal{L}_0(\rho, j) + \mathcal{R}^{\frac{1}{2}}_{F^{\mathrm{sym}}}(\rho) - \langle F^{\mathrm{sym}}(\rho), j\rangle \\ &= \Phi(\rho, j) + \Phi^*\big(\rho, F^{\mathrm{sym}}(\rho)\big) - \langle F^{\mathrm{sym}}(\rho), j\rangle, \end{aligned} \tag{1.8}$$

with the convex dual pair of *dissipation potentials* defined as $\Phi(\rho, j) := \mathcal{L}_0(\rho, j)$ and $\Phi^*(\rho, \zeta) := \sup_j \langle \zeta, j\rangle - \Phi(\rho, j)$. This decomposition of $\mathcal{L}$ is exactly the characterisation of dissipative systems in the density-flux setting [Mae18, Ren18b]; see Section 2.6 for a further elaboration.

Using (1.3), $F^{\mathrm{sym}} = -\frac{1}{2}\nabla d\mathcal{V}$ (see Corollary 2.19 for definition) and applying the contraction (1.7), we switch to the density setting

$$\begin{aligned} \hat{\mathcal{L}}(\rho, u) &= \inf\big\{\Phi(\rho, j) : u = -\operatorname{div} j\big\} + \Phi^*\big(\rho, F^{\mathrm{sym}}(\rho)\big) + \big\langle \tfrac{1}{2} d\mathcal{V}(\rho), u\big\rangle \\ &=: \Psi(\rho, u) + \Psi^*\big(\rho, -\tfrac{1}{2} d\mathcal{V}(\rho)\big) + \big\langle \tfrac{1}{2} d\mathcal{V}(\rho), u\big\rangle, \end{aligned} \tag{1.9}$$

where Ψ is the contraction of Φ and Ψ,Ψ^* are convex duals of each other (see [Ren18b, Thm. 3] for details).

The identity (1.9) is the standard decomposition of the density cost function that characterises a dissipative system or *generalised gradient flow* in the following sense. For the zero-cost velocity, the left-hand side satisfies $\hat{\mathcal{L}}(\rho, u^0(\rho)) = 0$, and the right-hand side of (1.9) is the Energy–Energy-Dissipation identity (EDI) [SS04, AGS08, RMS08], which is equivalent by convex duality to

$$u^0(\rho) = d_\xi \Psi^*\big(\rho, -\tfrac{1}{2} d\mathcal{V}(\rho)\big), \tag{1.10}$$

where d_ξ is the derivative with respect to the second argument. In the special case when $\Psi^*(\rho,\xi) = \frac{1}{2}\langle K(\rho)\xi, \xi\rangle$ is a quadratic form with an inverse metric tensor $K(\rho)$ of a manifold, we arrive at the usual gradient-flow representation of the zero-cost velocity on that manifold

$$u^0(\rho) = -\frac{1}{2} K(\rho) d\mathcal{V}(\rho) =: -\frac{1}{2} \operatorname{grad}_\rho \mathcal{V}(\rho).$$

This connection between generalised gradient flows and the symmetry $F = F^{\text{sym}}$ at the level of densities has been explored more directly in [MPR14], where it was shown that this symmetry holds if $\hat{\mathcal{L}}$ corresponds to the large-deviation principle of a Markov process in detailed balance. The density-flux formulation (1.8) of a dissipative system with quadratic dissipation has also been investigated extensively in the literature, see for instance [BDSG+15, Mae18, Ren18b]. Since we derived this decomposition from (1.5a) and (1.5b), these two decompositions can be thought of as the natural generalisations of the EDI to non-dissipative systems.

1.2.2 GENERIC

The GENERIC framework is specifically designed as a coupling between dissipative and non-dissipative effects in a thermodynamically consistent way [GÖ97, ÖG97, Ött05]. Although originally meant to describe evolution equations, recent work has also studied the following natural connection between GENERIC and large deviations from a variational perspective (see (1.9)),

$$\hat{\mathcal{L}}(\rho, u) = \Psi\big(\rho, u - \mathbb{J}(\rho) d\mathcal{E}(\rho)\big) + \Psi^*\big(\rho, -\tfrac{1}{2} d\mathcal{V}(\rho)\big) + \big\langle \tfrac{1}{2} d\mathcal{V}(\rho), u\big\rangle, \tag{1.11}$$

where the Poisson structure $\mathbb{J}$ and energy $\mathcal{E}$ define the Hamiltonian part of the dynamics, and additional non-interaction conditions are required to ensure that the zero-cost velocity

$$u^0(\rho) = d\Psi^*\big(\rho, -\tfrac{1}{2} d\mathcal{V}(\rho)\big) + \mathbb{J}(\rho) d\mathcal{E}(\rho) \tag{1.12}$$

dissipates $\mathcal{V}$ and conserves $\mathcal{E}$.

Such a connection is discussed in [DPZ13] in the particular setting of weakly interacting diffusions. More generally, the recent paper [KLMP20] shows that (1.11) can only hold if the underlying microscopic system consists of stochastic dynamics in detailed balance combined with a deterministic drift. The drift may be replaced by stochastic fluctuations as long as they appear deterministic on the large-deviation scale [Ren18b], but any larger scale fluctuations that are not in detailed balance will break down the GENERIC structure. Therefore, the class of large-deviation cost functions with a GENERIC structure is rather limited.

By contrast, the decompositions (1.5) *always* hold as soon as the quasipotential $\mathcal{V}$ is identified. The crucial difference is that our decompositions are based on a decomposition of forces, i.e.

$$u^0(\rho) = -\operatorname{div} j^0(\rho) = -\operatorname{div} d\Phi^*\big(\rho, F^{\text{sym}}(\rho) + F^{\text{asym}}(\rho)\big),$$

rather than a decomposition of fluxes or velocities as in GENERIC (1.12). Furthermore, generalised orthogonality between F^{sym} and F^{asym} (see Subsection 2.4) are a natural analogue of the non-interaction conditions used in GENERIC.

1.2.3 FIR inequalities

Using $\mathcal{L}_{F-2\lambda F^{\text{sym}}} \geq 0$ and $F^{\text{sym}} = -\frac{1}{2}\nabla d\mathcal{V}$ (as above) in the decomposition (1.5b), we find

$$\tfrac{1}{\lambda}\mathcal{L}(\rho, j) \geq \tfrac{1}{\lambda}\mathcal{R}^{\lambda}_{F^{\text{sym}}}(\rho) + \langle \nabla d\mathcal{V}, j\rangle.$$

Since ∇ is the dual of $-\operatorname{div}$, using the contraction principle (1.7) and the definition of the Fisher information (1.6) it follows that (see Corollary 2.32 for details)

$$\tfrac{1}{\lambda}\hat{\mathcal{L}}(\rho,u) \geq -\tfrac{1}{\lambda}\hat{\mathcal{H}}(\rho, d\mathcal{V}(\rho)) + \langle d\mathcal{V}(\rho), u\rangle, \tag{1.13}$$

where $\hat{\mathcal{H}}$ is the convex dual of $\hat{\mathcal{L}}$. This is a local-in-time version of the FIR inequality.

Assume that a smooth trajectory $[0,T] \ni t \mapsto \rho(t)$ satisfies (1.13) for every t. Substituting $u = \dot\rho$, formally applying the chain rule $\langle d\mathcal{V}(\rho), \dot\rho\rangle = \frac{d}{dt}\mathcal{V}(\rho)$, and integrating in time over $[0,T]$ we arrive at the F("free energy")-I("rate functional")-R("Fisher information") inequality [HPST20, Thm. 1.6]

$$\frac{1}{\lambda}\int_0^T \hat{\mathcal{L}}(\rho(t),\dot\rho(t))dt + \mathcal{V}(\rho(t)) \geq \mathcal{V}(\rho(T)) - \frac{1}{\lambda}\int_0^T \hat{\mathcal{H}}\big(\rho(t), d\mathcal{V}(\rho(t))\big)\,dt. \tag{1.14}$$

Therefore, the decomposition (1.5b) can be thought of as a generalisation of [HPST20] in various ways. First, (1.5b) holds fairly generally (in the abstract framework) and can be applied to systems well beyond independent copies of Markov jump processes studied in [HPST20]. Second, (1.5b) exactly characterises the gap in the inequality (1.13) via $\mathcal{L}_{F-2\lambda F^{\mathrm{sym}}}$ which we discarded in this discussion due to its non-negativity. And third, a different version of the FIR inequality can also be derived from (1.5c).

It should be noted that the FIR inequalities have been used in the literature as *a priori estimates* to study singular limits, and we expect that the decomposition (1.5b) and inequality (1.5b) will serve the same purpose for a considerably larger class of systems. However, in this paper we limit ourselves to the local-in-time decompositions (1.5b) as opposed to the global-in-time inequality (1.14) discussed in [HPST20], since moving from local to global descriptions is a nontrivial technical step outside the scope of this work.

1.2.4 MFT and (non-)quadratic cost function

As stated earlier, most MFT literature is concerned with the diffusive scaling of underlying stochastic particle systems which converge to diffusion-type macroscopic partial differential equations and corresponds to quadratic cost functions of the form [BDSG+15]

$$\mathcal{L}(\rho,j) = \frac{1}{2}\|j - j^0(\rho)\|_\rho^2, \quad \text{for some Hilbert norm } \|\cdot\|_\rho.$$

Crucial arguments in MFT are based on the fact that the dissipative and the non-dissipative effects are orthogonal in this Hilbert space, i.e.

$$\langle F^{\mathrm{sym}}(\rho), F^{\mathrm{asym}}(\rho)\rangle_\rho \equiv 0.$$

However, even the simple example of independent particles on a finite graph (see Example 2.1) yields a non-quadratic cost function $\mathcal{L}$, and the aforementioned orthogonality arguments break down. In [KJZ18] (for independent jump processes) and [RZ21] (for chemical reactions) these ideas are ported to the non-quadratic setting by introducing a generalised notion of orthogonality, where the pairing is no longer bilinear, and rather satisfies a relation of the form

$$\theta_\rho(F^{\mathrm{sym}}(\rho), F^{\mathrm{asym}}(\rho)) \equiv 0. \tag{1.15}$$

By contrast, the abstract framework that we develop is not necessarily based on such orthogonality relations, although we do borrow many notions such as time-reversed cost-functions and forces from MFT. However we will show that within our framework, one can also construct a generalised orthogonality pairing θ_ρ (fully characterised by $\mathcal{L}$) that satisfies (1.15), and coincides with the bilinear pairings $\langle\cdot,\cdot\rangle_\rho$ in case of quadratic cost functions and with $\theta_\rho(\cdot,\cdot)$ from [KJZ18, RZ21] in the case of specific non-quadratic cost functions. This will be the content of Subsection 2.4.

1.3 Summary of notation and outline of the article

$\mathcal{X}^2/2$	Half the edges on a finite graph $\mathcal{X}$	(2.2)
$s(\cdot\vert\cdot)$	Relative Boltzmann function (integrand/summand in relative entropy)	(2.7)
$\mathcal{Z}, \mathcal{W}, \phi$	State-flux triple	Def. 2.2
$T\mathcal{Z}$, $T^*\mathcal{Z}$	Tangent and cotangent bundle associated to $\mathcal{Z}$	
$T_\rho\mathcal{Z}$, $T^*_\rho\mathcal{Z}$	Tangent and cotangent space at $\rho \in \mathcal{Z}$	
$\mathcal{L}$, $\mathcal{H}$	L-function and its convex dual	Def. 2.4
$\hat{\mathcal{L}}$, $\hat{\mathcal{H}}$	Contracted L-function and its convex dual	(2.38)
$\mathcal{V}$	Quasipotential	Def. 2.5
$d\mathcal{F}$	Gateaux derivative of a functional $\mathcal{F}$	
χ^T	dual operator $\chi^\mathsf{T} : \mathcal{M}^* \to \mathcal{N}^*$ for $\chi : \mathcal{N} \to \mathcal{M}$	
$\mathrm{Dom}(A)$	domain of an operator A	
F	Driving force	Def. 2.8
Φ^*, Φ	Dissipation potential and its dual	Def. 2.8
Ψ^*, Ψ	Contracted dissipation potential and its dual	(2.40)
$\mathcal{L}_G$, $\mathcal{H}_G$	Tilted L-function and its convex dual	Def. 2.12
$\mathrm{Dom}_{\mathrm{symdiss}}(A)$	Subset of $\mathrm{Dom}(A)$ where the dissipation potential is symmetric	(2.16)
$\mathcal{R}^\lambda_\zeta$	Generalised Fisher information	Def. 2.15
$\overleftarrow{\mathcal{L}}$, $\overleftarrow{\mathcal{H}}$	Reversed L-function and its convex dual	Def. 2.17
F^{sym}, F^{asym}	Symmetric and antisymmetric force	Cor. 2.19
$\mathcal{M}(\mathcal{X})$	Space of signed measures on $\mathcal{X}$	
$\mathcal{P}(\mathcal{X})$	Space of probability measures on $\mathcal{X}$	
$\mathcal{P}_+(\mathcal{X})$	Space of strictly positive probability measures on a discrete state space $\mathcal{X}$	
∇, div	Discrete/continuous gradient and divergence	
$\mathbb{1}_x$	Indicator function associated to $\{x\}$	

In Section 2 we present the abstract framework and in Section 3 we connect the abstract framework to large deviations. In Section 4 we analyse the zero-cost velocity for the antisymmetric L-function in the setting of independent particles on a finite graph. In Section 5 we apply the abstract framework to various stochastic particle systems and conclude with discussion in Section 6.

2 Abstract framework

In the introduction we worked with the large-deviation cost; we now work with its abstraction, the so-called the L-function[1]. In what follows we first introduce the L-function and other key ingredients of the abstract framework in Section 2.1. Using these objects we introduce dissipation potentials, tilted L-functions and Fisher information in Section 2.2. Using time-reversal-type arguments from MFT, in Section 2.3 we introduce time-reversed L-functions, symmetric and antisymmetric forces, and in Section 2.4 we introduce a generalised notion of orthogonality satisfied by these forces. Section 2.5 contains various decompositions of the L-function and in Section 2.6 we study the symmetric and antisymmetric L-function. Throughout this section we will use the guiding example of Independent Markovian Particles on a Finite Graph (IPFG), which we now introduce.

Example (IPFG). 2.1. Consider n independent Markovian particles $X_1(t), \dots X_n(t)$ on a finite graph $\mathcal{X}$, with irreducible generator $Q \in \mathbb{R}^{\mathcal{X}\times\mathcal{X}}$. The particle density (also called empirical measure or mean-field), defined as $\rho^{(n)}(t) := n^{-1}\sum_{i=1}^n \delta_{X_i(t)}$, is a Markov process on the space of probability measures

[1] We use the terminology "L-function" from [MPR14, Def. 1.1] as opposed to 'Lagrangian' or 'cost', since in practice $\mathcal{L}$ need not correspond to a large-deviation principle, and it often plays a different role to the Lagrangian in mechanics.

$\mathcal{P}(\mathcal{X}) \subseteq \mathbb{R}^{\mathcal{X}}$ with generator

$$(\hat{\mathcal{Q}}^{(n)} f)(\rho) = n \sum\sum_{(x,y)\in\mathcal{X}\times\mathcal{X}} \rho_x Q_{xy} \big[f(\rho - \tfrac{1}{n}\mathbb{1}_x + \tfrac{1}{n}\mathbb{1}_y) - f(\rho) \big],$$

where $\mathbb{1}_x$ is the indicator function for $x \in \mathcal{X}$. With a suitable initial condition, Varadarajan's Theorem implies that the random process $\rho^{(n)}$ converges in the many-particle limit $n \to \infty$ to the deterministic solution of the ODE

$$\dot{\rho}(t) = Q^{\mathsf{T}} \rho(t). \tag{2.1}$$

In addition to the empirical measure, we will also track the number of jumps through each edge, which characterises the flux over an edge. For reasons that will be clarified in Section 2.2, it is important to consider net fluxes (over the usual one-sided fluxes), defined on half of the edges

$$\mathcal{X}^2/2 := \big\{ (x,y) \in \mathcal{X}\times\mathcal{X} : x < y \big\}. \tag{2.2}$$

More precisely, the so-called integrated net flux $W^{(n)}_{xy}(t)$ over the edge connecting $x, y \in \mathcal{X}$, is defined as the difference between the number of jumps from $x \to y$ and in the opposite direction from $y \to x$ in the time interval $[0,t]$, all rescaled by $\frac{1}{n}$. Then the pair $(\rho^{(n)}(t), W^{(n)}(t))$ is again a Markov process, now in $\mathcal{P}(\mathcal{X}) \times \mathbb{R}^{\mathcal{X}^2/2}$ with the generator

$$\begin{aligned}(\mathcal{Q}^{(n)} f)(\rho, w) = n \sum\sum_{(x,y)\in\mathcal{X}^2/2} & \rho_x Q_{xy} \big[f(\rho - \tfrac{1}{n}\mathbb{1}_x + \tfrac{1}{n}\mathbb{1}_y, w + \tfrac{1}{n}\mathbb{1}_{xy}) - f(\rho) \big] \\ & + \rho_y Q_{yx} \big[f(\rho - \tfrac{1}{n}\mathbb{1}_y + \tfrac{1}{n}\mathbb{1}_x, w - \tfrac{1}{n}\mathbb{1}_{xy}) - f(\rho) \big].\end{aligned}$$

This process converges as $n \to \infty$ to the solution of the macroscopic system

$$\begin{cases} \dot{w}_{xy}(t) = \rho_x(t) Q_{xy} - \rho_y(t) Q_{yx}, & (x,y) \in \mathcal{X}^2/2, \\ \dot{\rho}_x(t) = -\operatorname{div}_x \dot{w}(t), & x \in \mathcal{X}, \end{cases} \tag{2.3}$$

where the operator

$$\operatorname{div}_x j := \sum_{y\in\mathcal{X}: y>x} j_{xy} - \sum_{y\in\mathcal{X}: y<x} j_{yx}, \tag{2.4}$$

is the discrete divergence for net fluxes. Indeed the system (2.3) is of the form (1.1).

In the many-particle limit ($n \to \infty$), the random fluctuations around the mean behaviour decay fast due to averaging effects. The unlikeliness to observe an atypical flux for large but finite n is quantified by the large-deviation principle, formally written as

$$\operatorname{Prob}\Big((\rho^{(n)}, W^{(n)}) \approx (\rho, w) \Big) \overset{n\to\infty}{\sim} e^{-n\mathcal{I}_0(\rho) - n\mathcal{J}(\rho,w)}, \qquad \mathcal{J}(\rho, w) := \begin{cases} \int_0^T \mathcal{L}\big(\rho(t), \dot{w}(t)\big)\, dt, & \dot{\rho} = -\operatorname{div} \dot{w}, \\ \infty, & \text{otherwise}, \end{cases} \tag{2.5}$$

where the $\mathcal{L}$ is given by [Ren18a, Kra17] (we use j as a placeholder for $\dot{w}$)

$$\mathcal{L}(\rho, j) := \inf_{j^+ \in \mathbb{R}^{\mathcal{X}^2/2}_{\geq 0}} \sum\sum_{(x,y)\in\mathcal{X}^2/2} \big[s(j^+_{xy} \mid \rho_x Q_{xy}) + s(j^+_{xy} - j_{xy} \mid \rho_y Q_{yx}) \big], \tag{2.6}$$

$$s(a \mid b) := \begin{cases} a \log \frac{a}{b} - a + b, & a, b > 0, \\ b, & a = 0, \\ \infty, & b \leq 0, a > 0 \text{ or } a < 0, \end{cases} \tag{2.7}$$

and $\mathcal{I}_0$ is the large-deviation rate functional corresponding to the initial distribution of $\rho^{(n)}(0)$. Indeed $\mathcal{L}(\rho, j)$ is non-negative and minimised by (2.3). Due to the contraction principle [DZ09, Thm. 4.2.1], the infimum is taken over all non-negative one-way fluxes $(j^+_{xy})_{x<y}$ and $(j^+_{yx} - j_{yx})_{x>y}$.

Applying the contraction principle, the empirical measure satisfies the following large-deviation principle, where $\hat{\mathcal{L}}$ is related to $\mathcal{L}$ via (1.7),

$$\mathrm{Prob}\left(\rho^{(n)} \approx \rho\right) \overset{n\to\infty}{\sim} \exp\Big[-n\mathcal{I}_0(\rho(0)) - n\int_0^T \hat{\mathcal{L}}(\rho(t), \dot\rho(t))\,dt\Big].$$

2.1 Setup

We now introduce *state-flux triples*, *L-functions* and *quasipotentials*, which are the key ingredients of the abstract framework .

Definition 2.2 ([Ren18b, Sec. 4.1])**.** A triple $(\mathcal{Z}, \mathcal{W}, \phi)$ is called a *state-flux triple* if

(i) The state-space $\mathcal{Z}$ and the flux-space $\mathcal{W}$ are differentiable Banach manifolds.

(ii) $\phi : \mathcal{W} \to \mathcal{Z}$ is a surjective differentiable operator $\phi : \mathcal{W} \to \mathcal{Z}$.

(iii) $T_w\mathcal{W}$ depends on w only through $\rho = \phi[w]$, so that by a slight abuse of notation we can replace $T_w\mathcal{W}$ by $T_\rho\mathcal{W}$ and write $T\mathcal{W} := \{(\rho, j) : \rho \in \mathcal{Z}, j \in T_\rho\mathcal{W}\}$.

(iv) ϕ has a linear bounded differential that depends on w only through $\rho = \phi[w]$, so that by a slight abuse of notation we write $d\phi_\rho : T_\rho\mathcal{W} \to T_\rho\mathcal{Z}$.

(v) $T_\rho\mathcal{W}, T_\rho\mathcal{Z}$ have Banach pre-duals $T^*_\rho\mathcal{W}, T^*_\rho\mathcal{Z}$ respectively, paired by the duality pairing $\langle\cdot,\cdot\rangle$, where we omit the indices since it will be clear to which spaces the elements belong. Analogously we write $T^*\mathcal{W} := \{(\rho, \zeta) : \rho \in \mathcal{Z}, \zeta \in T^*_\rho\mathcal{W}\}$ and $T^*\mathcal{Z} := \{(\rho, \xi) : \rho \in \mathcal{Z}, \xi \in T^*_\rho\mathcal{Z}\}$.

The Banach structure should be seen as a reference norm only required for example to define the dual pairing $\langle\cdot,\cdot\rangle$, or the Gateaux derivative $d\mathcal{F}(\rho)$ of a functional $\mathcal{F} : \mathcal{Z} \to \mathbb{R}\cup\{\infty\}$. Observe that $T^*_\rho\mathcal{W}, T^*_\rho\mathcal{Z}$ as pre-duals is a slight abuse of notation. The choice to work with pre-duals instead of dual spaces is rather arbitrary, but fits better with the applications that we have in mind. In order to avoid confusion with convex duality, we will denote adjoint operators by T, e.g. $d\phi^{\mathsf{T}}_\rho : T^*_\rho\mathcal{Z} \to T^*_\rho\mathcal{W}$. Note that here we choose to work with Banach manifolds $\mathcal{Z}, \mathcal{W}$, but this can be generalised to more general structures which allow for derivatives in tangent vector spaces. Usually, a continuity equation satisfies $u = \operatorname{div} j$, and connects a tangent vector u to a tangent vector j via the div operator. As will become clear in the following discussion, the purpose of ϕ is to abstractly define the notion of div operator via $d\phi_\rho$. The assumption that $d\phi$ is bounded, ensures the existence of a well-defined adjoint.

Example (IPFG). 2.3. Consider the example of the independent particles on a finite graph $\mathcal{X}$. Due to mass conservation, the state space is

$$\mathcal{Z} := \mathcal{P}(\mathcal{X}) := \left\{\rho \in \mathbb{R}^{\mathcal{X}}_{\geq 0} : \textstyle\sum_{x\in\mathcal{X}} \rho_x = 1\right\}, \text{ with tangent space}$$
$$T_\rho\mathcal{Z} = \left\{u \in \mathbb{R}^{\mathcal{X}} : \rho_x = 0 \implies u_x \geq 0 \text{ for all } x \in \mathcal{X}\right\}.$$

The restriction in $T_\rho\mathcal{Z}$ is easily understood in the case when $\mathcal{X}$ contains only two points and therefore $\mathcal{Z}$ is the line connecting $(1, 0)$ and $(0, 1)$. The requirement that $\ell \geq 0$ corresponds to these two end-points of the line, and states that the tangents are contained within the line. For the dual space we choose $T^*_\rho\mathcal{Z} = \mathbb{R}^{\mathcal{X}}$, paired with $T_\rho\mathcal{Z}$ via the usual Euclidean inner product.

Recall that net fluxes do not necessarily have non-negative coordinates; the only restriction is that fluxes which push the state out the manifold $\mathcal{Z}$ are not allowed. For an arbitrary but fixed reference point $\rho^0 \in \mathcal{Z}$, this yields the manifold of integrated fluxes that preserve $\mathcal{Z}$ when starting from ρ^0

$$\mathcal{W} := \{w \in \mathbb{R}^{\mathcal{X}^2/2} : \rho^0 - \operatorname{div} w \in \mathcal{Z}\}, \text{ with tangent space}$$
$$T_\rho\mathcal{W} = \{j \in \mathbb{R}^{\mathcal{X}^2/2} : -\operatorname{div} j \in T_\rho\mathcal{Z}\},$$

where div is defined in (2.4). Again, $T^*_\rho\mathcal{W} = \mathbb{R}^{\mathcal{X}^2/2}$, paired with $T_\rho\mathcal{W}$ via the Euclidean inner product. In practice, one usually works with $j \in \mathbb{R}^{\mathcal{X}^2/2}$, setting $\mathcal{L}(\rho, j) = \infty$ when $j \notin T_\rho\mathcal{W}$.

The map $\phi : \mathcal{W} \to \mathcal{Z}$ is defined by $\phi[w] = \rho^0 - \operatorname{div} w$, and has the differential $d\phi_\rho = -\operatorname{div}$ and adjoint $d\phi_\rho^\mathsf{T} = \nabla$ where $\nabla_{xy}\zeta = \zeta_y - \zeta_x$. Note that $d\phi_\rho, d\phi_\rho^\mathsf{T}$ depend on ρ only via their domain of definition $T_\rho\mathcal{W}$.

Definition 2.4. For any $\mathcal{S} \subseteq \mathcal{Z}$ define $\mathcal{D}_\mathcal{S} := \{(\rho, j) : \rho \in \mathcal{S}, j \in T_\rho\mathcal{W}\}$. Then $\mathcal{L} : \mathcal{D}_\mathcal{S} \to \mathbb{R} \cup \{\infty\}$ is called an *L-function on* $\mathcal{S}$, if for all $\rho \in \mathcal{S}$ we have

(i) $\inf \mathcal{L}(\rho, \cdot) = 0$,

(ii) there exists a unique $j^0(\rho) \in T_\rho\mathcal{W}$, called the *zero-cost flow*, which satisfies $\mathcal{L}(\rho, j^0(\rho)) = 0$,

(iii) $\mathcal{L}(\rho, \cdot)$ is convex and lower semicontinuous (with respect to the Banach norm on $T_\rho\mathcal{W}$).

For the simplicity of notation, we will often drop the explicit dependence of the zero-cost flux j^0 on ρ. While this definition allows for flexibility in the domain, throughout this paper we will reserve the symbol $\mathcal{L}$ for L-functions on the full space $\mathcal{S} = \mathcal{Z}$. Section 2.2 onwards we will encounter functions $\mathcal{L}_G$ which are L-functions on proper subsets of $\mathcal{Z}$.

By lower semicontinuity and convexity, $\mathcal{L}(\rho, \cdot)$ is its own convex bidual with respect to the second variable [Pey15, Prop. 3.56], i.e. there exists an $\mathcal{H} : T^*\mathcal{W} \to \mathbb{R} \cup \{\infty\}$ such that

$$\mathcal{H}(\rho, \zeta) := \sup_{j \in T_\rho\mathcal{W}} \langle \zeta, j\rangle - \mathcal{L}(\rho, j) \qquad \text{and} \qquad \mathcal{L}(\rho, j) = \sup_{\zeta \in T^*_\rho\mathcal{W}} \langle \zeta, j\rangle - \mathcal{H}(\rho, \zeta). \tag{2.8}$$

It is easy to see that $\mathcal{L}$ is an L-function if and only if for any $\rho \in \mathcal{Z}$, $\mathcal{H}(\rho, 0) = 0$, $\mathcal{H}(\rho, \cdot)$ is convex, lower semicontinuous, proper and bounded from below by an affine function. Typically $\mathcal{L}(\rho, 0) < \infty$, so that $\mathcal{H}(\rho, \cdot)$ is bounded from below.

We use the following notion of the quasipotential.

Definition 2.5. A function $\mathcal{V} : \mathcal{Z} \to \mathbb{R} \cup \{\infty\}$ is called a *quasipotential* (corresponding to $\mathcal{L}$) if

(i) $\inf \mathcal{V} = 0$,

(ii) for any $\rho \in \mathcal{Z}$ where the Gateaux derivative $d\mathcal{V}$ is well defined, we have

$$\mathcal{H}(\rho, d\phi_\rho^\mathsf{T} d\mathcal{V}(\rho)) = 0. \tag{2.9}$$

We stress that this notion of a quasipotential is only related to the convex dual $\mathcal{H}$ of some abstract function $\mathcal{L}$, where a priori no stochastic particle system is involved. Both nowhere differentiable functions and the zero function are quasipotentials by definition, and our results are true but mostly trivial in this setting. In all the examples we consider, (2.9) will have at least one non-trivial solution and in fact this definition is consistent with the the usual definition from statistical physics when large deviations are involved (see Section 3.2). We envisage that (2.9) should be understood in the sense of viscosity solutions, however it is not clear how one can define a viscosity solution in the general setup of this section.

Example (IPFG). 2.6. In Example 2.1, the processes $X_1(t), X_2(t), \ldots$ are irreducible and $\mathcal{X}$ is finite which ensures the existence of an invariant measure $\pi \in \mathcal{P}_+(\mathcal{X})$ (space of strictly positive probability measures). Consequently, the n-particle density $\rho^{(n)}(t)$ admits an invariant measure $\Pi^{(n)} \in \mathcal{P}(\mathcal{P}(\mathcal{X}))$, where

$$\Pi^{(n)} = \Big(\bigotimes_{i=1}^n \pi\Big) \circ \eta_n^{-1}, \qquad \eta_n(x_1,\dots,x_n) := \tfrac{1}{n}\sum_{i=1}^n \delta_{x_i}.$$

By Sanov's theorem, the large-deviation rate functional corresponding to $\Pi^{(n)}$ is

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

where $s(\cdot \mid \cdot)$ is defined in (2.7), and hence $\mathcal{V}$ is indeed the quasipotential corresponding to $\mathcal{L}$ in the classical large-deviation sense (see Theorem 3.6).

This can also be checked macroscopically by verifying (2.9), without invoking any connection to large deviations of a microscopic particle system. The convex dual of $\mathcal{L}$ (2.6) is explicitly given by

$$\mathcal{H}(\rho,\zeta) := \sum\sum_{(x,y)\in\mathcal{X}^2/2} \big[\rho_x Q_{xy}\big(e^{\zeta_{xy}}-1\big) + \rho_y Q_{yx}\big(e^{-\zeta_{xy}}-1\big)\big].$$

Since $\pi_x > 0$ for every $x \in \mathcal{X}$, at points of differentiability of $\mathcal{V}$, i.e. when $\rho \in \mathcal{P}_+(\mathcal{Z}) \subseteq \mathcal{Z}$, using $Q^\mathsf{T}\pi = 0$ and $\sum_y Q_{xy} = 0$ we find

$$\begin{aligned}\mathcal{H}\big(\rho, d\phi_\rho^\mathsf{T} d\mathcal{V}(\rho)\big) = \mathcal{H}\big(\rho, \nabla \log \tfrac{\rho}{\pi}\big) &= \sum\sum_{(x,y)\in\mathcal{X}^2/2} \Big(\rho_x Q_{xy}\Big[\frac{\rho_y\pi_x}{\rho_x\pi_y}-1\Big] + \rho_y Q_{yx}\Big[\frac{\rho_x\pi_y}{\rho_y\pi_x}-1\Big]\Big)\\ &= \sum\sum_{\substack{x,y\in\mathcal{X}\\ x\neq y}} \frac{\rho_y}{\pi_y}\left(Q_{xy}\pi_x - Q_{yx}\pi_y\right) = \sum\sum_{x,y\in\mathcal{X}} Q_{xy}\pi_x\big(\frac{\rho_y}{\pi_y} - \frac{\rho_x}{\pi_x}\big) = \sum_{y\in\mathcal{X}} (Q^\mathsf{T}\pi)_y \frac{\rho_y}{\pi_y} = 0,\end{aligned}$$

where the third and fourth inequality follows by interchanging the indices in the second terms of the summation.

2.2 Dissipation potentials, tilted L-functions and Fisher information

While the concept of a dissipation potential is standard [CV90, LS95, Mie11], the connection to convex analysis [MPR14] and the application to flux spaces is more recent [MN08, Mae17, KJZ18, Ren18a, Ren18b]. Classically, a dissipation potential $\Phi(\rho, j)$ is convex, lower semicontinuous in the second variable, and satisfies $\inf \Phi(\rho,\cdot) = 0 = \Phi(\rho, 0)$. To define the dissipation potential in our context, we first present the following basic result on $\mathcal{L}$, which was originally derived in the context of gradient flows [MPR14, Lem. 2.1 & Prop. 2.1], where the driving force is the derivative of a certain free energy. As in the literature [Sch76, MN08, Mae17, KJZ18, Ren18a, RZ21], the setting with fluxes allows for more general driving forces. We first focus on a driving force $\hat\zeta \in T^*_\rho\mathcal{W}$ for a fixed ρ; and later introduce it as a ρ-dependent force field $F(\rho)$.

Theorem 2.7. *[MPR14, Prop. 2.1(i)] Let $\mathcal{L}$ be an L-function on $\mathcal{Z}$ and fix $\rho \in \mathcal{Z}$. For any $\hat\zeta \in T^*_\rho\mathcal{W}$ and convex lower-semicontinuous $\Phi(\rho,\cdot) : T_\rho\mathcal{W} \to \mathbb{R}\cup\{\infty\}$ with convex dual Φ^*, the following statements are equivalent*

(i) $\inf \Phi(\rho,\cdot) = 0 = \Phi(\rho,0)$, *and for any* $j \in T_\rho\mathcal{W}$

$$\mathcal{L}(\rho, j) = \Phi(\rho, j) + \Phi^*(\rho,\hat\zeta) - \langle\hat\zeta, j\rangle. \tag{2.10}$$

(ii) $-\hat\zeta \in \partial\mathcal{L}(\rho, 0)$ *with*

$$\Phi^*(\rho,\zeta) = \mathcal{H}(\rho,\zeta-\hat\zeta) - \mathcal{H}(\rho,-\hat\zeta). \tag{2.11}$$

Proof. The result is mathematically the same as the cited one, but applied to the context of the state-flux triple $(\mathcal{Z},\mathcal{W},\phi)$. We provide a short proof for convenience and completeness. For the forward implication, by Fermat's rule $0 \in \partial\Phi(\rho,0)$, and calculating the subdifferential of (2.10) at $j=0$ yields $-\hat\zeta \in \partial\mathcal{L}(\rho,0)$ as claimed. The convex dual of (2.10) is

$$\mathcal{H}(\rho,\zeta) = \Phi^*(\rho,\zeta+\hat\zeta) - \Phi^*(\rho,\hat\zeta). \tag{2.12}$$

Therefore $\mathcal{H}(\rho,-\hat\zeta) = \Phi^*(\rho,0) - \Phi^*(\rho,\hat\zeta) = -\Phi^*(\rho,\hat\zeta)$ and $\mathcal{H}(\rho,\zeta-\hat\zeta) = \Phi^*(\rho,\zeta) - \Phi^*(\rho,\hat\zeta) = \Phi^*(\rho,\zeta) + \mathcal{H}(\rho,-\hat\zeta)$. Here we have used $\Phi^*(\rho,0) = -\inf\Phi(\rho,\cdot) = 0$.

Next we prove the backward implication. By (2.11) and $\mathcal{H}(\rho,0) = \inf\mathcal{L}(\rho,\cdot) = 0$, we find $\Phi^*(\rho,0) = 0$ and $\Phi^*(\rho,\hat\zeta) = -\mathcal{H}(\rho,-\hat\zeta)$. Since $-\hat\zeta \in \partial\mathcal{L}(\rho,0)$, we have $0 \in \partial\mathcal{H}(\rho,-\hat\zeta)$, which by Fermat's rule implies that $-\hat\zeta$ is a minimiser of $\mathcal{H}(\rho,\cdot)$, and using (2.11) it follows that 0 is a minimiser of $\Phi^*(\rho,\cdot)$. Therefore we have $\inf\Phi^*(\rho,\cdot) = 0 = \Phi^*(\rho,0)$, which is equivalent to $\inf\Phi(\rho,\cdot) = 0 = \Phi(\rho,0)$ as claimed. Taking the convex dual of (2.11) yields

$$\Phi(\rho,j) = \mathcal{L}(\rho,j) + \mathcal{H}(\rho,-\hat\zeta) + \langle\hat\zeta,j\rangle = \mathcal{L}(\rho,j) - \Phi^*(\rho,\hat\zeta) + \langle\hat\zeta,j\rangle.$$

□

We would like to define the driving force as $F(\rho) = \hat\zeta$ and the dissipation potential $\Phi(\rho,j)$ as above. However these exist uniquely only if the subdifferential $\partial\mathcal{L}(\rho,0)$ consists of a singleton, i.e. $\mathcal{L}(\rho,\cdot)$ is Gateaux differentiable at 0, which motivates the following definitions.

Definition 2.8. Let $\mathcal{L}$ be an L-function on $\mathcal{Z}$. The driving force F and dissipation potentials (corresponding to $\mathcal{L}$) are defined as

$$\begin{aligned}
\mathrm{Dom}(F) \ni \rho &\mapsto F(\rho) := -d\mathcal{L}(\rho,0) \in T^*_\rho\mathcal{W}, && (2.13)\\
T^*_{\mathrm{Dom}(F)}\mathcal{W} \ni (\rho,\zeta) &\mapsto \Phi^*(\rho,\zeta) := \mathcal{H}\big(\rho,\zeta-F(\rho)\big) - \mathcal{H}\big(\rho,-F(\rho)\big), && (2.14)\\
T_{\mathrm{Dom}(F)}\mathcal{W} \ni (\rho,j) &\mapsto \Phi(\rho,j) := \sup_{\zeta\in T^*_\rho\mathcal{W}} \langle\zeta,j\rangle - \Phi^*(\rho,\zeta).
\end{aligned}$$

where

$$\begin{aligned}
\mathrm{Dom}(F) &:= \big\{\rho\in\mathcal{Z} : j\mapsto\mathcal{L}(\rho,j) \text{ is Gateaux differentiable at } j=0\big\},\\
T^*_{\mathrm{Dom}(F)}\mathcal{W} &:= \big\{(\rho,\zeta)\in T^*\mathcal{W} : \rho\in\mathrm{Dom}(F)\big\},\\
T_{\mathrm{Dom}(F)}\mathcal{W} &:= \big\{(\rho,j)\in T\mathcal{W} : \rho\in\mathrm{Dom}(F)\big\}.
\end{aligned}$$

Note that, Φ^* as defined in (2.14) indeed satisfies $\inf\Phi^*(\rho,\cdot) = 0 = \Phi(\rho,0)$, since $-F$ is a minimiser of $\mathcal{H}(\rho,\cdot)$ by (2.13), and consequently it is a dissipation potential in the classical sense. Furthermore combining Theorem 2.7 with Definition 2.8, for any $\rho\in\mathrm{Dom}(F)$ and $j\in T_\rho\mathcal{W}$ we have the decomposition

$$\mathcal{L}(\rho,j) = \Phi(\rho,j) + \Phi^*(\rho,F) - \langle F,j\rangle. \tag{2.15}$$

In what follows we will make use of

$$\mathrm{Dom}_{\mathrm{symdiss}}(F) := \Big\{\rho\in\mathrm{Dom}(F) : \mathcal{H}\big(\rho,\zeta+d\mathcal{L}(\rho,0)\big) = \mathcal{H}\big(\rho,-\zeta+d\mathcal{L}(\rho,0)\big) \text{ for all } (\rho,\zeta)\in T^*_{\mathrm{Dom}(F)}\mathcal{W}\Big\}. \tag{2.16}$$

The following lemma states that the dissipation potential is indeed symmetric in $\mathrm{Dom}_{\mathrm{symdiss}}(F)$.

Lemma 2.9 ([MPR14, Prop. 2.1(ii)])**.** *Let $\mathcal{L}$ be a L-function on $\mathcal{Z}$. For $\rho\in\mathrm{Dom}_{\mathrm{symdiss}}(F)$ the following statements are equivalent*

(i) $\mathcal{H}\big(\rho,\zeta-F(\rho)\big) = \mathcal{H}\big(\rho,-\zeta-F(\rho)\big)$ *for all* $\zeta\in T^*_\rho\mathcal{W}$,

(ii) $\mathcal{L}(\rho,j) = \mathcal{L}(\rho,-j) - 2\langle F(\rho),j\rangle$ *for all* $j\in T_\rho\mathcal{W}$,

(iii) $\Phi^*(\rho,\zeta) = \Phi^*(\rho,-\zeta)$ *for all* $\zeta\in T^*_\rho\mathcal{W}$,

(iv) $\Phi(\rho,j) = \Phi(\rho,-j)$ *for all* $j\in T_\rho\mathcal{W}$.

Example (IPFG). 2.10. In practice the force (2.13) is more easily calculated via the equivalent statement $d\mathcal{H}(\rho, -F(\rho)) = 0$. Since $\xi = \frac{1}{2}\log\frac{d}{c}$ minimises $\xi \mapsto c(e^{\xi}-1) + d(e^{-\xi}-1)$, we find

$$F_{xy}(\rho) = \frac{1}{2}\log\frac{\rho_x Q_{xy}}{\rho_y Q_{yx}}, \qquad \mathrm{Dom}(F) = \mathcal{P}_+(\mathcal{X}).$$

This definition of the driving force has been introduced in [KJZ18, Sec. 2.2]. Using (2.14), the dissipation potentials are given by

$$\begin{aligned}\Phi^*(\rho,\zeta) &= \sum\sum_{(x,y)\in\mathcal{X}^2/2} 2\sqrt{\rho_x Q_{xy}\rho_y Q_{yx}}\big(\cosh(\zeta_{xy}) - 1\big), \qquad (2.17)\\ \Phi(\rho,j) &= \sum\sum_{(x,y)\in\mathcal{X}^2/2} 2\sqrt{\rho_x Q_{xy}\rho_y Q_{yx}}\Big(\cosh^*\big(\tfrac{j_{xy}}{2\sqrt{\rho_x Q_{xy}\rho_y Q_{yx}}}\big) - 1\Big).\end{aligned}$$

These dissipation potentials are indeed symmetric (since cosh is even), and therefore $\mathrm{Dom}_{\mathrm{symdiss}}(F) = \mathrm{Dom}(F)$. Note that, while a priori Φ and Φ^* are only defined for strictly positive probability measures, they can easily be extended to the full space $\mathcal{Z} = \mathcal{P}(\mathcal{X})$. For instance, the observation that $\lim_{a\to 0} a\cosh^*(\frac{x}{a}) = 0$ if $x = 0$ and $+\infty$ otherwise, offers a trivial extension of Φ^* to $\mathcal{Z}$, which also reflects the idea that 0 rates guarantee no flux.

We note that the Hamiltonian corresponding to one-way fluxes is given by

$$\mathcal{H}^{\text{one-way}}(\rho,\zeta) := \sum\sum_{\substack{x,y\in\mathcal{X}\times\mathcal{X}\\ x\neq y}} \rho_x Q_{xy}(e^{\zeta_{xy}} - 1),$$

for which the corresponding driving force does not exist at all, i.e. $\mathrm{Dom}(F^{\text{one-way}}) = \emptyset$ (also see [Ren18a, Rem. 4.10]). Hence one can only construct a meaningful macroscopic fluctuation theory for net fluxes. This further justifies the net-flux approach used in this paper, as opposed to the one-way fluxes typically used for Markov jump processes.

Note that in the IPFG example above and all the other examples considered in Section 5, $\mathrm{Dom}_{\mathrm{symdiss}}(F) = \mathrm{Dom}(F)$, i.e. the dissipation potential is symmetric. However as discussed in the following remark, it is possible to construct non-symmetric dissipation potentials, and therefore in general $\mathrm{Dom}_{\mathrm{symdiss}}(F)$ is a subset of $\mathrm{Dom}(F)$.

Remark 2.11. Consider $\mathcal{Z} = \mathcal{W} = \mathbb{R}$ and $\phi = \mathrm{id}$. Let $\mathcal{H}(\rho,\zeta) = -\zeta + e^{\zeta} - 1$, which corresponds to a real-valued Markov process with generator $(\mathcal{Q}^{(n)}f)(\rho,w) := -\partial_\rho f(\rho,w) - \partial_w f(\rho,w) + n(f(\rho+\frac{1}{n}, w+\frac{1}{n}) - f(\rho,w))$. Then $F \equiv 0$ and clearly $\mathcal{H}(\rho, -\zeta - F(\rho)) \neq \mathcal{H}(\rho, \zeta - F(\rho))$, which implies that $\mathrm{Dom}_{\mathrm{symdiss}}(F) = \emptyset$. □

So far we have dealt with L-functions on $\mathcal{Z}$. Using (2.11), we now introduce L-functions defined on subsets of $\mathcal{Z}$. For a given $\mathcal{L}$ and an appropriate cotangent field $G(\rho)$, using (2.11) we can define a (G-tilted) L-function $\mathcal{L}_G$ defined on a subset of $\mathcal{Z}$. We call this a 'tilted' L-function since its definition is motivated by tilted Markov processes (see Section 3.1). Although, technically G is a cotangent field, in this paper we will often refer to it as a force field due to physical considerations.

Definition 2.12. For any $G : \mathrm{Dom}(G) \to T^*_{\mathrm{Dom}(G)}\mathcal{W}$ with $\mathrm{Dom}(G) \subseteq \mathcal{Z}$, the tilted function $\mathcal{H}_G : T^*_{\mathrm{Dom}(F)\cap\mathrm{Dom}(G)}\mathcal{W} \to \mathbb{R}\cup\{\infty\}$ is defined as

$$\mathcal{H}_G(\rho,\zeta) := \mathcal{H}\big(\rho, \zeta + G(\rho) - F(\rho)\big) - \mathcal{H}\big(\rho, G(\rho) - F(\rho)\big), \qquad (2.18)$$

and $\mathcal{L}_G : T_{\mathrm{Dom}(F)\cap\mathrm{Dom}(G)}\mathcal{W} \to \mathbb{R}\cup\{\infty\}$ denotes its convex dual in the second variable.

Lemma 2.13. *The tilted function $\mathcal{L}_G$ is an L-function on* $\mathrm{Dom}(F)\cap\mathrm{Dom}(G)$, *and satisfies the decomposition*

$$\begin{aligned}\mathcal{L}_G(\rho,j) &= \mathcal{L}(\rho,j) + \mathcal{H}\big(\rho, G(\rho) - F(\rho)\big) + \langle F(\rho) - G(\rho), j\rangle \qquad (2.19)\\ &= \Phi(\rho,j) + \Phi^*\big(\rho, G(\rho)\big) - \langle G(\rho), j\rangle.\end{aligned}$$

The two equalities follow by using convex duality and (2.10), (2.11) with $\hat{\zeta} = F$. For special choices of $G(\rho)$ we obtain

$$\mathcal{L}_F(\rho, j) = \mathcal{L}(\rho, j) \quad \text{and} \quad \mathcal{L}_0(\rho, j) = \Phi(\rho, j). \tag{2.20}$$

Example (IPFG). 2.14. For any force field $G(\rho) \in \mathbb{R}^{\mathcal{X}^2/2}$ we have

$$\mathcal{L}_G(\rho, j) = \inf_{j^+ \in \mathbb{R}^{\mathcal{X}^2/2}} \sum\sum_{(x,y)\in\mathcal{X}^2/2} s\big(j^+_{xy} \mid \sqrt{\rho_x Q_{xy} \rho_y Q_{yx}} e^{G_{xy}(\rho)}\big) + s\big(j^+_{xy} - j_{xy} \mid \sqrt{\rho_x Q_{xy} \rho_y Q_{yx}} e^{-G_{xy}(\rho)}\big),$$

$$\mathcal{H}_G(\rho, \zeta) = \sum\sum_{(x,y)\in\mathcal{X}^2/2} \sqrt{\rho_x Q_{xy} \rho_y Q_{yx}} \Big[e^{G_{xy}(\rho)}(e^{\zeta_{xy}} - 1) + e^{-G_{xy}(\rho)}(e^{-\zeta_{xy}} - 1)\Big].$$

We now define the notion of *generalised Fisher information* which was introduced in Section 1.1.

Definition 2.15. Let $\mathcal{L}$ be an L-function on $\mathcal{Z}$. For any $\rho \in \mathcal{Z}$, $\zeta \in T^*_\rho \mathcal{W}$, and $\lambda \in [0, 1]$, the generalised Fisher information is

$$\mathcal{R}^\lambda_\zeta(\rho) = -\mathcal{H}(\rho, -2\lambda\zeta).$$

As discussed in Section 1.1, it is important to choose λ and ζ such that $\mathcal{R}^\lambda_\zeta$ is non-negative, as this guarantees that the corresponding powers are non-negative along the zero-cost flux. The following result explores the set of force fields for which this is true (also see Figure 2).

Proposition 2.16. *Let $\mathcal{L}$ be a L-function on $\mathcal{Z}$. For any $\rho \in \mathcal{Z}$ we have*

(i) The set $\{\zeta \in T^*_\rho \mathcal{W} : \mathcal{R}^{\frac{1}{2}}_\zeta(\rho) \geq 0\}$ is convex and includes $\zeta = 0$.

(ii) In particular, if $\zeta \in T^*_\rho \mathcal{W}$ such that

$$\mathcal{R}^{\frac{1}{2}}_\zeta(\rho) \geq 0, \tag{2.21}$$

then for any $\lambda \in [0, 1]$

$$\mathcal{R}^\lambda_{\frac{1}{2}\zeta}(\rho) \geq 0. \tag{2.22}$$

(iii) For any $\zeta \in T^*_\rho \mathcal{W}$ we have

$$\lim_{\lambda \downarrow 0} \tfrac{1}{\lambda} \mathcal{R}^\lambda_\zeta(\rho) = 2\langle \zeta, j^0(\rho)\rangle. \tag{2.23}$$

where j^0 is the zero-cost flux for $\mathcal{L}$ (see Definition 2.4).

Proof. *(i)* Since $\mathcal{L}$ is an L-function, $\mathcal{H}(\rho, \cdot)$ is convex with $\mathcal{H}(\rho, 0) = 0$ and the assertion follows.
(ii) Using convexity, $-\mathcal{R}^\lambda_{\frac{1}{2}\zeta}(\rho) = \mathcal{H}(\rho, -\lambda\zeta) = \mathcal{H}(\rho, -\lambda\zeta + (1 - \lambda)0) \leq \lambda\mathcal{H}(\rho, -\zeta) + (1 - \lambda)\mathcal{H}(\rho, 0) \leq 0$.
(iii) By definition of L-functions, $\mathcal{L}(\rho, \cdot)$ has unique minimiser $j^0(\rho)$, which is equivalent to $\partial\mathcal{H}(\rho, 0) = \{j^0(\rho)\} = \{d\mathcal{H}(\rho, 0)\}$. The claim then follows from the definition of the Gateaux derivative. □

Note that [HPST20, Thm. 1.7] is a special case of this result for the IPFG example. Following [HPST20], we call $\mathcal{R}^\lambda$ the generalised Fisher information since it generalises the classical notion of Fisher information as the dissipation rate of free energy along the solutions of the zero-cost flux of the L-function. This property follows by using (2.23) with appropriate choices for ζ. In the next section we construct ζ for which $\mathcal{R}^{\frac{1}{2}}_\zeta(\rho) = 0$ and the above result can be applied.

2.3 Reversed L-function, symmetric and antisymmetric forces

Inspired by the notion of time-reversibility in MFT we now introduce the reversed L-function which will then be used to define symmetric and antisymmetric forces. From now on we assume that $\mathcal{V}$ is a quasi-potential associated to $\mathcal{L}$ in the sense of Definition 2.5.

Definition 2.17. Let $\mathcal{L}$ be a L-function on $\mathcal{Z}$. For any $\rho \in \mathcal{Z}$ where $\mathcal{V}$ is Gateaux differentiable and any $j \in T_\rho \mathcal{W}$, we define the *reversed L-function* as

$$\overleftarrow{\mathcal{L}}(\rho, j) := \mathcal{L}(\rho, -j) + \langle d\phi_\rho^\mathsf{T} d\mathcal{V}(\rho), j \rangle.$$

This notion of the reversed L-function is motivated by the large-deviations of time-reversed Markov processes (see Section 3.3 for details). Note that we use the name reversed L-function as opposed to time-reversed L-function since there is no time variable in this abstract setup.

The following result states that $\overleftarrow{\mathcal{L}}$ is indeed a L-function, and discusses the driving force and dissipation potential associated to it.

Proposition 2.18. *Let $\mathcal{L}$ be a L-function on $\mathcal{Z}$. For any $\rho \in \mathcal{Z}$ where $\mathcal{V}$ is Gateaux differentiable we have*

(i) The convex dual of $\overleftarrow{\mathcal{L}}(\rho, \cdot)$ is $\overleftarrow{\mathcal{H}}(\rho, \zeta) = \mathcal{H}\big(\rho, d\phi_\rho^\mathsf{T} d\mathcal{V}(\rho) - \zeta\big)$.

(ii) If $\overleftarrow{\jmath}^0(\rho)$ is the zero-cost flux in the sense that $\overleftarrow{\mathcal{L}}\big(\rho, \overleftarrow{\jmath}^0(\rho)\big) = 0$, then $-\overleftarrow{\jmath}^0(\rho) \in \partial \mathcal{H}\big(\rho, d\phi_\rho^\mathsf{T} d\mathcal{V}(\rho)\big)$, and it is unique if $\mathcal{H}(\rho, \cdot)$ is Gateaux differentiable at $d\phi_\rho^\mathsf{T} d\mathcal{V}(\rho)$. Furthermore $\overleftarrow{\mathcal{L}}$ is a L-function on $\mathrm{Dom}(F^{\mathrm{sym}})$*, i.e. any $\rho \in \mathcal{Z}$ for which $d\phi_\rho^\mathsf{T} d\mathcal{V}(\rho)$ is well defined (see* (2.24), (2.25) *for definition) and $\mathcal{V}$ is a quasipotential corresponding to $\overleftarrow{\mathcal{L}}$.*

(iii) Additionally, if $\rho \in \mathrm{Dom}(F)$, then the driving force and dissipation potentials corresponding to $\overleftarrow{\mathcal{L}}$ are given by

$$\overleftarrow{F}(\rho) = -F(\rho) - d\phi_\rho^\mathsf{T} d\mathcal{V}(\rho), \quad \overleftarrow{\Phi}(\rho, j) = \Phi(\rho, -j), \quad \overleftarrow{\Phi}^*(\rho, \zeta) = \Phi^*(\rho, -\zeta).$$

Proof. (i) Follows by a straightforward calculation of the convex dual.
(ii) Using the Fermat's rule $0 \in \partial \overleftarrow{\mathcal{L}}(\rho, \overleftarrow{\jmath}^0(\rho))$, and therefore $\overleftarrow{\jmath}^0(\rho) \in \partial \overleftarrow{\mathcal{H}}(\rho, 0)$. Using Definition 2.17 and since $\mathcal{L}$ is a L-function, $\overleftarrow{\mathcal{L}}$ is convex, lower semicontinuous and using (2.9) satisfies $\inf \overleftarrow{\mathcal{L}}(\rho, \cdot) = 0$. Consequently $\overleftarrow{\mathcal{L}}$ is a L-function on $\mathrm{Dom}(F^{\mathrm{sym}})$ (see (2.25) below) and $\mathcal{V}$ is a quasipotential associated to $\overleftarrow{\mathcal{L}}$.
(iii) Using (2.13) we find

$$-\overleftarrow{F}(\rho) := d\overleftarrow{\mathcal{L}}(\rho, 0) = -d\mathcal{L}(\rho, 0) + d\phi_\rho^\mathsf{T} d\mathcal{V}(\rho) = F(\rho) + d\phi_\rho^\mathsf{T} d\mathcal{V}(\rho)$$

and using (2.14) we find

$$\begin{aligned} \overleftarrow{\Phi}^*(\rho, \zeta) &:= \overleftarrow{\mathcal{H}}\big(\rho, \zeta - \overleftarrow{F}(\rho)\big) - \overleftarrow{\mathcal{H}}\big(\rho, -\overleftarrow{F}(\rho)\big) = \mathcal{H}\big(\rho, d\phi_\rho^\mathsf{T} d\mathcal{V}(\rho) + \overleftarrow{F}(\rho) - \zeta\big) - \mathcal{H}\big(\rho, d\phi_\rho^\mathsf{T} d\mathcal{V}(\rho) + \overleftarrow{F}(\rho)\big) \\ &= \mathcal{H}\big(\rho, -F(\rho) - \zeta\big) - \mathcal{H}\big(\rho, -F(\rho)\big) = \Phi^*(\rho, -\zeta). \end{aligned}$$

Consequently $\overleftarrow{\Phi}(\rho, j) = \Phi(\rho, -j)$. □

Motivated by this result, we decompose the driving force F (recall (2.13)) into a symmetric and antisymmetric part with respect to the reversal, i.e. $F^{\mathrm{sym}} = \frac{1}{2}(F + \overleftarrow{F})$ and $F^{\mathrm{asym}} = \frac{1}{2}(F - \overleftarrow{F})$. The following result summarises these ideas.

Corollary 2.19. *Let $\mathcal{L}$ be a L-function on $\mathcal{Z}$. Define*

$$\begin{aligned} \mathrm{Dom}(F^{\mathrm{sym}}) \ni \rho &\mapsto F^{\mathrm{sym}}(\rho) := -\tfrac{1}{2} d\phi_\rho^\mathsf{T} d\mathcal{V}(\rho), \\ \mathrm{Dom}(F^{\mathrm{asym}}) \ni \rho &\mapsto F^{\mathrm{asym}}(\rho) := F(\rho) + \tfrac{1}{2} d\phi_\rho^\mathsf{T} d\mathcal{V}(\rho), \end{aligned} \tag{2.24}$$

where

$$\begin{aligned}\mathrm{Dom}(F^{\mathrm{sym}}) &:= \{\rho \in \mathcal{Z} : \mathcal{V} \text{ is Gateaux differentiable at } \rho\}, \\ \mathrm{Dom}(F^{\mathrm{asym}}) &:= \mathrm{Dom}(F) \cap \mathrm{Dom}(F^{\mathrm{sym}}).\end{aligned} \tag{2.25}$$

Then for any $\rho \in \mathrm{Dom}(F^{\mathrm{asym}})$,

$$F(\rho) = F^{\mathrm{sym}}(\rho) + F^{\mathrm{asym}}(\rho), \quad \text{and} \quad \overleftarrow{F}(\rho) = F^{\mathrm{sym}}(\rho) - F^{\mathrm{asym}}(\rho). \tag{2.26}$$

Note that while we make use of the reversed L-function to construct the symmetric and antisymmetric force, it does not explicitly appear in their definition. In the case of zero antisymmetric force, i.e. $F^{\mathrm{asym}}(\rho) = 0$, the driving forces satisfy $F(\rho) = \overleftarrow{F}(\rho) = F^{\mathrm{sym}}(\rho)$, which is the setting of dissipative systems (see Section 2.6).

Example (IPFG). 2.20. We have

$$\begin{aligned}\overleftarrow{\mathcal{H}}(\rho,\zeta) &= \sum\sum_{(x,y)\in\mathcal{X}^2/2} \rho_x \frac{\pi_y}{\pi_x} Q_{yx}(e^{\zeta_{xy}} - 1) + \rho_y \frac{\pi_x}{\pi_y} Q_{xy}(e^{-\zeta_{xy}} - 1), \\ \overleftarrow{\mathcal{L}}(\rho,j) &= \inf_{j^+\in\mathbb{R}^{\mathcal{X}^2/2}_{\geq 0}} \sum\sum_{(x,y)\in\mathcal{X}^2/2} s\big(j^+_{xy} \mid \rho_x \frac{\pi_y}{\pi_x} Q_{yx}\big) + s\big(j^+_{xy} - j_{xy} \mid \rho_y \frac{\pi_x}{\pi_y} Q_{xy}\big), \\ \overleftarrow{F}_{xy}(\rho) &= \frac{1}{2} \log \frac{\rho_x \frac{\pi_y}{\pi_x} Q_{yx}}{\rho_y \frac{\pi_x}{\pi_y} Q_{xy}}.\end{aligned}$$

The expression $\frac{\pi_x}{\pi_y} Q_{xy}$ is the generator matrix for a single time-reversed jump process [Nor98, Thm. 3.7.1]. Again, beware that a priori $\overleftarrow{\mathcal{H}}$ and $\overleftarrow{\mathcal{L}}$ are only defined on $\mathcal{Z} = \mathrm{Dom}(F)$, but can be continuously extended to $\mathcal{P}(\mathcal{X})$ in a straightforward manner.

The symmetric and antisymmetric (with respect to the reversal) components of the driving force are (also see [KJZ18])

$$F^{\mathrm{sym}}_{xy}(\rho) = \frac{1}{2} \log \frac{\pi_y \rho_x}{\pi_x \rho_y} \quad \text{and} \quad F^{\mathrm{asym}}_{xy}(\rho) = \frac{1}{2} \log \frac{\pi_x Q_{xy}}{\pi_y Q_{yx}}, \tag{2.27}$$

with $\mathrm{Dom}(F) = \mathrm{Dom}(F^{\mathrm{sym}}) = \mathrm{Dom}(F^{\mathrm{asym}}) = \mathcal{P}_+(\mathcal{X})$. Note that for reversible Markov chains, i.e. those satisfying *detailed balance*, $F^{\mathrm{asym}} = 0$.

Recall the generalised Fisher information $\mathcal{R}^\lambda_\zeta$ from Definition 2.15, and that we are looking for force fields that make this quantity non-negative. The following result shows that $\mathcal{R}^{\frac{1}{2}}_\zeta(\rho) = 0$ for $\zeta = 2F(\rho), 2F^{\mathrm{sym}}(\rho), 2F^{\mathrm{asym}}(\rho)$. This will be crucial to derive the key decompositions of $\mathcal{L}$ in Section 2.5.

In this result we make use of

$$\mathrm{Dom}_{\mathrm{symdiss}}(F^{\mathrm{asym}}) := \Big\{\rho \in \mathrm{Dom}(F^{\mathrm{asym}}) : \ \mathcal{H}\big(\rho, \zeta + d\mathcal{L}(\rho,0)\big) = \mathcal{H}\big(\rho, -\zeta + d\mathcal{L}(\rho,0)\big), \ \forall \zeta \in T^*_\rho \mathcal{W}\Big\}. \tag{2.28}$$

Note that $\mathrm{Dom}_{\mathrm{symdiss}}(F^{\mathrm{asym}}) \subseteq \mathrm{Dom}_{\mathrm{symdiss}}(F)$ since $\mathrm{Dom}(F^{\mathrm{asym}}) \subseteq \mathrm{Dom}\, F$.

Lemma 2.21. *Let $\mathcal{L}$ be a L-function on $\mathcal{Z}$. We have*

(i) $\forall \rho \in \mathrm{Dom}(F) : \ \mathcal{R}^{\frac{1}{2}}_F(\rho) \geq 0$ *and* $\forall \rho \in \mathrm{Dom}_{\mathrm{symdiss}}(F) : \ \mathcal{R}^{\frac{1}{2}}_{2F}(\rho) = 0$,

(ii) $\forall \rho \in \mathrm{Dom}(F^{\mathrm{sym}}) : \ \mathcal{R}^{\frac{1}{2}}_{2F^{\mathrm{sym}}}(\rho) = 0$,

(iii) $\forall \rho \in \mathrm{Dom}_{\mathrm{symdiss}}(F^{\mathrm{asym}}) : \ \mathcal{R}^{\frac{1}{2}}_{2F^{\mathrm{asym}}}(\rho) = 0.$

Proof. *(i)* Since $-F$ minimises $\mathcal{H}$, it follows that $\mathcal{H}(\rho,-F) = \inf \mathcal{H}(\rho,\cdot) \le \mathcal{H}(\rho,0) = -\inf \mathcal{L}(\rho,\cdot) = 0$, and therefore $\mathcal{R}^{\frac{1}{2}}_{F}(\rho) = -\mathcal{H}(\rho,-F) \ge 0$. If the dissipation potential is symmetric, the choice $\zeta = -F(\rho)$ in Lemma 2.9(i) gives $\mathcal{R}^{\frac{1}{2}}_{2F}(\rho) = \mathcal{H}\big(\rho,-2F(\rho)\big) = \mathcal{H}(\rho,0) = 0$.
(ii) The claim follows since (2.9) holds for all $\rho \in \mathrm{Dom}(F^{\mathrm{sym}})$.
(iii) With $\zeta = \overleftarrow{F}(\rho) = F^{\mathrm{sym}}(\rho) - F^{\mathrm{asym}}(\rho)$ in Lemma 2.9(i) we find $\mathcal{H}\big(\rho,-2F^{\mathrm{asym}}(\rho)\big) = \mathcal{H}\big(\rho,-2F^{\mathrm{sym}}(\rho)\big) = 0$. □

Figure 2 is a schematic digram of force fields ζ for which $\mathcal{R}^{\lambda}_{\zeta}$ is non-negative. Note that, while there are various possibilities for such ζ, we focus on $\zeta = 2F(\rho), 2F^{\mathrm{sym}}(\rho), 2F^{\mathrm{asym}}(\rho)$ since they correspond to the physically relevant powers defined in (1.3) and (1.4).

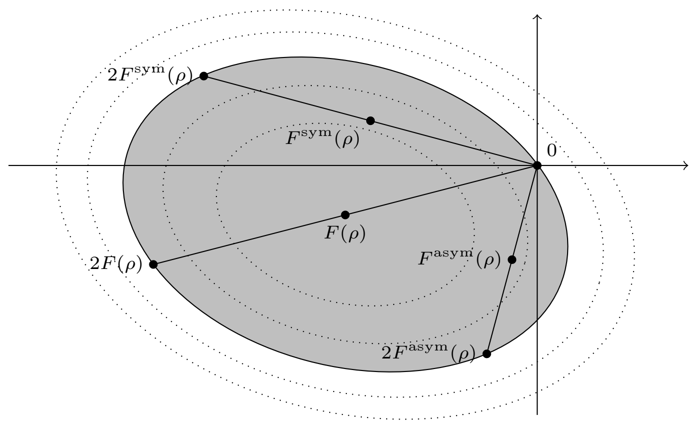

Figure 2: Contour lines of a possible concave function $\zeta \mapsto \mathcal{R}^{\frac{1}{2}}_{\zeta}(\rho)$ for a fixed ρ, where the superlevel set $\{\zeta \in T^*_\rho\mathcal{W} : \mathcal{R}^{\frac{1}{2}}_{\zeta}(\rho) \ge 0\}$ is depicted in gray. By Definitions 2.8 and 2.15, $F(\rho)$ is a maximiser for $\zeta \mapsto \mathcal{R}^{\frac{1}{2}}_{\zeta}(\rho)$, and assuming $\rho \in \mathrm{Dom}_{\mathrm{symdiss}}(F^{\mathrm{asym}})$, Lemma 2.21 says that $2F(\rho)$, $2F^{\mathrm{sym}}(\rho)$ and $2F^{\mathrm{asym}}(\rho)$ all lie on the 0-contour line. By the convexity of the superlevel set $\{\mathcal{R}^{\frac{1}{2}}_{\zeta}(\rho) \ge 0\}$ (see Proposition 2.16), any convex combination ζ between 0 and $2F(\rho)$, $2F^{\mathrm{sym}}(\rho)$ or $2F^{\mathrm{asym}}(\rho)$, drawn by the three lines, yield non-negative $\mathcal{R}^{\frac{1}{2}}_{\zeta}(\rho) \ge 0$. This picture should be seen as a schematic sketch; it is difficult to construct a two-dimensional example with a non-trivial asymmetric force.

Remark 2.22. For all $\rho \in \mathrm{Dom}(F^{\mathrm{asym}})$, we can write the reversed function as a tilting in the sense of (2.18)

$$\overleftarrow{\mathcal{H}}(\rho,\zeta) = \mathcal{H}_{-\overleftarrow{F}}(\rho,-\zeta).$$

Using (2.19), the corresponding reversed L-function then satisfies

$$\overleftarrow{\mathcal{L}}(\rho,j) = \mathcal{L}_{-\overleftarrow{F}}(\rho,j) = \mathcal{L}(\rho,j) + \mathcal{H}\big(\rho, d\phi_\rho^{\mathsf{T}} d\mathcal{V}(\rho)\big) - \langle d\phi_\rho^{\mathsf{T}} d\mathcal{V}(\rho), j\rangle = \Phi(\rho,j) + \Phi^*\big(\rho,-\overleftarrow{F}\big) + \langle -\overleftarrow{F}, j\rangle,$$

where we have used $F + \overleftarrow{F} = -d\phi_\rho^{\mathsf{T}} d\mathcal{V}(\rho)$. □

2.4 Generalised orthogonality

Before we continue with deriving the main decompositions (1.5) of the L-function, we elaborate further on the decomposition of the driving force F into the symmetric force F^{sym} and antisymmetric force F^{asym}, and investigate the natural question whether these forces are orthogonal in some sense. It turns out that they are indeed orthogonal in a generalised sense, and using this notion of orthogonality we can already derive decompositions (1.5) for $\lambda = \frac{1}{2}$. As discussed in the introduction, in MFT the dissipation potentials are often squares of appropriate Hilbert norms $\|\cdot\|_\rho$, and in that setting one can write

$$\begin{aligned}\Phi^*\big(\rho,\zeta^1+\zeta^2\big) &:= \tfrac12\|\zeta^1+\zeta^2\|_\rho^2 = \tfrac12\|\zeta^1\|_\rho^2 + \langle\zeta^1,\zeta^2\rangle_\rho + \tfrac12\|\zeta^2\|_\rho^2\\ &= \Phi^*\big(\rho,\zeta^1\big) + \langle\zeta^1,\zeta^2\rangle_\rho + \Phi^*\big(\rho,\zeta^2\big),\end{aligned}$$

where $\langle\cdot,\cdot\rangle_\rho$ is the inner product induced by the norm. Typically F^{sym} and F^{asym} are orthogonal in the sense that $\langle F^{\mathrm{sym}},F^{\mathrm{asym}}\rangle_\rho = 0$. We reiterate these ideas more clearly in Section 5.3 which deals with the classical MFT setting of lattice gases. However this orthogonality relation is specific to the quadratic setting. A generalised notion of orthogonality was introduced in [KJZ18] for non-quadratic dissipation potential (2.17) corresponding to independent Markov chains which have cosh-type structure (see Example 2.10) and this principle was further generalised to chemical reaction networks in [RZ21] (see Section 5.2 for details). Based on these results, we now provide a notion of generalised orthogonality which applies to arbitrary dissipation potentials arising within the abstract framework of this section (and does not require any specific structure).

Definition 2.23. For any $\rho\in\mathrm{Dom}(F)$ and $\zeta^2\in T^*_\rho\mathcal{W}$, define the *modified dissipation potential* $\Phi^*_{\zeta^2} : T^*_\rho\mathcal{W}\to\mathbb{R}\cup\{\infty\}$ and the *generalised orthogonality pairing* $\theta_\rho : T^*_\rho\mathcal{W}\times T^*_\rho\mathcal{W}\to\mathbb{R}\cup\{\infty\}$ as

$$\begin{aligned}\Phi^*_{\zeta^2}(\rho,\zeta^1) &:= \tfrac12\left[\mathcal{H}\big(\rho,\zeta^1+\zeta^2-F(\rho)\big)+\mathcal{H}\big(\rho,-\zeta^1+\zeta^2-F(\rho)\big)\right]-\mathcal{H}\big(\rho,\zeta^2-F(\rho)\big),\\ &= \tfrac12\left[\Phi^*(\rho,\zeta^1+\zeta^2)+\Phi^*(\rho,-\zeta^1+\zeta^2)\right]-\Phi^*(\rho,\zeta^2),\\ \theta_\rho(\zeta^1,\zeta^2) &:= \tfrac12\left[\mathcal{H}\big(\rho,\zeta^1+\zeta^2-F(\rho)\big)-\mathcal{H}\big(\rho,-\zeta^1+\zeta^2-F(\rho)\big)\right]\\ &= \tfrac12\left[\Phi^*(\rho,\zeta^1+\zeta^2)-\Phi^*(\rho,-\zeta^1+\zeta^2)\right],\end{aligned}$$

where we have used (2.14) to arrive at the equalities.

The following result collects the properties of Φ_{ζ^2} and θ_ρ clarifying the notion of orthogonality in the abstract setup. Recall the definition of $\mathrm{Dom}_{\mathrm{symdiss}}(F^{\mathrm{asym}})$ from (2.28).

Proposition 2.24. *Let $\mathcal{L}$ be a L-function on $\mathcal{Z}$. For any $\rho\in\mathrm{Dom}(F)$, $\Phi^*_{\zeta^2}(\rho,\cdot)$ is convex, lower semicontinuous and* $\inf\Phi^*_{\zeta^2}(\rho,\cdot)=0=\Phi^*_{\zeta^2}(\rho,0)$*. Furthermore, for any $\zeta^1,\zeta^2\in T^*_\rho\mathcal{W}$, the dissipation potential Φ^* admits the decomposition*

$$\Phi^*(\rho,\zeta^1+\zeta^2) = \Phi^*(\rho,\zeta^1)+\theta_\rho(\zeta^2,\zeta^1)+\Phi^*_{\zeta^1}(\rho,\zeta^2) = \Phi^*(\rho,\zeta^2)+\theta_\rho(\zeta^1,\zeta^2)+\Phi^*_{\zeta^2}(\rho,\zeta^1).$$

Moreover the generalised orthogonality pairing satisfies

$$\begin{aligned}\forall\rho\in\mathrm{Dom}(F^{\mathrm{asym}}):&\ \ \theta_\rho\big(F^{\mathrm{sym}}(\rho),F^{\mathrm{asym}}(\rho)\big)=0,\\ \forall\rho\in\mathrm{Dom}_{\mathrm{symdiss}}(F^{\mathrm{asym}}):&\ \ \theta_\rho\big(F^{\mathrm{asym}}(\rho),F^{\mathrm{sym}}(\rho)\big)=0,\end{aligned}$$

and therefore we have

$$\begin{aligned}\forall\rho\in\mathrm{Dom}(F^{\mathrm{asym}}):&\ \ \Phi^*\big(\rho,F(\rho)\big)=\Phi^*\big(\rho,F^{\mathrm{asym}}(\rho)\big)+\Phi^*_{F^{\mathrm{asym}}(\rho)}\big(F^{\mathrm{sym}}(\rho)\big),\\ \forall\rho\in\mathrm{Dom}_{\mathrm{symdiss}}(F^{\mathrm{asym}}):&\ \ \Phi^*\big(\rho,F(\rho)\big)=\Phi^*\big(\rho,F^{\mathrm{sym}}(\rho)\big)+\Phi^*_{F^{\mathrm{sym}}(\rho)}\big(F^{\mathrm{asym}}(\rho)\big).\end{aligned}\tag{2.29}$$

Proof. The convexity, lower semicontinuity of $\Phi^*_{\zeta^2}$ follows from the convexity, lower semicontinuity of Φ^* and $\Phi^*_{\zeta^2}(\rho,0)=0$ follows from the definition. Using convexity of Φ^* we find

$$\Phi^*_{\zeta^2}(\rho,\zeta^1)\ge\Phi^*\left(\rho,\tfrac12(\zeta^1+\zeta^2)+\tfrac12(-\zeta^1+\zeta^2)\right)-\Phi^*(\rho,\zeta^2)=0,$$

and therefore $\inf\Phi^*_{\zeta^2}(\rho,\cdot)=0$. The two decompositions follow immediately by adding $\Phi^*_{\zeta^2}$ and θ_ρ. Using Lemma 2.21 we find

$$\begin{aligned}2\theta_\rho\big(F^{\mathrm{sym}}(\rho),F^{\mathrm{asym}}(\rho)\big) &= \mathcal{H}\big(\rho,F^{\mathrm{sym}}(\rho)+F^{\mathrm{asym}}(\rho)-F(\rho)\big)-\mathcal{H}\big(\rho,-F^{\mathrm{sym}}(\rho)+F^{\mathrm{asym}}(\rho)-F(\rho)\big)\\ &= \mathcal{H}(\rho,0)-\mathcal{H}\big(\rho-2F^{\mathrm{sym}}(\rho)\big)=0,\\ 2\theta_\rho\big(F^{\mathrm{asym}}(\rho),F^{\mathrm{sym}}(\rho)\big) &= \mathcal{H}\big(\rho,F^{\mathrm{sym}}(\rho)+F^{\mathrm{asym}}(\rho)-F(\rho)\big)-\mathcal{H}\big(\rho,F^{\mathrm{sym}}(\rho)-F^{\mathrm{asym}}(\rho)-F(\rho)\big)\\ &= \mathcal{H}(\rho,0)-\mathcal{H}\big(\rho-2F^{\mathrm{asym}}(\rho)\big)=0.\end{aligned}$$

where the second decomposition additionally requires that $\rho\in\mathrm{Dom}_{\mathrm{symdiss}}(F^{\mathrm{asym}})$. ☐

From the general decomposition (2.15) and the generalised orthogonality result above, we can already provide two distinct decompositions of $\mathcal{L}$, as derived in [RZ21, Cor. 4.3] for the case of chemical reactions.

Corollary 2.25. *Let $\mathcal{L}$ be an L-function on $\mathcal{Z}$. Then for all $\rho \in \mathrm{Dom}(F^{\mathrm{asym}}(\rho))$, $j \in T_\rho\mathcal{W}$,*

$$\mathcal{L}(\rho, j) = \Phi(\rho, j) + \Phi^*\big(\rho, F^{\mathrm{asym}}(\rho)\big) - \langle F^{\mathrm{asym}}(\rho), j\rangle + \Phi^*_{F^{\mathrm{asym}}}\big(\rho, F^{\mathrm{sym}}(\rho)\big) - \langle F^{\mathrm{sym}}(\rho), j\rangle,$$

and for all $\rho \in \mathrm{Dom}_{\mathrm{symdiss}}(F^{\mathrm{asym}}(\rho))$, $j \in T_\rho\mathcal{W}$,

$$\mathcal{L}(\rho, j) = \Phi(\rho, j) + \Phi^*\big(\rho, F^{\mathrm{sym}}(\rho)\big) - \langle F^{\mathrm{sym}}(\rho), j\rangle + \Phi^*_{F^{\mathrm{sym}}}\big(\rho, F^{\mathrm{asym}}(\rho)\big) - \langle F^{\mathrm{asym}}(\rho), j\rangle.$$

In both decompositions, we may interpret the first three terms as an L-function with a modified force, the fourth term as a Fisher information, and the last term as a power (see Remark 2.30 for details).

Example (IPFG). 2.26. Using Definition 2.23 we have (see also [KJZ18])

$$\begin{aligned}\Phi^*_{\zeta^2}(\rho, \zeta^1) &= 2 \sum\sum_{(x,y)\in\mathcal{X}^2/2} \sqrt{\rho_x Q_{xy} \rho_y Q_{yx}} \cosh(\zeta^2_{xy})\big(\cosh(\zeta^1_{xy}) - 1\big),\\ \theta_\rho(\zeta^1, \zeta^2) &= 2 \sum\sum_{(x,y)\in\mathcal{X}^2/2} \sqrt{\rho_x Q_{xy} \rho_y Q_{yx}} \sinh(\zeta^2_{xy}) \sinh(\zeta^1_{xy}).\end{aligned}$$

2.5 Decomposing the L-function

We now present decompositions of the L-function, which are the main results of the abstract framework presented so far. Using $G = F, F^{\mathrm{sym}}, F^{\mathrm{asym}}$ in (2.19) and encoding convex combinations via the parameter λ, we arrive at three distinct decompositions of $\mathcal{L}$; this corresponds to all the points on the three lines depicted in Figure 2.

Theorem 2.27. *Let $\mathcal{L}$ be an L-function on $\mathcal{Z}$. It admits the following decompositions*

(i) For any $\rho \in \mathrm{Dom}_{\mathrm{symdiss}}(F)$, $j \in T_\rho\mathcal{W}$ and $\lambda \in [0,1]$,

$$\mathcal{L}(\rho, j) = \mathcal{L}_{(1-2\lambda)F}(\rho, j) + \mathcal{R}^\lambda_F(\rho) - 2\lambda\langle F(\rho), j\rangle \quad \textit{with } \mathcal{R}^\lambda_F(\rho) \geq 0. \tag{2.30}$$

(ii) For any $\rho \in \mathrm{Dom}(F^{\mathrm{asym}})$, $j \in T_\rho\mathcal{W}$ and $\lambda \in [0,1]$,

$$\mathcal{L}(\rho, j) = \mathcal{L}_{F-2\lambda F^{\mathrm{sym}}}(\rho, j) + \mathcal{R}^\lambda_{F^{\mathrm{sym}}}(\rho) - 2\lambda\langle F^{\mathrm{sym}}(\rho), j\rangle \quad \textit{with } \mathcal{R}^\lambda_{F^{\mathrm{sym}}}(\rho) \geq 0. \tag{2.31}$$

(iii) For any $\rho \in \mathrm{Dom}_{\mathrm{symdiss}}(F^{\mathrm{asym}})$ and all $j \in T_\rho\mathcal{W}$ and $\lambda \in [0,1]$,

$$\mathcal{L}(\rho, j) = \mathcal{L}_{F-2\lambda F^{\mathrm{asym}}}(\rho, j) + \mathcal{R}^\lambda_{F^{\mathrm{asym}}}(\rho) - 2\lambda\langle F^{\mathrm{asym}}(\rho), j\rangle \textit{ with } \mathcal{R}^\lambda_{F^{\mathrm{asym}}}(\rho) \geq 0. \tag{2.32}$$

Proof. The decompositions follow directly from Lemma 2.13. The non-negativity of the Fisher informations follows from Proposition 2.16 and Lemma 2.21. □

Remark 2.28. The decomposition (2.30) holds for $\rho \in \mathrm{Dom}_{\mathrm{symdiss}}(F)$. Since by Lemma 2.21(i), $\mathcal{R}^{\frac{1}{2}}_F(\rho) \geq 0$ for any $\rho \in \mathrm{Dom}(F)$, we also have the following decomposition for any $\rho \in \mathrm{Dom}(F)$, $j \in T_\rho\mathcal{W}$ and $\lambda \in [0, \frac{1}{2}]$

$$\mathcal{L}(\rho, j) = \mathcal{L}_{(1-\lambda)F}(\rho, j) + \mathcal{R}^\lambda_F(\rho) - \lambda\langle F(\rho), j\rangle \quad \text{with } \mathcal{R}^\lambda_F(\rho) \geq 0.$$

The non-negativity of $\mathcal{R}^\lambda_F(\rho)$ follows by repeating the proof of Proposition 2.16(ii) for $\lambda \in [0, \frac{1}{2}]$. □

The following result exhibits the significance of the choices $\lambda = \frac{1}{2}, 1$, and that the decompositions for other values can be seen as generalisations.

Corollary 2.29 ($\lambda = \frac{1}{2}, 1$)**.** *With the choice $\lambda = \frac{1}{2}$, the decompositions* (2.30), (2.31) *and* (2.32) *respectively become*

$$\mathcal{L}(\rho, j) = \mathcal{L}_0(\rho, j) + \mathcal{R}_F^{\frac{1}{2}}(\rho) - \langle F(\rho), j\rangle = \Phi(\rho, j) + \Phi^*\big(\rho, F(\rho)\big) - \langle F(\rho), j\rangle, \tag{2.33}$$

$$\mathcal{L}(\rho, j) = \mathcal{L}_{F^{\text{asym}}}(\rho, j) + \mathcal{R}_{F^{\text{sym}}}^{\frac{1}{2}}(\rho) - \langle F^{\text{sym}}(\rho), j\rangle, \tag{2.34}$$

$$\mathcal{L}(\rho, j) = \mathcal{L}_{F^{\text{sym}}}(\rho, j) + \mathcal{R}_{F^{\text{asym}}}^{\frac{1}{2}}(\rho) - \langle F^{\text{asym}}(\rho), j\rangle. \tag{2.35}$$

With the choice $\lambda = 1$, the decompositions (2.30), (2.31) *and* (2.32) *respectively become*

$$\begin{aligned} \mathcal{L}(\rho, j) &= \mathcal{L}_{-F}(\rho, j) - 2\langle F(\rho), j\rangle, \\ \mathcal{L}(\rho, j) &= \mathcal{L}_{-\overleftarrow{F}}(\rho, j) - 2\langle F^{\text{sym}}(\rho), j\rangle = \overleftarrow{\mathcal{L}}(\rho, -j) - 2\langle F^{\text{sym}}(\rho), j\rangle, \\ \mathcal{L}(\rho, j) &= \mathcal{L}_{\overleftarrow{F}}(\rho, j) - 2\langle F^{\text{asym}}(\rho), j\rangle, \end{aligned} \tag{2.36}$$

where $F, \overleftarrow{F}$ satisfy the relations (2.26).

The second equality in (2.33) follows from (2.20) and (2.14) where we use $\mathcal{H}(\rho, 0) = 0$ and the Fisher-information term vanishes by Lemma 2.21. The second equality in (2.36) follows by Remark 2.22. A careful analysis of the zero-cost flux for $\mathcal{L}_{F^{\text{sym}}}$ and $\mathcal{L}_{F^{\text{asym}}}$ will be presented in Subsection 2.6 and Section 4.

Remark 2.30. Using (2.15), we see that (2.34) and (2.35) are the same decompositions as those in Corollary 2.25 which use generalised orthogonality, and that the two corresponding Fisher informations are in fact modified dissipation potentials (as introduced in Section 2.4)

$$\mathcal{R}_{F^{\text{sym}}}^{\frac{1}{2}}(\rho) = \Phi^*_{F^{\text{asym}}}\big(\rho, F^{\text{sym}}(\rho)\big), \quad \mathcal{R}_{F^{\text{asym}}}^{\frac{1}{2}}(\rho) = \Phi^*_{F^{\text{sym}}}\big(\rho, F^{\text{asym}}(\rho)\big).$$

This also explains the non-negativity of these Fisher informations for $\lambda = \frac{1}{2}$. □

Example (IPFG). 2.31. Decompositions (2.30), (2.31) and (2.32) hold with the tilted L-functions

$$\begin{aligned} \mathcal{L}_{(1-2\lambda)F}(\rho, j) = \inf_{j^+ \in \mathbb{R}_{\geq 0}^{\mathcal{X}^2/2}} \sum\sum_{(x,y)\in\mathcal{X}^2/2} & s\big(j^+_{xy} \mid (\rho_x Q_{xy})^{1-\lambda}(\rho_y Q_{yx})^{\lambda}\big) \\ & + s\big(j^+_{xy} - j_{xy} \mid (\rho_y Q_{yx})^{1-\lambda}(\rho_x Q_{xy})^{\lambda}\big), \\ \mathcal{L}_{F-2\lambda F^{\text{sym}}}(\rho, j) = \inf_{j^+ \in \mathbb{R}_{\geq 0}^{\mathcal{X}^2/2}} \sum\sum_{(x,y)\in\mathcal{X}^2/2} & s\big(j^+_{xy} \mid (\rho_x Q_{xy})^{1-\lambda}(\rho_y \tfrac{\pi_x}{\pi_y} Q_{xy})^{\lambda}\big) \\ & + s\big(j^+_{xy} - j_{xy} \mid (\rho_y Q_{yx})^{1-\lambda}(\rho_x \tfrac{\pi_y}{\pi_x} Q_{yx})^{\lambda}\big), \\ \mathcal{L}_{F-2\lambda F^{\text{asym}}}(\rho, j) = \inf_{j^+ \in \mathbb{R}_{\geq 0}^{\mathcal{X}^2/2}} \sum\sum_{(x,y)\in\mathcal{X}^2/2} & s\big(j^+_{xy} \mid (\rho_x Q_{xy})^{1-\lambda}(\rho_x \tfrac{\pi_y}{\pi_x} Q_{yx})^{\lambda}\big) \\ & + s\big(j^+_{xy} - j_{xy} \mid (\rho_y Q_{yx})^{1-\lambda}(\rho_y \tfrac{\pi_x}{\pi_y} Q_{xy})^{\lambda}\big), \end{aligned}$$

and the corresponding Fisher informations

$$\begin{aligned} \mathcal{R}^{\lambda}_F(\rho) = -\mathcal{H}\big(\rho, -2\lambda F(\rho)\big) &= \sum\sum_{\substack{x,y\in\mathcal{X} \\ x\neq y}} \rho_x Q_{xy} - (\rho_x Q_{xy})^{1-\lambda}(\rho_y Q_{yx})^{\lambda}, \\ \mathcal{R}^{\lambda}_{F^{\text{sym}}}(\rho) = -\mathcal{H}\big(\rho, -2\lambda F^{\text{sym}}(\rho)\big) &= \sum\sum_{\substack{x,y\in\mathcal{X} \\ x\neq y}} \rho_x Q_{xy} - (\rho_x Q_{xy})^{1-\lambda}(\rho_y \tfrac{\pi_x}{\pi_y} Q_{xy})^{\lambda}, \\ \mathcal{R}^{\lambda}_{F^{\text{asym}}}(\rho) = -\mathcal{H}\big(\rho, -2\lambda F^{\text{asym}}(\rho)\big) &= \sum\sum_{\substack{x,y\in\mathcal{X} \\ x\neq y}} \rho_x Q_{xy} - (\rho_x Q_{xy})^{1-\lambda}(\rho_x \tfrac{\pi_y}{\pi_x} Q_{yx})^{\lambda}. \end{aligned}$$

While non-negativity of these Fisher informations is guaranteed by construction, it can also be proven directly by using $(1-\lambda)a + \lambda b \geq a^{1-\lambda}b^{\lambda}$. For $\lambda = \frac{1}{2}$, all three Fisher informations are of the form $\sum\sum_{x\neq y}(\sqrt{\cdot} - \sqrt{\cdot})^2$; interpreting the difference as an abstract discrete gradient, this is reminiscent of the usual Fisher information in continuous space $\frac{1}{2}\int(\nabla\sqrt{\rho(x)})^2\,dx$.

All three L-functions $\mathcal{L}_{(1-2\lambda)F}$, $\mathcal{L}_{F-2\lambda F^{\mathrm{sym}}}$ and $\mathcal{L}_{F-2\lambda F^{\mathrm{asym}}}$ are the large-deviation cost functions for processes with altered jump rates. In particular, $\mathcal{L}_{F^{\mathrm{sym}}} = \mathcal{L}_{F-F^{\mathrm{asym}}}$ is the large-deviation cost function corresponding to the jump process with jump rates for a particle to jump from x to y given by

$$\kappa^{\mathrm{sym}}_{xy}(\rho) := \rho_x\sqrt{Q_{xy}Q_{yx}\frac{\pi_y}{\pi_x}} = \rho_x\sqrt{Q_{xy}\overleftarrow{Q}_{xy}},$$

where we write $\overleftarrow{v}_{xy} := v_{yx}\frac{\pi_y}{\pi_x}$ for the jump rate of a single time-reversed jump process [Nor98, Thm. 3.7.1]. The linearity in ρ_x reflects that the system consists of *independent* Markov particles with generator $\sqrt{Q_{xy}\overleftarrow{Q}_{xy}}$ [Ren18a, Kra17].

Similarly, $\mathcal{L}_{F^{\mathrm{asym}}} = \mathcal{L}_{F-F^{\mathrm{sym}}}$ is the large-deviation cost function corresponding to a system with jump rates for one particle to jump from x to y given by [PR19]

$$\kappa^{\mathrm{asym}}_{xy}(\rho) := Q_{xy}\sqrt{\rho_x\rho_y\frac{\pi_x}{\pi_y}} = \sqrt{\rho_x\rho_y}\sqrt{Q_{xy}\overleftarrow{Q}_{yx}}. \tag{2.37}$$

We can interpret $\mathcal{L}_{F^{\mathrm{asym}}}(\rho, j)$ as the flux large-deviation cost function corresponding to a system of interacting particles with jump rates $n\kappa^{\mathrm{asym}}_{xy}(\rho)$ [AAPR21]. It should be noted that the usual large-deviation proof techniques break down in this particular case due to the non-uniqueness of solution to the limiting antisymmetric ODE (see Theorem 4.2).

The next corollary connects the decomposition (2.31) to an (abstract-)FIR inequality (recall Section 1.2.3) only defined on the state-space $\mathcal{Z}$ and with no dependence on the flux-space $\mathcal{W}$. In order to make this connection we introduce the contracted L-function $\hat{\mathcal{L}} : T_\rho\mathcal{Z} \to \mathbb{R}\cup\{\infty\}$ defined as

$$\hat{\mathcal{L}}(\rho, u) := \inf_{j\in T_\rho\mathcal{W}:\, u = d\phi_\rho j} \mathcal{L}(\rho, j). \tag{2.38}$$

The definition of $\hat{\mathcal{L}}$ is inspired by the contraction principle in large-deviation theory, where $\hat{\mathcal{L}}$ is the large-deviation rate functional only on the state space (recall Example 2.1). This connection will be further clarified in Proposition 3.3.

Corollary 2.32 (FIR inequality)**.** *Let $\mathcal{L}$ be an L-function on $\mathcal{Z}$. For any $\rho \in \mathrm{Dom}(F^{\mathrm{asym}})$, $u \in T_\rho\mathcal{Z}$ and $\lambda \in [0,1]$ we have*

$$\hat{\mathcal{L}}(\rho, u) \geq \mathcal{R}^{\lambda}_{F^{\mathrm{sym}}}(\rho) + \lambda\langle d\mathcal{V}(\rho), u\rangle,$$

where $\hat{\mathcal{L}}$ (with convex dual $\hat{\mathcal{H}}$) is defined in (2.38) *and $\mathcal{R}^{\lambda}_{F^{\mathrm{sym}}}(\rho) = -\hat{\mathcal{H}}(\rho, \lambda d\mathcal{V})$.*

Proof. Using convex duality and (2.38) it follows that $\mathcal{R}^{\lambda}_{F^{\mathrm{sym}}}(\rho) = -\mathcal{H}(\rho, \lambda d\phi_\rho^{\mathsf{T}} d\mathcal{V}) = -\hat{\mathcal{H}}(\rho, \lambda d\mathcal{V})$. Using (2.31) and the definition of F^{sym} (2.24) we find

$$\begin{aligned}
\hat{\mathcal{L}}(\rho, u) &= \inf_{j\in T_\rho\mathcal{W}:\, u = d\phi_\rho j}\big[\mathcal{L}_{F-2\lambda F^{\mathrm{sym}}}(\rho, j) - 2\lambda\langle F^{\mathrm{sym}}(\rho), j\rangle\big] + \mathcal{R}^{\lambda}_{F^{\mathrm{sym}}}(\rho) \\
&= \inf_{j\in T_\rho\mathcal{W}:\, u = d\phi_\rho j}\big[\mathcal{L}_{F-2\lambda F^{\mathrm{sym}}}(\rho, j)\big] + \mathcal{R}^{\lambda}_{F^{\mathrm{sym}}}(\rho) + \lambda\langle d\mathcal{V}(\rho), u\rangle \\
&\geq \mathcal{R}^{\lambda}_{F^{\mathrm{sym}}}(\rho) + \lambda\langle d\mathcal{V}(\rho), u\rangle,
\end{aligned}$$

where the second equality follows since $\langle d\phi_\rho^{\mathsf{T}}\eta, j\rangle = \langle \eta, d\phi_\rho j\rangle$ and the inequality follows since tilted L-functions are non-negative by definition (see Lemma 2.13 & Definition 2.4). □

Example (IPFG). 2.33. We now comment on the connection with the FIR inequality in [HPST20]. Let $\rho \in C^1([0,T];\mathrm{Dom}(F^{\mathrm{sym}}))$, where we have abused notation so that ρ is now a trajectory, and recall that $\mathrm{Dom}(F^{\mathrm{sym}}) = \mathcal{P}_+(\mathcal{X})$. Since $\dot\rho(t) \in T_{\rho(t)}\mathcal{Z}$, using Corollary 2.32, for any $t \in [0,T]$ and $\lambda \in [0,1]$ we have

$$\hat{\mathcal{L}}(\rho(t),\dot\rho(t)) \geq \mathcal{R}^{\lambda}_{F^{\mathrm{sym}}}(\rho(t)) + \lambda \tfrac{d}{dt}\mathcal{V}(\rho(t)),$$

where we have used $\langle d\mathcal{V}(\rho(t)), \dot\rho(t)\rangle = \frac{d}{dt}\mathcal{V}(\rho(t))$. Integrating in time, which is allowed since ρ is a sufficiently smooth curve we find

$$\frac{1}{\lambda}\int_0^T \hat{\mathcal{L}}(\rho(t),\dot\rho(t))dt + \mathcal{V}(\rho(0)) \geq \frac{1}{\lambda}\int_0^T \mathcal{R}^{\lambda}_{F^{\mathrm{sym}}}(\rho(t))dt + \mathcal{V}(\rho(T)).$$

This is exactly the FIR inequality in [HPST20, Thm. 1.6] with two crucial differences. First, using approximation arguments, in [HPST20] the class of admissible curves is extended to $\rho \in AC([0,T];\mathcal{Z})$, i.e. absolutely continuous curves in $\mathcal{Z} = \mathcal{P}(\mathcal{X})$ instead of $\mathcal{P}_+(\mathcal{X})$ discussed above (recall the discussion in Section 1.2.3). Second, in [HPST20] relative entropy $\mathrm{RelEnt}(\rho(t)|\mu(t))$ with respect to any time-dependent solution μ of the corresponding macroscopic dynamics (which is the forward Kolmogorov equation)

$$\dot\mu(t) = Q^{\mathsf{T}}\mu(t), \tag{2.39}$$

is used as opposed to the quasipotential $\mathcal{V}(\rho) = \mathrm{RelEnt}(\rho(t)|\pi)$, where π is the invariant measure of (2.39). We believe that this generalisation from the invariant measure π to any time dependent solution $\mu(t)$ is a feature of the linear forward Kolmogorov equations (similar results also hold for linear Fokker-Planck equations [BRS16, Thm. 1.1], [DLP+18, Thm. 4.18] arising from diffusion processes), and cannot be expected to hold in the setup of our paper where we are interested in nonlinear macroscopic equations. This is also the case for nonlinear diffusion processes [DLPS17, Thm. 2.3].

2.6 Symmetric and antisymmetric L-functions

In this section we focus on the two terms $\mathcal{L}_{F^{\mathrm{sym}}}$ and $\mathcal{L}_{F^{\mathrm{asym}}}$ in the decompositions (2.35) and (2.34) respectively. Observe that $\mathcal{L} = \mathcal{L}_{F^{\mathrm{sym}}}$ if $F^{\mathrm{asym}} = 0$, and therefore $\mathcal{L}_{F^{\mathrm{sym}}}$ corresponds to a system with a purely symmetric force. The relation between such systems with gradient flows is well known and follows from the theory in the previous sections, but for completeness we will make this connection explicit here. Similarly, $\mathcal{L}_{F^{\mathrm{asym}}}$ corresponds to a system with a purely antisymmetric force; in the level of abstraction of our current paper such systems are less understood. Motivated by our analysis in Section 4 and the examples in Section 5 we conjecture below that these L-functions are related to Hamiltonian systems.

We first discuss the purely symmetric case. Note that when particle systems and large-deviations are involved, $\mathcal{L}_{F^{\mathrm{sym}}}$ is the large-deviation cost function of a microscopic system in detailed balance (see Corollary 3.10). In what follows we will make use of the contracted dissipation potential $\Psi : T_\rho\mathcal{Z} \to \mathbb{R}\cup\{\infty\}$ defined as

$$\Psi(\rho,u) := \inf_{j\in T_\rho\mathcal{W}:\, u=d\phi_\rho j} \Phi(\rho,j). \tag{2.40}$$

Corollary 2.34 (EDI)**.** *Let $\mathcal{L}$ be an L-function on $\mathcal{Z}$ and $\rho \in \mathrm{Dom}(F^{\mathrm{asym}})$. For any $j \in T_\rho\mathcal{W}$ we have*

$$\mathcal{L}_{F^{\mathrm{sym}}}(\rho,j) = \Phi(\rho,j) + \Phi^*(\rho, -\tfrac12 d\phi_\rho^{\mathsf{T}} d\mathcal{V}(\rho)) + \tfrac12\langle d\phi_\rho^{\mathsf{T}} d\mathcal{V}(\rho), j\rangle, \tag{2.41}$$

and for any $u \in T_\rho\mathcal{Z}$ we have

$$\hat{\mathcal{L}}_{F^{\mathrm{sym}}}(\rho,u) = \Psi(\rho,u) + \Psi^*\big(\rho, -\tfrac12 d\mathcal{V}(\rho)\big) + \tfrac12\langle d\mathcal{V}(\rho), u\rangle, \tag{2.42}$$

where $\hat{\mathcal{L}}_{F^{\mathrm{sym}}}$, Ψ are defined in (2.38), (2.40) *and $\Psi^*(\rho,\xi) = \Phi^*(\rho, d\phi_\rho^{\mathsf{T}}\xi)$ is the convex dual of Ψ. Additionally if $\rho \in \mathrm{Dom}_{\mathrm{symdiss}}(F^{\mathrm{asym}})$, then for any $j \in T_\rho\mathcal{W}$ and $u \in T_\rho\mathcal{Z}$ we have the symmetry relations*

$$\mathcal{L}_{F^{\mathrm{sym}}}(\rho,j) - \mathcal{L}_{F^{\mathrm{sym}}}(\rho,-j) = \langle d\phi_\rho^{\mathsf{T}} d\mathcal{V}(\rho), j\rangle, \quad \hat{\mathcal{L}}(\rho,u) - \hat{\mathcal{L}}(\rho,-u) = \langle d\mathcal{V}(\rho), u\rangle. \tag{2.43}$$

Proof. Using $F^{\mathrm{asym}} = 0$ we have $F(\rho) = F^{\mathrm{sym}}(\rho)$, and the decomposition (2.41) then follows from (2.34) since $\mathcal{L}_0(\rho, j) = \Phi(\rho, j)$ (see (2.20)), $\mathcal{R}^{\frac{1}{2}}_{F^{\mathrm{sym}}}(\rho) = \Phi^*(\rho, F^{\mathrm{sym}}(\rho))$ and using the definition of F^{sym} (2.24). The decomposition (2.42) follows by applying the infimum in (2.38) to (2.41) and noting that by definition of convex duality $\Psi^*(\rho, \xi) = \Phi^*(\rho, d\phi^{\mathsf{T}}\xi)$ for any $\xi \in T^*_\rho\mathcal{Z}$. The first symmetry relation follows by Lemma 2.9(ii) and the second symmetry relation following by taking the infimum of the first symmetry relation on both sides. ☐

Note that the decomposition (2.41) also follows from (2.35) by using (2.10), but for $\rho \in \mathrm{Dom}_{\mathrm{symdiss}}(F^{\mathrm{asym}})$. Let us first comment on the *contracted* symmetric function $\hat{\mathcal{L}}_{F^{\mathrm{sym}}}$. Clearly, its zero-cost velocity $u^0(\rho)$ satisfies the EDI

$$\Psi\big(\rho, u^0(\rho)\big) + \Psi^*\big(\rho, -\tfrac{1}{2}d\mathcal{V}(\rho)\big) + \tfrac{1}{2}\langle d\mathcal{V}(\rho), u^0(\rho)\rangle = 0,$$

which is equivalent by convex duality to a generalised gradient flow (1.10). Summarising Corollaries 3.10 and 2.34, if a microscopic system is in detailed balance, the large-deviation cost function $\mathcal{L} = \mathcal{L}_{F^{\mathrm{sym}}}$ has a purely symmetric force, and hence induces a generalised gradient flow. This connection between gradient flows and detailed balance was first discussed in this generality in [MPR14]. For the IPFG example, the second symmetry relation in (2.43) correspond to the classical gradient structure for finite-state Markov chains in detailed balance [MPR14, Sec. 4.1] and the decomposition (2.41) is the corresponding flux formulation of the gradient structure for this example [Ren18a, Sec. 4.5]. Note that, strictly speaking (2.41) is not a gradient flow in the density-flux space. However a careful rewriting allows us to see $\mathcal{L}_{F^{\mathrm{sym}}}$ as a gradient flow, as summarised in the following remark.

Remark 2.35. With $\mathcal{L}^{\mathcal{W}}_{F^{\mathrm{sym}}}(w, j) := \mathcal{L}_{F^{\mathrm{sym}}}(\phi[w], j)$, and applying the chain rule $d_w\mathcal{V}^{\mathcal{W}}(w) = d\phi^{\mathsf{T}}_{\phi[w]}d_\rho\mathcal{V}(\phi[w])$, we arrive at

$$\mathcal{L}^{\mathcal{W}}_{F^{\mathrm{sym}}}(w, j) = \Phi^{\mathcal{W}}(w, j) + \Phi^{\mathcal{W}*}\big(w, -\tfrac{1}{2}d_w\mathcal{V}^{\mathcal{W}}(w)\big) + \tfrac{1}{2}\langle d_w\mathcal{V}^{\mathcal{W}}(\rho), j\rangle. \tag{2.44}$$

In this formulation $\mathcal{L}_{F^{\mathrm{sym}}}$ is indeed a gradient flow in the density-flux space [Ren18b]. ☐

As far as we are aware, the purely antisymmetric cost $\mathcal{L}_{F^{\mathrm{asym}}}$ has not been studied in the literature, and we could not produce rigorous results for it in the abstract setting of this section. However, as will be discussed in forthcoming sections, we are able to show that for certain examples the zero-cost *velocity* associated to $\mathcal{L}_{F^{\mathrm{asym}}}$ is non-dissipative, in the sense that one can associate a non-trivial conserved energy and a skew-symmetric operator to it, which motivates the following conjecture.

Conjecture 2.36. *Let $\mathcal{L}$ be an L-function on $\mathcal{Z}$ and $\hat{\mathcal{L}}_{F^{\mathrm{asym}}}$ be the contracted L-function corresponding to $\hat{\mathcal{L}}_{F^{\mathrm{asym}}}$, i.e.*

$$\hat{\mathcal{L}}_{F^{\mathrm{asym}}}(\rho, u) := \inf_{j \in T_\rho\mathcal{W}:\, u = d\phi_\rho j} \mathcal{L}_{F^{\mathrm{asym}}}(\rho, j).$$

Then there exists an energy $\mathcal{E} : \mathcal{Z} \to \mathbb{R}$ and a skew-symmetric operator $\mathbb{J} : \rho \mapsto (T^*_\rho\mathcal{Z} \to T_\rho\mathcal{Z})$ such that the zero-cost velocity of $\hat{\mathcal{L}}_{F^{\mathrm{asym}}}$ can be written as

$$u^0(\rho) = \mathbb{J}(\rho)D\mathcal{E}(\rho).$$

Clearly, the skew-symmetry of $\mathbb{J}(\rho)$ implies that the energy $\mathcal{E}(\rho(t))$ will be conserved along solutions of $\dot{\rho}(t) = \mathbb{J}(\rho(t))D\mathcal{E}(\rho(t))$. In fact, for the IPFG and lattice gas examples, the corresponding $\mathbb{J}$ even satisfies the Jacobi identity, so that the purely antisymmetric velocity has a Hamiltonian structure (see Sections 4, 5.3 for details).

3 Large deviations and dynamics

In Section 2 we focussed on the purely macroscopic setting. In this section we motivate the abstract structures introduced therein by connecting them to Markov processes and their large deviations. Although the results presented in this section are largely known in the literature in specific settings, we include them here in a more general setting to provide rationale for the abstract framework discussed in the last section. While these results are formal due to the level of generality at which we work, they can be made rigorous case by case.

Throughout this section we assume a *microscopic* dynamics described by a sequence of Markov processes $\big(\rho^{(n)}(t), W^{(n)}(t)\big)$ defined on $\mathcal{Z} \times \mathcal{W}$. Typically, $\rho^{(n)}(t)$ is the empirical measure, concentration or density corresponding to $\mathcal{O}(n)$ particles, and $W^{(n)}(t)$ is the integrated/cumulative particle flux (recall Example 2.1 and see Section 5 for further examples). For now, we assume a fixed deterministic initial condition $\rho^{(n)}(0)$ for the empirical measure; this will be relaxed later on. We always assume that the initial condition for the flux satisfies $W^{(n)}(0) = 0$ almost surely, since the particles have not moved yet at initial time. For any $t \geq 0$, the integrated flux $W^{(n)}(t)$ contains all information required to reconstruct the current state of the system, i.e. almost surely

$$\rho^{(n)}(t) = \phi[W^{(n)}(t)].$$

Equivalently, if the random paths allow for a notion of (measure-valued) time-integration, we write

$$\dot{\rho}^{(n)}(dt) = d\phi_{\rho^{(n)}(t)} \dot{W}^{(n)}(dt).$$

We assume that the sequence $\big(\rho^{(n)}(t), W^{(n)}(t)\big)$ satisfies a law of large numbers, whereby the microscopic process $\big(\rho^{(n)}(t), W^{(n)}(t)\big)$ converges to a macroscopic, deterministic trajectory $(\rho(t), w(t))$, which satisfies an equation of the form (1.1), where at this stage we are only interested in the instantaneous flux $j = \dot{w}$. Consequently, the corresponding path probability measures $\mathbb{P}^{(n)} = \mathrm{law}(\rho^{(n)}, W^{(n)})$ will concentrate on that path (ρ, w) as $n \to \infty$.

Finally we assume that the sequence $\big(\rho^{(n)}(t), W^{(n)}(t)\big)$ satisfies a corresponding large-deviation principle, which can informally be written as

$$\mathbb{P}^{(n)}\big((\rho^{(n)}, W^{(n)}) \approx (\rho, w)\big) \sim e^{-n \int_0^T \mathcal{L}(\rho(t), \dot{w}(t))\, dt}. \tag{3.1}$$

This large-deviation principle characterises the exponentially vanishing probability of paths starting from the fixed deterministic initial conditions which do not converge to the macroscopic path (ρ, w). The function $\mathcal{L}$ is non-negative and its zero-cost flux corresponds to the macroscopic path, since for that path $\mathbb{P}^{(n)} \sim 1$.

In what follows, we first focus on the classical technique for proving the aforementioned large-deviation statement, using which we motivate the tilted L-function introduced in Lemma 2.13. Consequently we motivate the Definition 2.5 of the quasipotential via the large deviations of invariant measures, and the Definition 2.17 of the reversed L-function using time-reversal.

3.1 Tilting, contraction and mixture

Rigorous proofs of large-deviation principles for Markov processes tend to be rather technical. We nevertheless briefly review the classical proof technique, since it is closely related to the macroscopic framework introduced in Subsection 2.2. For an example of this technique see [KL99, Chap. 10].

Formal Theorem 3.1. *Let $\mathcal{Q}^{(n)}$ be the generator of the Markov process $(\rho^{(n)}(t), W^{(n)}(t))$, define*

$$\mathcal{H}^{(n)}(\rho, w, \zeta) := \frac{1}{n} e^{-n\langle \zeta, w\rangle} \mathcal{Q}^{(n)} e^{n\langle \zeta, w\rangle},$$

and let the limit $\mathcal{H}(\rho, \zeta) = \lim_{n\to\infty} \mathcal{H}^{(n)}(\rho, w, \zeta)$ exist and be dependent on w only via the relation $\rho = \phi[w]$. Then the process $(\rho^{(n)}, W^{(n)})$ satisfies the large-deviation principle (3.1) *with*

$$\mathcal{L}(\rho, j) := \sup_{\zeta \in T^*_\rho \mathcal{W}} \langle \zeta, j\rangle - \mathcal{H}(\rho, \zeta).$$

The assumption that $\mathcal{H}$ depends on w only via $\rho = \phi[w]$ will generally be justified if the noise only depends on the state ρ of the system.

Main proof technique. In order to derive the large deviations (3.1) for a given, atypical path (ρ, w), one changes the probability measure $\mathbb{P}^{(n)}$ to a *tilted* probability measure $\mathbb{P}^{(n)}_\zeta$. The tilting is defined via a time-dependent force field $\zeta(t)$ to be chosen later, and the Radon-Nikodym derivative is explicitly given by (see [PR02] for the generator of the tilted process and related technical details)

$$\frac{d\mathbb{P}^{(n)}_\zeta}{d\mathbb{P}^{(n)}}(\hat\rho,\hat w) = \exp\Big[n\int_0^T \Big(\langle \zeta(t), \dot{\hat w}(dt)\rangle - \mathcal{H}^{(n)}\big(\hat\rho(t),\hat w(t),\zeta(t)\big)\Big)\,dt\Big]. \tag{3.2}$$

One can then (formally) estimate, for a small ball $\mathcal{B}_\varepsilon(\rho,w)$ around the given atypical path (ρ,w),

$$\begin{aligned}
-\frac{1}{n}\log \mathbb{P}^{(n)}\big(\mathcal{B}_\varepsilon(\rho,w)\big) &= -\frac{1}{n}\log\int_{\mathcal{B}_\varepsilon(\rho,w)} \frac{d\mathbb{P}^{(n)}}{d\mathbb{P}^{(n)}_\zeta}(\hat\rho,\hat w)\,\mathbb{P}^{(n)}_\zeta\big(d(\hat\rho,\hat w)\big)\\
&\approx \frac{1}{n}\log\frac{d\mathbb{P}^{(n)}_\zeta}{d\mathbb{P}^{(n)}}(\rho,w) - \frac{1}{n}\log \mathbb{P}^{(n)}_\zeta\big(\mathcal{B}_\varepsilon(\rho,w)\big) \qquad \text{(for small } \varepsilon)\\
&= \int_0^T \Big(\langle\zeta(t),\dot w(dt)\rangle - \mathcal{H}^{(n)}\big(\rho(t),w(t),\zeta(t)\big)\Big)\,dt - \frac{1}{n}\log\mathbb{P}^{(n)}_\zeta\big(\mathcal{B}_\varepsilon(\rho,w)\big).
\end{aligned}$$

We choose $\zeta(t)$ to be optimum in $\sup_{\hat\zeta}\langle\hat\zeta,\dot w(t)\rangle - \mathcal{H}(\rho(t),\hat\zeta)$. It turns out that with this choice, the tilted probability $\mathbb{P}^{(n)}_\zeta$ will concentrate on the given path (ρ,w) and therefore the final term in the right hand side vanishes (even for small ε), which results in

$$-\frac{1}{n}\log\mathbb{P}^{(n)}\big(\mathcal{B}_\varepsilon(\rho,w)\big) \overset{n\to\infty}{\approx} \int_0^T \sup_\zeta\Big(\langle\zeta,\dot w(dt)\rangle - \mathcal{H}\big(\rho(t),\zeta\big)\Big)\,dt = \int_0^T \mathcal{L}\big(\rho(t),\dot w(t)\big)\,dt.$$

□

Following similar arguments one can derive the large deviations of the tilted measures.

Corollary 3.2. *For a given path $\zeta(t)$, the tilted probability $\mathbb{P}^{(n)}_\zeta$ from* (3.2) *satisfies the large-deviation principle*

$$\mathbb{P}^{(n)}_\zeta\big((\rho^{(n)},W^{(n)})\approx(\rho,w)\big) \sim e^{-n\int_0^T \mathcal{L}_{\zeta(t)}(\rho(t),\dot w(t))\,dt}, \tag{3.3}$$

where $\mathcal{L}_\zeta$ is the convex dual of

$$\mathcal{H}_\zeta(\rho,\hat\zeta) := \mathcal{H}(\rho,\zeta+\hat\zeta) - \mathcal{H}(\rho,\zeta).$$

The proof follows from the same arguments as Formal Theorem 3.1, with (3.2) replaced by

$$\begin{aligned}
\frac{d\mathbb{P}^{(n)}_{\zeta+\hat\zeta}}{d\mathbb{P}^{(n)}_\zeta}(\hat\rho,\hat w) &= \frac{d\mathbb{P}^{(n)}_{\zeta+\hat\zeta}}{d\mathbb{P}^{(n)}}(\hat\rho,\hat w)\frac{d\mathbb{P}^{(n)}}{d\mathbb{P}^{(n)}_\zeta}(\hat\rho,\hat w)\\
&= \exp\Big[n\int_0^T\Big(\langle\hat\zeta(t),\dot{\hat w}(dt)\rangle - \mathcal{H}^{(n)}\big(\hat\rho(t),\hat w(t),\zeta(t)+\hat\zeta(t)\big) + \mathcal{H}^{(n)}\big(\hat\rho(t),\hat w(t),\zeta(t)\big)\Big)\,dt\Big].
\end{aligned}$$

Note that $\mathcal{H}_{\zeta-F}$ is exactly as in (2.12) and consequently we interpret the tilted L-functions introduced in Definition 2.12 as the large-deviation cost functions for the tilted probability measures.

From the Formal Theorem 3.1, one immediately obtains the following large-deviation principle for the state by applying the contraction principle [DZ09, Thm. 4.2.1], which motivates the definition (1.7).

Proposition 3.3. *Assume that the large-deviation principle* (3.1) *holds for the pair $(\rho^{(n)},W^{(n)})$. Then the large-deviation principle also holds for $\rho^{(n)}$, i.e.*

$$\mathbb{P}^{(n)}\big(\rho^{(n)}\approx\rho\big)\sim e^{-n\int_0^T\hat{\mathcal{L}}(\rho(t),\dot\rho(t))\,dt}, \quad \text{with} \quad \hat{\mathcal{L}}(\rho,\dot\rho) := \inf_{j:\dot\rho=d\phi_\rho j}\mathcal{L}(\rho,j). \tag{3.4}$$

Moreover, $\hat{\mathcal{H}}(\rho,\xi) := \sup_{\dot\rho\in T_\rho\mathcal{Z}}\langle\xi,\dot\rho\rangle - \hat{\mathcal{L}}(\rho,\dot\rho) = \mathcal{H}(\rho, d\phi_\rho^\mathsf{T}\xi)$.

So far we have assumed that the initial condition $\rho^{(n)}(0)$ is fixed and deterministic. If the initial condition is random then we have the following result, which will be useful in what follows.

Proposition 3.4 (Mixing [Big04])**.** *Assume that the large-deviation principle* (3.1) *holds for the pair* $(\rho^{(n)}, W^{(n)})$ *with a deterministic initial condition. If the initial condition is replaced by a sequence* $\rho^{(n)}(0) \in \mathcal{Z}$ *which satisfies the large-deviation principle*

$$\mathbb{P}^{(n)}\big(\rho^{(n)}(0) \approx \rho\big) \sim e^{-n\mathcal{I}_0(\rho)}$$

for some functional $\mathcal{I}_0 : \mathcal{Z} \to [0, \infty]$ *and* $W^{(n)}(0) = 0$ *almost surely, then the pair* $(\rho^{(n)}, W^{(n)})$ *with random initial condition* $\rho^{(n)}(0) \in \mathcal{Z}$ *satisfies the large deviation principle*

$$\mathbb{P}^{(n)}\big((\rho^{(n)}, W^{(n)}) \approx (\rho, w)\big) \sim e^{-n\mathcal{I}_0(\rho(0)) - n\int_0^T \mathcal{L}(\rho(t), \dot{w}(t))\,dt}. \tag{3.5}$$

Remark 3.5. The abstract setup introduced in Subsection 2.1 automatically fixes the state $\rho(0) = \phi[0]$, which coincides with deterministic initial conditions in context of large deviations. Strictly speaking, to work with varying random initial conditions would require additional flexibility in the abstract framework. This can be achieved by either replacing the mapping ϕ (recall Definition 2.2) by a family of mappings $(\phi_{\rho(0)})_{\rho(0)}$, or by keeping a fixed reference state $\phi[0]$, and redefining the initial integrated flux as $w(0) \in \phi^{-1}[\rho(0)]$, exploiting the surjectivity of ϕ. To keep the notation simple, we stick to the setup of a deterministic initial condition, and with a slight abuse of notation always tacitly assume that $\rho(t) = \phi(w(t)) = \phi_{\rho(0)}(w(t))$. □

3.2 Quasipotential

We now motivate Definition 2.5 of the quasipotential $\mathcal{V}$. The following result is largely known in the literature, see for instance [BDSG+02, Sec. 2.2] and [Bou20, Sec. 3.3], although it is not often made explicit at the level of generality used in this section.

Theorem 3.6. *Assume that the Markov process* $\rho^{(n)}(t)$ *satisfies the large-deviation principle* (3.4) *and has an invariant measure* $\Pi^{(n)} \in \mathcal{P}(\mathcal{Z})$ *that satisfies the large-deviation principle*

$$\Pi^{(n)}\big(\mu^{(n)} \approx \mu\big) \sim e^{-n\mathcal{V}(\mu)}, \tag{3.6}$$

where $\mu^{(n)}$ *denotes a random variable distributed with* $\Pi^{(n)}$*. Then we have*

(i) $\mathcal{V}(\mu) \equiv \inf_{\substack{\hat\rho \in C_b^1([0,T];\mathcal{Z}):\\ \hat\rho(T)=\mu}} \Big\{\mathcal{V}\big(\hat\rho(0)\big) + \int_0^T \hat{\mathcal{L}}\big(\hat\rho(t), \dot{\hat\rho}(t)\big)\,dt\Big\}$ *for any* $T \geq 0$,

(ii) $\mathcal{H}\big(\mu, d\phi_\mu^{\mathsf{T}} d\mathcal{V}(\mu)\big) = \hat{\mathcal{H}}\big(\mu, d\mathcal{V}(\mu)\big) \equiv 0$,

where $\hat{\mathcal{L}}, \hat{\mathcal{H}}$ *are defined in Proposition 3.3.*

Formal proof. For arbitrary $T > 0$ and fixed deterministic initial condition $\rho^{(n)}(0) = \rho(0)$, the state $\rho_T^{(n)}$ satisfies the large-deviation principle [DZ09, Thm. 4.2.1],

$$\begin{aligned} P_T^{(n)}\big(d\mu \mid \rho(0)\big) &:= \mathbb{P}^{(n)}\big(\rho^{(n)}(T) \approx \mu \mid \rho^{(n)}(0) = \rho(0)\big) \sim e^{-nI_T(\mu \mid \rho(0))}, \quad \text{with} \\ I_T(\mu \mid \rho(0)) &:= \inf_{\substack{\hat\rho \in C_b^1([0,T];\mathcal{Z}):\\ \hat\rho(0)=\rho(0), \hat\rho(T)=\mu}} \int_0^T \hat{\mathcal{L}}\big(\hat\rho(t), \dot{\hat\rho}(t)\big)\,dt. \end{aligned} \tag{3.7}$$

By definition the invariant measure is invariant under the transition probability, i.e. for any $T > 0$,

$$\Pi^{(n)}(d\mu) = \int P_T^{(n)}(d\mu \mid \rho(0))\Pi^{(n)}(d\rho(0)).$$

Hence the large-deviation functional of the left-hand side is equal to the large-deviation rate of the right-hand side, which using a mixing argument [Big04] is given by

$$\mathcal{V}(\mu) = \inf_{\rho(0)\in\mathcal{Z}} \bigl\{\mathcal{V}(\rho(0)) + I_T\bigl(\mu \mid \rho(0)\bigr)\bigr\} = \inf_{\rho(0)\in\mathcal{Z}} \inf_{\substack{\hat\rho\in C_b^1([0,T];\mathcal{Z}):\\ \hat\rho(0)=\rho(0),\hat\rho(T)=\mu}} \Bigl\{\mathcal{V}(\rho(0)) + \int_0^T \hat{\mathcal{L}}\bigl(\hat\rho(t),\dot{\hat\rho}(t)\bigr)\,dt\Bigr\}$$

which proves the first claim. From here on the arguments are purely macroscopic. We proceed by noting that

$$\Xi_T(\rho) := \inf_{\substack{\hat\rho\in C_b^1([0,T];\mathcal{Z}):\\ \hat\rho(T)=\rho}} \mathcal{V}\bigl(\hat\rho(0)\bigr) + \int_0^T \hat{\mathcal{L}}\bigl(\hat\rho(t),\dot{\hat\rho}(t)\bigr)\,dt,$$

which has the form of the value function from classical control theory, and hence solves the Hamilton-Jacobi-Bellman equation

$$\dot\Xi_T(\rho) = -\hat{\mathcal{H}}\bigl(\rho, d\Xi_T(\rho)\bigr), \quad \Xi_0(\rho) = \mathcal{V}(\rho). \tag{3.8}$$

We have already shown that $\Xi_T \equiv \mathcal{V}$ does not depend on T, and therefore $\dot\Xi_T(\rho) \equiv 0$, which proves the second claim. □

Remark 3.7. Strictly speaking, $\mathcal{V}$ should be a *viscosity solution* of the Hamilton-Jacobi-Bellman (3.8) and hence also of the stationary version Theorem 3.6(ii). However, it is not precisely clear to us which boundary conditions should be imposed in the definition of the viscosity solution. This issue is particularly challenging since most classical Hamilton-Jacobi-Bellman theory is developed for quadratic $\hat{\mathcal{H}}$ only. Therefore, Theorem 3.6(ii) should be seen as formal. We remind the reader that a viscosity solution $\mathcal{V}(\rho)$ is a solution in the classical sense at points of differentiability. At least on a formal level, this already suffices for the applications in this paper. □

Remark 3.8. In Theorem 3.6(ii) we do not require that the invariant measure is unique, neither do we claim that the quasipotential $\mathcal{V}(\rho)$ will be unique. In particular, we do not require stable points $\pi \in \mathcal{Z}$ for which $\hat{\mathcal{L}}(\pi, 0) = 0$ to be unique. In case of uniqueness, the quasipotential from Theorem 3.6(ii) will also satisfy the classical definition of the quasipotential [FW94]

$$\mathcal{V}(\rho) = \inf_{\substack{\hat\rho\in C_b^1(-\infty,0;\mathcal{Z}):\\ \hat\rho(0)=\rho}} \int_{-\infty}^0 \hat{\mathcal{L}}\bigl(\hat\rho(t),\dot{\hat\rho}(t)\bigr)\,dt.$$

In case of multiple stable points, one usually defines a family of *non-equilibrium quasipotentials* indexed by the stable points [FW94]. Any one of these will also satisfy Theorem 3.6(ii), which is sufficient for our purpose. Therefore the abstract framework from Section 2 can be constructed with any of these quasipotentials. □

3.3 Time reversal

In the following proposition we relate the large-deviation rate functions for Markov processes and their time-reversed counterparts, which motivates the notion of reversed L-function introduced in Definition 2.17. Since the proof below is standard in MFT, we only outline the proof idea for completeness.

Proposition 3.9 ([BDSG+15, Sec. II.C], [Ren18a, Sec. 4.2])**.** *Let $\bigl(\rho^{(n)}(t), W^{(n)}(t)\bigr)$ be a Markov process with random initial distribution $\Pi^{(n)}$ for $\rho^{(n)}(0)$ and $W^{(n)}(0) = 0$ almost surely, where $\Pi^{(n)} \in \mathcal{P}(\mathcal{Z})$ is the invariant measure of $\rho^{(n)}(t)$. Define the time-reversed process* [2]

$$\overleftarrow{\rho}^{(n)}(t) := \rho^{(n)}(T-t), \quad \overleftarrow{W}^{(n)}(t) := W^{(n)}(T-t) - W^{(n)}(T).$$

[2] This construction requires a vector structure on the manifold $\mathcal{W}$. For all applications that we have in mind this holds trivially, as long as we work with net fluxes (see the discussion in Example 2.10).

Assume that $\Pi^{(n)}$ satisfies a large-deviation principle (3.6)*, $\big(\rho^{(n)}(t), W^{(n)}(t)\big)$ with deterministic initial condition satisfies a large-deviation principle* (3.1) *with cost function $\mathcal{L}$, and $\big(\overleftarrow{\rho}^{(n)}(t), \overleftarrow{W}^{(n)}(t)\big)$ with deterministic initial condition satisfies a large-deviation principle* (3.1) *with cost function $\overleftarrow{\mathcal{L}}$. Then for any $(\mu, j) \in \mathcal{Z}\times\mathcal{W}$, $\overleftarrow{\mathcal{L}}$ is related to $\mathcal{L}$ and $\mathcal{V}$ via the relation*

$$\overleftarrow{\mathcal{L}}(\mu, j) = \mathcal{L}(\mu, -j) + \langle d\phi_\rho^{\mathsf{T}} d\mathcal{V}(\mu), j\rangle.$$

Proof. Note that if $\rho^{(n)}(0)$ is distributed according to $\Pi^{(n)}$, then so is $\overleftarrow{\rho}^{(n)}(0)$, and if $W^{(n)}(0) = 0$ almost surely, then $\overleftarrow{W}^{(n)}(0) = 0$ almost surely as well. Since

$$\mathbb{P}^{(n)}\big(\big(\rho^{(n)}, W^{(n)}\big) \in (d\rho, dW)\big) = \mathbb{P}^{(n)}\big(\big(\overleftarrow{\rho}^{(n)}, \overleftarrow{W}^{(n)}\big) \in (d\overleftarrow{\rho}, d\overleftarrow{W})\big),$$

using Proposition 3.4, we find for all paths (ρ, w),

$$\mathcal{V}(\rho(0)) + \int_0^T \mathcal{L}\big(\rho(t), \dot w(t)\big)\, dt = \mathcal{V}(\rho(T)) + \int_0^T \overleftarrow{\mathcal{L}}\big(\rho(t), -\dot w(t)\big)\, dt.$$

Since the equality above holds for any $T > 0$, we can write

$$\begin{aligned}\big\langle d\phi_{\rho(0)}^{\mathsf{T}} d\mathcal{V}(\rho(0)), \dot w(0)\big\rangle &= \big\langle d\mathcal{V}(\rho(0)), \dot\rho(0)\big\rangle = \lim_{T\to 0} \frac{\mathcal{V}(\rho(T)) - \mathcal{V}(\rho(0))}{T} \\ &= \lim_{T\to 0} \frac{1}{T}\int_0^T \big[\mathcal{L}(\rho(t), \dot w(t)) - \overleftarrow{\mathcal{L}}(\rho(t), -\dot w(t))\big]\, dt = \mathcal{L}\big(\rho(0), \dot w(0)\big) - \overleftarrow{\mathcal{L}}\big(\rho(0), -\dot w(0)\big),\end{aligned}$$

for any $\rho(0)$ and $\dot w(0)$ (assuming sufficient regularity on $t \mapsto \mathcal{L}(\rho(t), \dot w(t)) - \overleftarrow{\mathcal{L}}(\rho(t), -\dot w(t))$). The claimed result then follows by choosing any path ρ, w for which $\rho(0) = \mu$ and $\dot w(0) = j$. □

A special and important case of the previous result pertains to detailed balance.

Corollary 3.10. *Let $\big(\rho^{(n)}(t), W^{(n)}(t)\big)$ and $\big(\overleftarrow{\rho}^{(n)}(t), \overleftarrow{W}^{(n)}(t)\big)$ be as in Proposition 3.9. If, under initial distribution $\Pi^{(n)} \in \mathcal{P}(\mathcal{Z})$ of $\rho^{(n)}(0)$ and $\overleftarrow{\rho}^{(n)}(0)$ and $W^{(n)}(0) = \overleftarrow{W}^{(n)}(0) = 0$ almost surely,*

$$\mathbb{P}^{(n)}\big(\big(\rho^{(n)}, W^{(n)}\big) \in (d\rho, dW)\big) = \mathbb{P}^{(n)}\big(\big(\overleftarrow{\rho}^{(n)}, \overleftarrow{W}^{(n)}\big) \in (d\rho, dW)\big), \tag{3.9}$$

then $\mathcal{L} = \overleftarrow{\mathcal{L}}$.

For the applications that we have in mind, the condition (3.9) holds precisely when $\rho^{(n)}(t)$ is in detailed balance with respect to $\Pi^{(n)}$, see for example [Ren18a, Prop. 4.1]. The relation $\mathcal{L} = \overleftarrow{\mathcal{L}}$ is the time-reversal symmetry from [MPR14], which implies that $\mathcal{L}$ induces a gradient flow, or $F^{\mathrm{asym}} = 0$ in the context of this paper.

4 Zero-cost velocity for IPFG antisymmetric L-function

In Subsection 2.6 we argued that the both the purely symmetric flux and velocity are dissipative, that is, they are generalised gradient flows of the energy $\frac{1}{2}\mathcal{V}$ (and $\frac{1}{2}\mathcal{V}^{\mathcal{W}}$ respectively). Moreover, $\mathcal{L}_{F^{\mathrm{sym}}}$ *defines* the variational structure of those gradient flows via the equalities (2.41) and (2.44).

The interpretation of $\mathcal{L}_{F^{\mathrm{asym}}}$ is more complicated. In general $\mathcal{L}_{F^{\mathrm{asym}}}$ will not have $\mathcal{V}$ as its quasipotential, and using Lemmas 2.9 and 2.13 for any $\rho \in \mathrm{Dom}_{\mathrm{symdiss}}(F^{\mathrm{asym}})$ and $j \in T_\rho\mathcal{W}$ it satisfies the time-reversal relation

$$\mathcal{L}_{-F^{\mathrm{asym}}}(\rho, j) = \mathcal{L}_{F^{\mathrm{asym}}}(\rho, -j).$$

This relation in fact holds for any tilted L-function, but $-F^{\mathrm{asym}}$ can be interpreted as the time-reversed counterpart of F^{asym} in the sense that $\overleftarrow{F^{\mathrm{sym}} + F^{\mathrm{asym}}} = F^{\mathrm{sym}} - F^{\mathrm{asym}}$ (see Remark 2.22). Formally this means that time-reversal reverses the fluxes, which is a physical indication that $\mathcal{L}_{F^{\rm asym}}$ might correspond to Hamiltonian dynamics, as stated in Conjecture 2.36.

In this section we illustrate this principle for the IPFG example with L-function $\mathcal{L}$ from Example 2.3. As far as we are aware this is has not been studied in the literature, and as a first step we will focus solely on the trajectories of the zero-cost velocity $u(t) = \dot\rho(t) = u^0(\rho(t))$ of $\mathcal{L}_{F^{\rm asym}}$, largely ignoring fluxes as well as the variational structure.

Let (ρ, j) satisfy $\mathcal{L}_{F^{\rm asym}}\big(\rho(t), j(t)\big) = 0$ or equivalently $j(t) \in \partial\Phi^*\big(\rho(t), F^{\rm asym}(\rho(t))\big)$, where the subdifferential is with respect to the second variable. Substituting $\lambda = \frac{1}{2}$ in $\mathcal{L}_{F-2\lambda F^{\rm sym}}$ (defined in Example 2.31), for any $x \in \mathcal{X}$, $\rho : [0,T] \to \mathcal{P}(\mathcal{X})$ satisfies the ODE

$$\dot\rho_x(t) = -\operatorname{div}_x j(t) = \sum_{\substack{y\in\mathcal{X}\\ y\neq x}} \Big(Q_{yx}\sqrt{\frac{\pi_y}{\pi_x}} - Q_{xy}\sqrt{\frac{\pi_x}{\pi_y}}\Big)\sqrt{\rho_x(t)\,\rho_y(t)}. \tag{4.1}$$

Introducing the change of variables $\omega_x(t) := \sqrt{\rho_x(t)}$, the zero-cost velocity (4.1) transforms into a linear ODE with a matrix $A \in \mathbb{R}^{|\mathcal{X}|\times|\mathcal{X}|}$, i.e.

$$\dot\omega(t) = \frac{1}{2}A\omega(t), \quad \text{with} \quad A_{xy} := Q_{yx}\sqrt{\frac{\pi_y}{\pi_x}} - Q_{xy}\sqrt{\frac{\pi_x}{\pi_y}}. \tag{4.2}$$

Solutions to this equation have a nice geometric interpretation, see Figure 3 for an example in three dimensions. Clearly, $|\omega(t)|_2^2 = |\rho(t)|_1 = 1$ and so the solutions are confined to (the positive octant of) the unit sphere $S^{\mathcal{X}-1}$. On the other hand, the matrix A is skewsymmetric with imaginary eigenvalues and represents rotations around the axis $\sqrt{\pi}$, implying that the solutions are confined to a plane perpendicular to $\sqrt{\pi}$. Therefore, solutions $\omega(t)$ lie on the intersection of these planes with the unit sphere, resulting in periodic orbits that conserve the distance of the plane to the origin. In the following result we show that this transformed system is indeed a Hamiltonian system with a suitable energy and Poisson structure which satisfies the Jacobi identity (see Lemma A.1 for a useful alternate characterisation of the Jacobi identity in our context).

Proposition 4.1. *The ODE* (4.2) *admits a Hamiltonian structure* $(\mathbb{R}^{|\mathcal{X}|\times|\mathcal{X}|}, \tilde{\mathcal{E}}, \widetilde{\mathbb{J}})$*, i.e.* $\dot\omega = \widetilde{\mathbb{J}}(\omega)D\tilde{\mathcal{E}}(\omega)$*, where the linear energy* $\tilde{\mathcal{E}} : \mathbb{R}^{|\mathcal{X}|} \to \mathbb{R}$ *and Poisson structure* $\widetilde{\mathbb{J}} : \mathbb{R}^{|\mathcal{X}|} \to \mathbb{R}^{|\mathcal{X}|\times|\mathcal{X}|}$ *are given by*

$$\tilde{\mathcal{E}}(\omega) := 1 - \sqrt{\pi}\cdot\omega, \qquad \widetilde{\mathbb{J}}(\omega) := \frac{1}{2}\Big(\sqrt{\pi}\otimes(A\omega) - (A\omega)\otimes\sqrt{\pi}\Big).$$

Here $\omega \cdot v$ *is the standard Euclidean inner product and* $\omega\otimes v$ *is the outer product of vectors* ω, v.

Proof. In Appendix A we present a Hamiltonian structure for a general class of ODEs, which includes the transformed system (4.2). The proof of Proposition 4.2 follows directly from Theorem A.2 with the choice $n = |\mathcal{X}|$, $\omega_* = \sqrt{\pi}$ and observing that $|\omega_*|^2 = \sum_x \pi_x = 1$ and $A\sqrt{\pi} = A^T\sqrt{\pi} = 0$ since π is the invariant solution corresponding to the original dynamics (4.1). ☐

We would now like to transform the Hamiltonian structure of the transformed ODE (4.2) back to obtain a Hamiltonian structure for the original non-linear equation (4.1). This transforms the positive octant of the sphere in Figure 3 to the simplex in Figure 1(c). However, transforming back via $\omega_x(t) = \sqrt{\rho}_x(t)$ is valid only if $\omega_x(t) \geq 0$ for every $x \in \mathcal{X}$. In the following result we state the criterion for this to hold.

Proposition 4.2. *Define the threshold*

$$\sigma := \min_{x\in\mathcal{X}}\big(1 - \sqrt{1-\pi_x}\big),$$

the energy $\mathcal{E} : \mathbb{R}^{|\mathcal{X}|} \to \mathbb{R}$ *and the Poisson structure* $\mathbb{J} : \mathbb{R}^{|\mathcal{X}|} \to \mathbb{R}^{|\mathcal{X}|\times|\mathcal{X}|}$ *as*

$$\mathcal{E}(\rho) := 1 - \sqrt{\pi}\cdot\sqrt{\rho}, \quad (\mathbb{J}(\rho))_{xy} := 2\sum_{z\in\mathcal{X}}\big(\sqrt{\pi_x}A_{yz} - \sqrt{\pi_y}A_{xz}\big)\sqrt{\rho_x\rho_y\rho_z},$$

where A is defined in (4.2). If the energy of the initial distribution $\rho^0 \in \mathcal{P}(\mathcal{X})$ for the ODE (4.1) satisfies $0 \le \mathcal{E}(\rho^0) < \sigma$, then (4.1) has a unique solution and admits a Hamiltonian structure $(\mathbb{R}^{|\mathcal{X}|\times|\mathcal{X}|}, \mathcal{E}, \mathbb{J})$, i.e. $\dot\rho = \mathbb{J}(\rho)D\mathcal{E}(\rho)$. If the energy of the initial distribution satisfies $\mathcal{E}(\rho^0) \ge \sigma$, then (4.1) has non-unique, non-energy-conserving solutions.

Proof. We first analyse the critical case, where the periodic orbit $\omega(t)$ of (4.2) touches one of the boundaries of $S^{\mathcal{X}-1} \cap \mathbb{R}^{\mathcal{X}}_{\ge 0}$. The energy level of such an orbit can be calculated by solving the constrained minimisation problem

$$\min\left\{\tilde{\mathcal{E}}(\omega) : \omega \in S^{\mathcal{X}-1}, \omega_x = 0 \text{ for some } x \in \mathcal{X}\right\} = \min_{x\in\mathcal{X}} \min\left\{\tilde{\mathcal{E}}(\omega) : \omega \in S^{\mathcal{X}-1},\ \omega_x = 0\right\}.$$

For the interior minimisation problem, the optimal ω with $\omega_x = 0$ solves

$$0 = \partial_{\omega_y}\left[\tilde{\mathcal{E}}(\omega) + \tfrac{1}{2}\lambda|\omega|_2^2\right] = -\sqrt{\pi_y} + \lambda\omega_y, \quad \text{for all } y \ne x,$$

where the Lagrange multiplier $\lambda \ge 0$ is such that the constraint $|\omega|_2^2 = 1$ holds. It follows that $\omega_y = \sqrt{\pi_y}/\sqrt{1-\pi_x}$, and so $\tilde{\mathcal{E}}(\omega) = 1 - \sqrt{1-\pi_x} =: \sigma$, yielding the critical case.

Using Proposition 4.1 we thus find that if $\mathcal{E}(\rho^0) = \tilde{\mathcal{E}}(\omega^0) < \omega$, the solution $\omega(t)$ of the linear system satisfies $\tilde{\mathcal{E}}(\omega(t)) = \tilde{\mathcal{E}}(\omega^0)$ and remains positive (coordinate-wise), so that $\rho(t) = \sqrt{\omega(t)}$ solves (4.1), and has the corresponding transformed Hamiltonian structure. Note that this is possible since Poisson structures are preserved by coordinate transformations [Mie91, Sec. 4.2]. The uniqueness of the thus constructed solution $\rho(t)$ follows since $\sqrt{\rho_x(t)\rho_y(t)}$ is strictly bounded away from zero, and therefore the right hand side of (4.1) is Lipschitz.

On the other hand, if $\mathcal{E}(\rho^0) \ge \sigma$, then after a finite time the solution $\rho(t)$ will touch a boundary (i.e. one of its components becomes zero), and therefore the right hand side of (4.1) fails to be Lipschitz, allowing for multiple solutions that move along the boundary for an arbitrary time before entering the interior of the simplex again (see Figure 1(c)). □

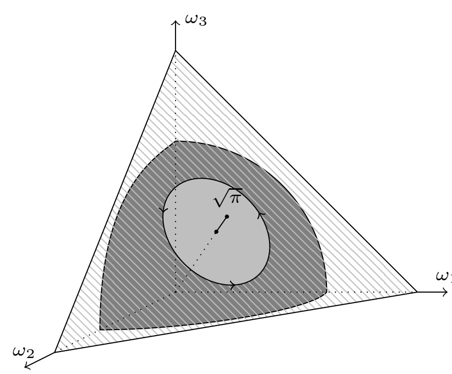

Figure 3: For $|\mathcal{X}| = 3$, the trajectories $\omega(t)$ rotate around the $\sqrt{\pi}$-axis, and lie at the intersection of the two-dimensional sphere S^2 and a plane perpendicular to the $\sqrt{\pi}$-axis. The transformation $\rho_x = \sqrt{\omega}_x$ maps the (octant) sphere to the simplex of Figure 1(c).

In the following remark we comment on the role of $\lambda \ne \frac{1}{2}$ in $\mathcal{L}_{F-2\lambda F^{\text{sym}}}$.

Remark 4.3. One can also study the zero-cost velocity associated to to $\mathcal{L}_{F-2\lambda F^{\text{sym}}}$ from (2.31) for $\lambda \in (0,1)$. For $\lambda < \frac{1}{2}$, the symmetric part is dominant and the trajectories spiral inwards towards π, i.e. π is a spiral sink, and for $\lambda > \frac{1}{2}$, the antisymmetric part is dominant and the trajectories spiral outwards from π, i.e. π is a spiral source (compare with Figure 1(c) for $\lambda = \frac{1}{2}$). □

5 Examples

Throughout Section 2 we applied the abstract framework developed therein to the example of independent Markovian particles. We now apply the abstract framework to three examples of interacting particle systems. In Section 5.1 we consider the example of zero-range processes with an atypical scaling limit which leads to an ODE system in the limit as opposed to the usual parabolic scaling. Section 5.2 deals with the case of chemical reaction networks in complex balance. Finally in Section 5.3 we consider the case of lattice gases with parabolic scaling (which lead to diffusive systems) and arrive at well known results in MFT. While MFT often deals with additional boundary effects and consequent non-equilibrium steady states arising from it, in our analysis we avoid these boundary effects to keep the presentation less technical.

5.1 Zero-range processes

Microscopic particle system. To simplify and unify notation, we first consider the irreducible Markov process on a finite graph $\mathcal{X}$ from the IPFG example, with generator (represented by a matrix) $Q \in \mathbb{R}^{\mathcal{X}\times\mathcal{X}}$, and assume that it has a unique and coordinate-wise positive invariant measure $\pi \in \mathcal{P}_+(\mathcal{X})$. Similar to the setup in Example 2.1 we study the Markov process $(\rho^{(n)}(t), W^{(n)}(t))$ on $\mathcal{P}(\mathcal{X}) \times \mathcal{X}^2/2$, where $\rho^{(n)}(t)$ is the particle density of *interacting* particles and $W^{(n)}(t)$ is the integrated net flux (both defined in Example 2.1). The interaction between the particles is so that the jump rate $n\kappa_{xy}(\rho)$ from x to y only depends on the density at the source node x ("zero-range")

$$\kappa_{xy}(\rho) = \kappa_{xy}(\rho_x) = Q_{xy}\pi_x\eta_x\big(\frac{\rho_x}{\pi_x}\big),$$

for a family of strictly increasing functions $\eta_x : [0,\infty) \to [0,\infty)$ with $\eta_x(0) = 0$ and $\eta_x(1) = 1$. The condition $\eta_x(0) = 0$ ensures that $\rho_x \geq 0$, i.e. there are no negative densities. The condition $\eta_x(1) = 1$ ensures that π is also an invariant measure for the many-particle limit (5.1), and is assumed only for convenience (see Remark 5.2 below). Observe that the particular choice $\eta_x \equiv \mathrm{id}$ corresponds to the IPFG model.

The pair $\big(\rho^{(n)}, W^{(n)}(t)\big)$ has the n-particle generator

$$\begin{aligned}(\mathcal{Q}^{(n)}f)(\rho,w) = n \sum\sum_{(x,y)\in\mathcal{X}^2/2} &\kappa_{xy}(\rho_x)\big[f(\rho - \tfrac{1}{n}\mathbb{1}_x + \tfrac{1}{n}\mathbb{1}_y, w + \tfrac{1}{n}\mathbb{1}_{xy}) - f(\rho,w)\big] \\ &+ \kappa_{yx}(\rho_y)Q_{yx}\big[f(\rho - \tfrac{1}{n}\mathbb{1}_y + \tfrac{1}{n}\mathbb{1}_x, w - \tfrac{1}{n}\mathbb{1}_{xy}) - f(\rho,w)\big].\end{aligned}$$

As opposed to the typical diffusive scaling for zero-range processes [BDSG+15], we keep the graph $\mathcal{X}$ fixed. The many-particle limit for this process as $n \to \infty$ is the solution to the ODE system [RZ21, Sec. 3.1]

$$\begin{cases}\dot{w}_{xy}(t) = \kappa_{xy}(\rho_x(t)) - \kappa_{yx}(\rho_y(t)), & (x,y) \in \mathcal{X}^2/2,\\ \dot{\rho}_x(t) = -\operatorname{div}_x \dot{w}(t), & x \in \mathcal{X}\end{cases} \tag{5.1}$$

where div is again the discrete divergence defined in (2.4). The Markov process $(\rho^{(n)}(t), W^{(n)}(t))$ satisfies a large-deviation principle with the rate functional (2.5) where the corresponding $\mathcal{L}$ and its dual $\mathcal{H}$ are now given by [PR19, GR20]

$$\begin{aligned}\mathcal{L}(\rho,j) &= \inf_{j^+\in\mathbb{R}^{\mathcal{X}^2/2}_{\geq 0}} \sum\sum_{(x,y)\in\mathcal{X}^2/2} \big[s\big(j^+_{xy} \mid \kappa_{xy}(\rho_x)\big) + s\big(j^+_{xy} - j_{xy} \mid \kappa_{yx}(\rho_y)\big)\big],\\ \mathcal{H}(\rho,\zeta) &= \sum\sum_{(x,y)\in\mathcal{X}^2/2} \big[\kappa_{xy}(\rho_x)\big(e^{\zeta_{xy}} - 1\big) + \kappa_{yx}(\rho_y)\big(e^{-\zeta_{xy}} - 1\big)\big],\end{aligned} \tag{5.2}$$

and $s(\cdot \mid \cdot)$ is defined in (2.7).

State-flux triple and L-function. The manifolds $\mathcal{Z}, \mathcal{W}$ with the corresponding tangent and cotangent spaces and the map $\phi : \mathcal{Z} \to \mathcal{W}$ with $d\phi_\rho = -\operatorname{div},\ d\phi^\mathsf{T} = \nabla$ are exactly as in Example 2.3.

Quasipotential. Define $\mathcal{V}:\mathcal{Z}\to\mathbb{R}\cup\{\infty\}$ as

$$\mathcal{V}(\rho)=\begin{cases}\displaystyle\sum_{x\in\mathcal{X}}\int_{\bar\rho_x}^{\rho_x}\log\eta_x\Big(\frac{z}{\pi_x}\Big)\,dz+C, & \rho\geq\bar\rho \text{ coordinate-wise},\\ \infty, & \text{otherwise},\end{cases}\tag{5.3}$$

where each $\bar\rho_x\geq 0$ is chosen as small as possible so that $\log\eta_x$ is still integrable, and C is the normalisation constant for which $\inf\mathcal{V}=0$. Note that $\mathcal{V}$ does not depend on Q. This functional can be found as the large-deviation rate of the explicitly known invariant measure $\Pi^{(n)}$ using Theorem 3.6, [KL99, Prop. 3.2] and [GR20, Sec. 4.1]. However, we can also show that it is the correct quasipotential without any reference to a microscopic particle system, in the macroscopic sense of Definition 2.5.

Proposition 5.1. *The function $\mathcal{V}$ defined in* (5.3) *satisfies $\mathcal{H}(\rho,d\phi^{\mathsf{T}}d\mathcal{V}(\rho))=0$ at all points of differentiability $\{\rho\in\mathcal{Z}=\mathcal{P}(\mathcal{X}):\rho_x\geq\bar\rho_x\,\forall x\in\mathcal{X}\}$ of $\mathcal{V}$.*

Proof. At the points of differentiability of $\mathcal{V}$ we have

$$\begin{aligned}\mathcal{H}\big(\rho,d\phi_\rho^{\mathsf{T}}d\mathcal{V}(\rho)\big)&=\mathcal{H}\big(\rho,\nabla\log\eta(\tfrac{\rho}{\pi})\big)=\sum\sum_{(x,y)\in\mathcal{X}^2/2}\Big(\kappa_{xy}(\rho_x)\Big[\frac{\eta_y(\rho_y/\pi_y)}{\eta_x(\rho_x/\pi_x)}-1\Big]+\kappa_{yx}(\rho_y)\Big[\frac{\eta_x(\rho_x/\pi_x)}{\eta_y(\rho_y/\pi_y)}-1\Big]\Big)\\&=\sum\sum_{\substack{x,y\in\mathcal{X}\\x\neq y}}\big(\pi_xQ_{xy}\eta_y\big(\tfrac{\rho_y}{\pi_y}\big)-Q_{xy}\eta_x\big(\tfrac{\rho_x}{\pi_x}\big)\big)=\sum_{y\in\mathcal{X}}\eta_y\big(\tfrac{\rho_y}{\pi_y}\big)\sum_{\substack{x\in\mathcal{X}\\x\neq y}}(\pi_xQ_{xy}-\pi_yQ_{yx})=0,\end{aligned}$$

where the fourth and fifth equality follows by exchanging indices and the final equality follows since $Q^{\mathsf{T}}\pi=0$. ☐

The following remark discusses the various assumptions on η_x.

Remark 5.2. Since η_x is nonnegative and strictly increasing, it follows that $\mathcal{V}(\rho)$ is strictly convex for any $\rho\in\mathcal{P}(\mathcal{X})$, and consequently has a unique minimiser. The property $\eta(1)=1$ ensures that π is this unique minimiser of $\mathcal{V}$. If this condition is not satisfied then, as we show below, one can always construct $\overline{Q}\in\mathbb{R}^{\mathcal{X}\times\mathcal{X}}$, $\overline{\pi}\in\mathcal{P}_+(\mathcal{X})$ and family $\overline{\eta}_x$ with $\overline{\eta}_x(1)=1$, such that $\kappa_{xy}(\rho)=\overline{Q}_{xy}\overline{\pi}_x\overline{\eta}_x\big(\frac{\rho_x}{\overline{\pi}_x}\big)$, $\overline{Q}^{\mathsf{T}}\overline{\pi}=0$, and $\overline{\pi}$ is the unique stable point of (5.1). To calculate these modified objects, we minimise $\mathcal{V}(\rho)$ for $\rho\in\mathcal{P}(\mathcal{X})$, which gives the minimiser

$$\overline{\pi}_x:=\pi_x\eta_x^{-1}(e^{-\lambda}),\quad\text{where }\lambda\in\mathbb{R}\ \text{ satisfies }\ \sum_{x\in\mathcal{X}}\pi_x\eta_x^{-1}(e^{-\lambda})=1,$$

and define

$$\overline{\eta}_x(z):=\eta_x\big(z\eta_x^{-1}(e^{0\lambda})\big)e^{\lambda},\quad\overline{Q}_{xy}:=Q_{xy}\frac{e^{-\lambda}}{\eta_x^{-1}(e^{-\lambda})}.$$

It is easily checked that these modified objects satisfy all the properties described above, and one can work with these objects instead. ☐

Dissipation potential, forces and orthogonality. As in Example (2.10), using Definition 2.8 the driving force is

$$F_{xy}(\rho)=\frac12\log\frac{\kappa_{xy}(\rho_x)}{\kappa_{yx}(\rho_y)}=\frac12\log\frac{\pi_xQ_{xy}\eta_x(\frac{\rho_x}{\pi_x})}{\pi_yQ_{yx}\eta_y(\frac{\rho_y}{\pi_y})},\quad\mathrm{Dom}(F)=\mathcal{P}_+(\mathcal{X}).$$

with the dissipation potentials

$$\begin{aligned}\Phi^*(\rho,\zeta)&=2\sum\sum_{(x,y)\in\mathcal{X}^2/2}\sqrt{\kappa_{xy}(\rho_x)\kappa_{yx}(\rho_y)}\,(\cosh(\zeta_{xy})-1),\\\Phi(\rho,j)&=2\sum\sum_{(x,y)\in\mathcal{X}^2/2}\sqrt{\kappa_{xy}(\rho_x)\kappa_{yx}(\rho_y)}\,\Big(\cosh^*\Big(\frac{j_{xy}}{2\sqrt{\kappa_{xy}(\rho_x)\kappa_{yx}(\rho_y)}}\Big)+1\Big).\end{aligned}$$

Since $\ell \mapsto \cosh(\ell)$ is an even function, using Lemma 2.9 it follows that $\mathrm{Dom}_{\mathrm{symdiss}}(F) = \mathrm{Dom}(F)$, i.e. the dissipation potential is symmetric.

Using Corollary 2.19 we find

$$F^{\mathrm{sym}}_{xy}(\rho) = -\Big(\frac{1}{2} d\phi_\rho^{\mathsf{T}} d\mathcal{V}(\rho)\Big)_{xy} = \frac{1}{2}\log\frac{\eta_x(\frac{\rho_x}{\pi_x})}{\eta_y(\frac{\rho_y}{\pi_y})}, \quad F^{\mathrm{asym}}_{xy}(\rho) = F_{xy}(\rho) - F^{\mathrm{sym}}_{xy}(\rho) = \frac{1}{2}\log\frac{\pi_x Q_{xy}}{\pi_y Q_{yx}},$$

with $\mathrm{Dom}(F^{\mathrm{sym}}) = \mathrm{Dom}(F^{\mathrm{asym}}) = \big\{\rho \in \mathcal{P}(\mathcal{X}) : \rho_x \geq \bar\rho_x\big\}$. Observe that the expressions of F^{sym} and F^{asym} imply that their domains can be easily extended to $\mathcal{P}_+(\mathcal{X})$ and $\mathcal{Z} = \mathcal{P}(\mathcal{X})$ respectively; however the theory of Section 2 will not automatically be valid on that extension. Also note that $F^{\mathrm{asym}}_{xy} = 0$ if the particle system satisfies detailed balance with respect to π. The orthogonality relations in Proposition 2.24 apply with (see [RZ21])

$$\begin{aligned}
\Phi^*_{\zeta^2}(\rho,\zeta^1) &= 2 \sum\sum_{(x,y)\in\mathcal{X}^2/2} \sqrt{\kappa_{xy}(\rho_x)\kappa_{yx}(\rho_y)}\, \cosh(\zeta^2_{xy})[\cosh(\zeta^1_{xy}) - 1],\\
\theta_\rho(\zeta^1,\zeta^2) &= 2 \sum\sum_{(x,y)\in\mathcal{X}^2/2} \sqrt{\kappa_{xy}(\rho_x)\kappa_{yx}(\rho_y)}\, \sinh(\zeta^1_{xy})\sinh(\zeta^2_{xy}).
\end{aligned}$$

Decomposition of the L-function. The decompositions in Theorem 2.27 hold with the L-functions

$$\begin{aligned}
\mathcal{L}_{(1-2\lambda)F}(\rho,j) = \inf_{j^+\in\mathbb{R}^{\mathcal{X}^2/2}_{\geq 0}} \sum\sum_{(x,y)\in\mathcal{X}^2/2} & s\big(j^+_{xy} \mid (\pi_x Q_{xy}\eta_x(\tfrac{\rho_x}{\pi_x}))^{1-\lambda}(\pi_y Q_{yx}\eta_y(\tfrac{\rho_y}{\pi_y}))^\lambda\big)\\
&+ s\big(j^+_{xy} - j_{xy} \mid (\pi_x Q_{xy}\eta_x(\tfrac{\rho_x}{\pi_x}))^{\lambda}(\pi_y Q_{yx}\eta_y(\tfrac{\rho_y}{\pi_y}))^{1-\lambda}\big),\\
\mathcal{L}_{F-2\lambda F^{\mathrm{sym}}}(\rho,j) = \inf_{j^+\in\mathbb{R}^{\mathcal{X}^2/2}_{\geq 0}} \sum\sum_{(x,y)\in\mathcal{X}^2/2} & s\big(j^+_{xy} \mid (\pi_x Q_{xy}\eta_x(\tfrac{\rho_x}{\pi_x}))^{1-\lambda}(\pi_x Q_{xy}\eta_y(\tfrac{\rho_y}{\pi_y}))^\lambda\big)\\
&+ s\big(j^+_{xy} - j_{xy} \mid (\pi_y Q_{yx}\eta_y(\tfrac{\rho_y}{\pi_y}))^{1-\lambda}(\pi_y Q_{yx}\eta_x(\tfrac{\rho_x}{\pi_x}))^{\lambda}\big),\\
\mathcal{L}_{F-2\lambda F^{\mathrm{asym}}}(\rho,j) = \inf_{j^+\in\mathbb{R}^{\mathcal{X}^2/2}_{\geq 0}} \sum\sum_{(x,y)\in\mathcal{X}^2/2} & s\big(j^+_{xy} \mid (\pi_x Q_{xy}\eta_x(\tfrac{\rho_x}{\pi_x}))^{1-\lambda}(\pi_y Q_{yx}\eta_x(\tfrac{\rho_x}{\pi_x}))^\lambda\big)\\
&+ s\big(j^+_{xy} - j_{xy} \mid (\pi_y Q_{yx}\eta_y(\tfrac{\rho_y}{\pi_y}))^{1-\lambda}(\pi_x Q_{xy}\eta_y(\tfrac{\rho_y}{\pi_y}))^{\lambda}\big),
\end{aligned}$$

and the corresponding Fisher informations

$$\begin{aligned}
\mathcal{R}^\lambda_F(\rho) = -\mathcal{H}\big(\rho,-2\lambda F(\rho)\big) &= \sum\sum_{\substack{x,y\in\mathcal{X}\\ x\neq y}} \pi_x Q_{xy}\eta_x(\tfrac{\rho_x}{\pi_x}) - (\pi_x Q_{xy}\eta_x(\tfrac{\rho_x}{\pi_x}))^{1-\lambda}(\pi_y Q_{yx}\eta_y(\tfrac{\rho_y}{\pi_y}))^\lambda,\\
\mathcal{R}^\lambda_{F^{\mathrm{sym}}}(\rho) = -\mathcal{H}\big(\rho,-2\lambda F^{\mathrm{sym}}(\rho)\big) &= \sum\sum_{\substack{x,y\in\mathcal{X}\\ x\neq y}} \pi_x Q_{xy}\eta_x(\tfrac{\rho_x}{\pi_x}) - (\pi_x Q_{xy}\eta_x(\tfrac{\rho_x}{\pi_x}))^{1-\lambda}(\pi_x Q_{xy}\eta_y(\tfrac{\rho_y}{\pi_y}))^\lambda,\\
\mathcal{R}^\lambda_{F^{\mathrm{asym}}}(\rho) = -\mathcal{H}\big(\rho,-2\lambda F^{\mathrm{asym}}(\rho)\big) &= \sum\sum_{\substack{x,y\in\mathcal{X}\\ x\neq y}} \pi_x Q_{xy}\eta_x(\tfrac{\rho_x}{\pi_x}) - (\pi_x Q_{xy}\eta_x(\tfrac{\rho_x}{\pi_x}))^{1-\lambda}(\pi_y Q_{yx}\eta_x(\tfrac{\rho_x}{\pi_x}))^\lambda.
\end{aligned}$$

In particular, with $\eta_x \equiv \mathrm{id}$, we indeed arrive at the expressions in Example 2.31.

With the expressions above the zero-range model satisfies the FIR inequality from Corollary 2.32 for $\lambda = \frac{1}{2}$, which is consistent with [RZ21, Cor. 4.3] but also holds more generally for $\lambda \in [0,1]$. We also mention that the zero-cost flux for the symmetric $\mathcal{L}_{F^{\mathrm{sym}}}$ satisfies EDI (see Corollary 2.34), i.e. it induces a gradient flow structure. We now turn our attention to its antisymmetric counterpart.

Zero-cost velocity for antisymmetric L-function. As in the IPFG case in Section 4, we now consider the zero-cost velocity associated to $\mathcal{L}_{F^{\mathrm{asym}}}$ which for any $x \in \mathcal{X}$ solves the ODE

$$\dot{\rho}_x(t) = \sum_{\substack{y\in\mathcal{X}\\ y\neq x}} A_{xy}\sqrt{\pi_x\pi_y\eta_x\big(\tfrac{\rho_x(t)}{\pi_x}\big)\eta_y\big(\tfrac{\rho_y(t)}{\pi_y}\big)}, \quad \text{with} \quad A_{xy} := Q_{yx}\sqrt{\frac{\pi_y}{\pi_x}} - Q_{xy}\sqrt{\frac{\pi_x}{\pi_y}}. \tag{5.4}$$

Note that the corresponding ODE for IPFG (4.1) follows with $\eta_x \equiv 1$. The geometric arguments of Section 4 cannot be fully repeated, because it is unclear how to transform (5.4) into a linear equation. However, by analogy to that section, we make a smart guess for the energy and the Poisson structure, which is summarised in the following result. We will make use of the following family of functions $g_x : [0,1] \to \mathbb{R}$

$$g_x(a) := \int_0^a \frac{1}{\sqrt{\eta_x(\frac{b}{\pi_x})}}\, db,$$

for every $x \in \mathcal{X}$. Using these functions we now show that the Conjecture 2.36 holds for the zero-range process.

Proposition 5.3. *Assume that η_x is such that g_x is well defined for any $x \in \mathcal{X}$. Define the threshold*

$$\sigma := \min_{x\in\mathcal{X}}\Big[1 - \sum_{z\in\mathcal{X}} g_z(\rho_z) + \lambda\Big(\sum_{\substack{z\in\mathcal{X}\\ x\neq x}} \rho_z - 1\Big)\Big], \qquad \textit{where } \lambda \in \mathbb{R} \;\; \textit{satisfies} \;\; \sum_{z\in\mathcal{X}} \pi_y\eta_y^{-1}\Big(\frac{1}{4\lambda^2}\Big) = 1, \tag{5.5}$$

and the energy $\mathcal{E} : \mathbb{R}^{|\mathcal{X}|} \to \mathbb{R}\cup\{\infty\}$ and the skew-symmetric matrix field $\mathbb{J} : \mathbb{R}^{|\mathcal{X}|} \to \mathbb{R}^{|\mathcal{X}|\times|\mathcal{X}|}$ as

$$\mathcal{E}(\rho) := 1 - \sum_{x\in\mathcal{X}} g_x(\rho_x), \quad (\mathbb{J}(\rho))_{xy} := 2\sum_{z\in\mathcal{X}} \sqrt{\pi_x\pi_y\pi_z\eta_x\big(\tfrac{\rho_x}{\pi_x}\big)\eta_y\big(\tfrac{\rho_y}{\pi_y}\big)\eta_z\big(\tfrac{\rho_z}{\pi_z}\big)}\Big(\sqrt{\pi_x}A_{yz} - \sqrt{\pi_y}A_{xz}\Big),$$

where A is defined in (5.4). If the energy of initial distribution $\rho^0 \in \mathcal{P}(\mathcal{X})$ for the ODE (5.4) satisfies $0 \le \mathcal{E}(\rho^0) < \sigma$, then (4.1) has a unique solution and $\dot{\rho} = \mathbb{J}(\rho)D\mathcal{E}(\rho)$. If the energy of the initial distribution satisfies $\mathcal{E}(\rho^0) \ge \sigma$, then (5.4) has non-unique, non-energy-conserving solutions.

Proof. For any $x \in \mathcal{X}$ we have

$$\begin{aligned}(\mathbb{J}(\rho)D\mathcal{E}(\rho))_x &= \sum_{y\in\mathcal{X}} (\mathbb{J}(\rho))_{xy}(D\mathcal{E}(\rho))_y = \sum_{y,z\in\mathcal{X}} \sqrt{\pi_x\pi_z\eta_x\big(\tfrac{\rho_x}{\pi_x}\big)\eta_z\big(\tfrac{\rho_z}{\pi_z}\big)}\Big(\pi_y A_{xz} - \sqrt{\pi_x\pi_y}A_{yz}\Big)\\ &= \sum_{z\in\mathcal{X}} \sqrt{\pi_x\pi_z\eta_x\big(\tfrac{\rho_x}{\pi_x}\big)\eta_z\big(\tfrac{\rho_z}{\pi_z}\big)}A_{xz} = \dot{\rho}_x(t),\end{aligned}$$

where the third equality follows since $\sum_y \pi_y = 1$ and $(A^\mathsf{T}\sqrt{\pi})_y = 0$ for any $y \in \mathcal{X}$. Finally, note that (5.4) has unique solutions if the right hand side is Lipschitz, which follows if $\rho_x > 0$, since $\eta_x(0) = 0$, for every $x \in \mathcal{X}$. The expression (5.5) for this threshold follows by solving

$$\min\big\{\mathcal{E}(\rho) : \rho \in \mathcal{P}(\mathcal{X}), \rho_x = 0 \text{ for some } x \in \mathcal{X}\big\} = \min_{x\in\mathcal{X}} \min\big\{\mathcal{E}(\rho) : \rho \in \mathcal{P}(\mathcal{X}),\ \rho_x = 0\big\},$$

where λ in (5.5) is the Lagrange multiplier for the constraint $\sum_x \rho_x = 1$. The non-uniqueness of solutions follows if $\mathcal{E}(\rho^0) \ge \sigma$ due to non-Lipschitz right-hand side in (5.4). ☐

The equation (5.4) may have an underlying Hamiltonian structure, but while the matrix field $\mathbb{J}(\rho)$ proposed here is skew-symmetric, it generally does not satisfy the Jacobi identity.

5.2 Complex-balanced chemical reaction networks

Microscopic particle system. We now describe a particle system that is commonly used to model chemical reactions. For a detailed review of this particle system with motivation and connections to related particle systems see [AK11].

Let $\mathcal{X}$ be a finite set of species, R be the finite set of reactions between the species, and let the vectors $\gamma^{(r)} \in \mathbb{R}^{\mathcal{X}}$ denote the net number of particles of each species that are created/annihilated during a reaction $r \in \mathrm{R}$. Furthermore, let $\mathrm{R} = \mathrm{R}_{\mathrm{fw}} \cup \mathrm{R}_{\mathrm{bw}}$ such that each forward reaction $r \in \mathrm{R}_{\mathrm{fw}}$ corresponds to a backward reaction $\mathrm{bw}(r) \in \mathrm{R}_{\mathrm{bw}}$, meaning that $\gamma^{(\mathrm{bw}(r))} = -\gamma^{(r)}$ for all $r \in \mathrm{R}_{\mathrm{fw}}$. The set R_{fw} will play the role of $\mathcal{X}^2/2$ from Example 2.1.

The microscopic model involves a finite volume V that controls the number of randomly reacting particles in the system. For a fixed V, we study the random *concentration* or *empirical measure* $\rho_x^{(V)}(t)$, which is the number of particles belonging to species $x \in \mathcal{X}$. Note that the total number of particles may not be conserved here, as opposed to the setting of Example 2.1. We also consider the *integrated net reaction flux* for $r \in \mathrm{R}_{\mathrm{fw}}$,

$$W_r^{(V)}(t) = \frac{1}{V}\#\big\{\text{reactions } r \text{ occurred in time } (0,t]\big\} - \frac{1}{V}\#\big\{\text{reactions bw}(r) \text{ occurred in time } (0,t]\big\}.$$

Forward and backward microscopic reactions r take place with given microscopic jump rates $V\kappa_r^{(V)}$ and $V\kappa_{\mathrm{bw}(r)}^{(V)}$ respectively. Typically these jump rates are modelled with combinatoric terms in the so-called chemical master equation (see [AK11]). Since our framework is purely macroscopic, the precise expressions for the microscopic jump rates are not relevant; the only crucial point is that both converge sufficiently strongly to macroscopic reaction rates κ_r and $\kappa_{\mathrm{bw}(r)}$. The pair $(\rho^{(V)}(t), W^{(V)}(t))$ is a Markov process on $\mathbb{R}^{\mathcal{X}} \times \mathbb{R}^{\mathrm{R}_{\mathrm{fw}}}$ with generator

$$(\mathcal{Q}^{(V)}f)(\rho,w) = \\ V \sum_{r\in\mathrm{R}_{\mathrm{fw}}} \kappa_r^{(V)}(\rho)\big[f(\rho + \tfrac{1}{V}\gamma^{(r)}, w + \tfrac{1}{V}\mathbb{1}_r) - f(\rho,w)\big] + \kappa_{\mathrm{bw}(r)}^{(V)}(\rho)\big[f(\rho+\tfrac{1}{V}\gamma^{(\mathrm{bw}(r))}, w + \tfrac{1}{V}\mathbb{1}_{\mathrm{bw}(r)}) - f(\rho,w)\big].$$

Using the matrix notation $\Gamma := [\gamma^{(r)}]_{r\in\mathrm{R}_{\mathrm{fw}}} \in \mathbb{R}^{\mathcal{X}\times\mathrm{R}_{\mathrm{fw}}}$, in the limit $V \to \infty$ the pair $(\rho^{(V)}, W^{(V)})$ converges to the solution of (see [Kur70] and [RZ21, Sec. 3.1])

$$\begin{cases} \dot{w}_r(t) = \kappa_r(\rho(t)) - \kappa_{\mathrm{bw}(r)}(\rho(t)), & r \in \mathrm{R}_{\mathrm{fw}} \\ \dot{\rho}_x(t) = (\Gamma\dot{w}(t))_x, & x \in \mathcal{X}. \end{cases} \tag{5.6}$$

The Markov process $(\rho^{(V)}(t), W^{(V)}(t))$ satisfies a large-deviation principle (2.5) where $\mathcal{L}, \mathcal{H}$ are now given by (see [PR19, Thm. 1.1] and [RZ21, Cor. 3.1])

$$\mathcal{L}(\rho, j) = \inf_{j^+\in\mathbb{R}_{\geq 0}^{\mathrm{R}_{\mathrm{fw}}}} \sum_{r\in\mathrm{R}_{\mathrm{fw}}} s(j_r^+ \mid \kappa_r(\rho)) + s(j_r^+ - j_r \mid \kappa_{\mathrm{bw}(r)}(\rho)),$$
$$\mathcal{H}(\rho,\zeta) = \sum_{r\in\mathrm{R}_{\mathrm{fw}}} \kappa_r(\rho)(e^{\zeta_r} - 1) + \kappa_{\mathrm{bw}(r)}(\rho)(e^{-\zeta_r} - 1),$$

and $s(\cdot \mid \cdot)$ is defined in (2.7). As in the IPFG and zero-range models, the infimum over one-way fluxes j^+ can be derived using the contraction principle.

We mention that at this level of generality one can already derive many interesting MFT properties, see [RZ21]. After all, the IPFG and zero-range models fall within this class. However, in order to apply our framework and obtain explicit results, the quasipotential needs to be known. To this aim we make two crucial assumptions.

First, the system satisfies *mass-action kinetics* i.e. there exists *stoichiometric vectors* or *complexes* $\alpha^{(r)} \in \mathbb{R}_{\geq 0}^{\mathcal{X}}$ (encoding the number of reactants involved) and *reaction constants* $c_r > 0$ for each $r \in \mathrm{R}$ such that

$$\gamma^{(r)} = \alpha^{(\mathrm{bw}(r))} - \alpha^{(r)}, \qquad \gamma^{(\mathrm{bw}(r))} = \alpha^{(r)} - \alpha^{(\mathrm{bw}(r))},$$

and the forward and backward rates satisfy, setting $\rho^{\alpha^{(r)}} := \prod_{x\in\mathcal{X}} \rho_x^{\alpha_x^{(r)}}$,

$$\kappa_r(\rho) = c_r \rho^{\alpha^{(r)}}, \qquad \forall r \in \mathrm{R}. \tag{5.7}$$

Second, we assume that the system satisfies *complex balance* [ACK10, Sec. 3.2], i.e. there exists a $\pi \in \mathbb{R}^{\mathcal{X}}_{>0}$ such that

$$\forall\ \psi \in \mathbb{R}^{\mathbb{C}}: \sum_{r\in\mathrm{R_{fw}}} (c_r \pi^{\alpha^{(r)}} - c_{\mathrm{bw}(r)} \pi^{\alpha^{(\mathrm{bw}(r))}})(\psi_{\alpha^{(r)}} - \psi_{\alpha^{(\mathrm{bw}(r))}}) = 0, \tag{5.8}$$

where $\mathbb{C} := \{\alpha^{(r)} : r \in \mathrm{R}\}$ signifies the set of *complexes*. As a consequence, this π is an equilibrium point of the dynamics (5.6). Complex balance says that each complex is in balance, and is a somewhat weaker condition than detailed balance and hence allows for non-dissipative effects. Since the chemical reaction network described here is, as a graph, "reversible", such an equilibrium point π exists *if* the reaction network has deficiency zero (see [ACK10, Thm. 3.3]).

State-flux triple and L-function. Fix a reference or initial concentration $\rho^0 \in \mathbb{R}^{\mathcal{X}}_{\geq 0}$. The state space consists of all concentrations that can be produced from ρ^0 via reactions:

$$\mathcal{Z} = \big\{\rho \in \mathbb{R}^{\mathcal{X}}_{\geq 0} : \exists w \in \mathbb{R}^{\mathrm{R_{fw}}} \text{ so that } \rho = \rho^0 + \Gamma w\big\}, \qquad \text{with tangent space}$$
$$T_\rho\mathcal{Z} = \big\{u \in \mathbb{R}^{\mathcal{X}} : \rho_x = 0 \implies u_x = 0 \text{ for all } x \in \mathcal{X}\big\}, \qquad T^*_\rho\mathcal{Z} = \mathbb{R}^{\mathcal{X}}.$$

This set $\mathcal{Z}$ is also known in the literature as the non-negative stoichiometric compatibility class or stoichiometric simplex [3]. The flux space and the associated tangent space are

$$\mathcal{W} = \big\{w \in \mathbb{R}^{\mathrm{R_{fw}}} :\ \rho^0 + \Gamma w \in \mathcal{Z}\big\},\ \ T_\rho\mathcal{W} = \big\{j \in \mathbb{R}^{\mathrm{R_{fw}}} :\ \Gamma j \in T_\rho\mathcal{Z}\big\},\ \ T^*_\rho\mathcal{W} = \mathbb{R}^{\mathrm{R_{fw}}},$$

where recall that $\Gamma w = \sum_{r\in\mathrm{R_{fw}}} \gamma^{(r)} w_r$. For an arbitrary $\rho^0 \in \mathcal{Z}$, the continuity map $\phi : \mathcal{W} \to \mathcal{Z}$ is defined as

$$\phi(w) = \rho^0 + \Gamma w,$$

with $d\phi_\rho = \Gamma$ and $d\phi_\rho^\mathsf{T} = \Gamma^\mathsf{T}$. Note that with this setup, ϕ is indeed surjective.

Quasipotential. The quasipotential is again the relative entropy with respect to the invariant measure,

$$\mathcal{V}(\rho) = \sum_{x\in\mathcal{X}} s(\rho_x \mid \pi_x). \tag{5.9}$$

Recall the relation between the quasipotential and the large-deviation rate functional for the invariant measure of the microscopic system from Theorem 3.6. Whereas in the IPFG model this relative entropy appears as the large-deviation rate functional for independent particles by Sanov's Theorem, in the complex balance case this is the rate functional of the explicitly known invariant measure of the microscopic particle system [ACK10, Thm. 4.1]. As in the previous examples, it can also be checked purely macroscopically that this is the correct quasipotential satisfying (2.9).

Proposition 5.4. *At the points of differentiability of $\mathcal{V}$, we have $\mathcal{H}(\rho, d\phi_\rho^\mathsf{T} d\mathcal{V}(\rho)) = 0$.*

Proof. Under the assumption of mass-action kinetics (5.7) we find[4]

$$\begin{aligned}
\mathcal{H}(\rho, d\phi_\rho^\mathsf{T} d\mathcal{V}(\rho)) &= \sum_{r\in\mathrm{R_{fw}}} \kappa_r(\rho)\Big[\big(\tfrac{\rho}{\pi}\big)^{\gamma^{(r)}} - 1\Big] + \kappa_{\mathrm{bw}(r)}(\rho)\Big[\big(\tfrac{\rho}{\pi}\big)^{-\gamma^{(r)}} - 1\Big] \\
&= \sum_{r\in\mathrm{R_{fw}}} c_r\big(\pi^{\alpha^{(r)}-\alpha^{(\mathrm{bw}(r))}} \rho^{\alpha^{(\mathrm{bw}(r))}} - \rho^{\alpha^{(r)}}\big) + c_{\mathrm{bw}(r)}\big(\pi^{\alpha^{(\mathrm{bw}(r))}-\alpha^{(r)}} \rho^{\alpha^{(r)}} - \rho^{\alpha^{(\mathrm{bw}(r))}}\big) \\
&= \sum_{r\in\mathrm{R_{fw}}} \big(c_r \pi^{\alpha^{(r)}} - c_{\mathrm{bw}(r)} \pi^{\alpha^{(\mathrm{bw}(r))}}\big)\Big[\big(\tfrac{\rho}{\pi}\big)^{\alpha^{(\mathrm{bw}(r))}} - \big(\tfrac{\rho}{\pi}\big)^{\alpha^{(r)}}\Big] = 0,
\end{aligned}$$

[3] Under the complex balance assumption the equilibrium point π is unique and stable within this simplex [ACK10, Thm. 3.2].

[4] The complex balance assumption (5.8) is only needed to show that (5.9) is indeed the quasipotential. However, the proof only requires (5.8) to hold for all $\psi_\alpha = (\frac{\rho}{\pi})^\alpha$.

where the final equality follows by choosing $\psi_\alpha = (\frac{\rho}{\pi})^\alpha$ in the complex-balance condition (5.8). ☐

Dissipation potential, forces and orthogonality. The driving force is

$$F_r(\rho) = \frac{1}{2}\log\frac{\kappa_r(\rho)}{\kappa_{\mathrm{bw}(r)}(\rho)} = \frac{1}{2}\log\Big(\frac{c_r}{c_{\mathrm{bw}(r)}}\rho^{-\gamma^{(r)}}\Big), \qquad \mathrm{Dom}(F) = \big\{\rho\in\mathcal{Z} : \rho_x > 0 \text{ for all } x\in\mathcal{X}\big\},$$

where recall that $\kappa_r(\rho) = c_r\rho^{\alpha^{(r)}}$. The dissipation potentials are

$$\Phi^*(\rho,\zeta) = 2\sum_{r\in\mathrm{R}_{\mathrm{fw}}}\sqrt{\kappa_r(\rho)\kappa_{\mathrm{bw}(r)}(\rho)}\;(\cosh(\zeta_r)-1),$$
$$\Phi(\rho,j) = 2\sum_{r\in\mathrm{R}_{\mathrm{fw}}}\sqrt{\kappa_r(\rho)\kappa_{\mathrm{bw}(r)}(\rho)}\;\Big(\frac{\cosh^*(j_r)}{2\sqrt{\kappa_r(\rho)\kappa_{\mathrm{bw}(r)}(\rho)}}+1\Big).$$

Note that $\mathrm{Dom}_{\mathrm{symdiss}}(F) = \mathrm{Dom}(F)$, i.e. the dissipation potential is symmetric.

Following Corollary 2.19, the symmetric and antisymmetric forces are

$$F^{\mathrm{sym}}_r(\rho) = -\Big(\frac{1}{2}d\phi_\rho^{\mathsf{T}}d\mathcal{V}(\rho)\Big)_r = -\frac{1}{2}\log\Big(\frac{\rho}{\pi}\Big)^{\gamma^{(r)}},\ F^{\mathrm{asym}}_r(\rho) = F_r(\rho) - F^{\mathrm{sym}}_r(\rho) = \frac{1}{2}\log\Big(\frac{c_r}{c_{\mathrm{bw}(r)}}\pi^{-\gamma^{(r)}}\Big),$$

with $\mathrm{Dom}(F^{\mathrm{sym}}) = \mathrm{Dom}(F^{\mathrm{asym}}) = \mathrm{Dom}(F)$. The orthogonality relations in Proposition 2.24 apply with

$$\Phi^*_{\zeta^2}(\rho,\zeta^1) = 2\sum_{r\in\mathrm{R}_{\mathrm{fw}}}\sqrt{\kappa_r(\rho)\kappa_{\mathrm{bw}(r)}(\rho)}\;\cosh(\zeta^2_r)[\cosh(\zeta^1_r)-1],$$
$$\theta_\rho(\zeta^1,\zeta^2) = 2\sum_{r\in\mathrm{R}_{\mathrm{fw}}}\sqrt{\kappa_r(\rho)\kappa_{\mathrm{bw}(r)}(\rho)}\;\sinh(\zeta^1 r)\sinh(\zeta^2_r).$$

This notion of generalised orthogonality is consistent with the derivations in [RZ21].

Decomposition of the L-function. The decompositions in Theorem 2.27 hold with the L-functions

$$\mathcal{L}_{(1-2\lambda)F}(\rho,j) = \inf_{j^+\in\mathbb{R}^{\mathrm{R}_{\mathrm{fw}}}_{\geq 0}}\sum_{r\in\mathrm{R}_{\mathrm{fw}}} s\big(j^+_r \mid (\kappa_r(\rho))^{1-\lambda}(\kappa_{\mathrm{bw}(r)}(\rho))^{\lambda}\big) + s\big(j^+_r - j_r \mid (\kappa_r(\rho))^{\lambda}(\kappa_{\mathrm{bw}(r)}(\rho))^{1-\lambda}\big),$$
$$\mathcal{L}_{F-2\lambda F^{\mathrm{sym}}}(\rho,j) = \inf_{j^+\in\mathbb{R}^{\mathrm{R}_{\mathrm{fw}}}_{\geq 0}}\sum_{r\in\mathrm{R}_{\mathrm{fw}}} s\Big(j^+_r \mid \kappa_r(\rho)\big(\frac{\rho}{\pi}\big)^{\lambda\gamma^{(r)}}\Big) + s\Big(j^+_r - j_r \mid \kappa_{\mathrm{bw}(r)}(\rho)\big(\frac{\rho}{\pi}\big)^{-\lambda\gamma^{(r)}}\Big),$$
$$\mathcal{L}_{F-2\lambda F^{\mathrm{asym}}}(\rho,j) = \inf_{j^+\in\mathbb{R}^{\mathrm{R}_{\mathrm{fw}}}_{\geq 0}}\sum_{r\in\mathrm{R}_{\mathrm{fw}}} s\Big(j^+_r \mid (\kappa_r(\rho))^{1-\lambda}(\kappa_{\mathrm{bw}(r)}(\rho))^{\lambda}\big(\frac{\rho}{\pi}\big)^{-\lambda\gamma^{(r)}}\Big)$$
$$+ s\Big(j^+_r - j_r \mid (\kappa_r(\rho))^{\lambda}(\kappa_{\mathrm{bw}(r)}(\rho))^{1-\lambda}\big(\frac{\rho}{\pi}\big)^{\lambda\gamma^{(r)}}\Big),$$

with the corresponding Fisher informations

$$\mathcal{R}^\lambda_F(\rho) = -\mathcal{H}\big(\rho,-2\lambda F(\rho)\big) = \sum_{r\in\mathrm{R}}\kappa_r(\rho) - (\kappa_r(\rho))^{1-\lambda}(\kappa_{\mathrm{bw}(r)}(\rho))^{\lambda},$$
$$\mathcal{R}^\lambda_{F^{\mathrm{sym}}}(\rho) = -\mathcal{H}\big(\rho,-2\lambda F^{\mathrm{sym}}(\rho)\big) = \sum_{r\in\mathrm{R}}\kappa_r(\rho) - \kappa_r(\rho)\big(\frac{\rho}{\pi}\big)^{\lambda\gamma^{(r)}},$$
$$\mathcal{R}^\lambda_{F^{\mathrm{asym}}}(\rho) = -\mathcal{H}\big(\rho,-2\lambda F^{\mathrm{asym}}(\rho)\big) = \sum_{r\in\mathrm{R}}\kappa_r(\rho) - (\kappa_r(\rho))^{1-\lambda}(\kappa_{\mathrm{bw}(r)}(\rho))^{\lambda}\big(\frac{\pi}{\rho}\big)^{\lambda\gamma^{(r)}}.$$

The zero-cost flux for $\mathcal{L}_{F^{\mathrm{sym}}}$ is related to a gradient flow by Corollary 2.34; this has been discussed in [Ren18a, Cor. 4.8]. As opposed to IPFG and zero-range examples, the construction of a Poisson structure for $\mathcal{L}_{F^{\mathrm{asym}}}$ is difficult in the chemical reaction setting due to the non-locality of the jump rates and the interplay with the stoichiometric vectors, and remains an open question.

5.3 Lattice gases

In this section we focus on the typical setting of MFT [BDSG+15], namely discrete state-space particle systems whose hydrodynamic limit is the following drift-diffusion equation on the torus $\mathbb{T}^d$

$$\begin{aligned} \dot\rho(t) &= -\operatorname{div} j(t), \\ j(t) &= j^0\big(\rho(t)\big), \qquad \text{with } j^0(\rho) := -\nabla\rho - \chi(\rho)(\nabla U + A). \end{aligned} \tag{5.10}$$

As before $\rho \in \mathcal{P}(\mathbb{T}^d)$ is the limiting density of the particle system, but now $\nabla, \operatorname{div}$ denote the continuous differential operators in $\mathbb{R}^d$. We are given a smooth, strictly-positive potential $U \in C^\infty(\mathbb{T}^d;\mathbb{R})$ and a smooth divergence-free covector field $A \in C^\infty(\mathbb{T}^d;\mathbb{R}^d)$, i.e. $\operatorname{div} A = 0$, that satisfies $\nabla U \cdot A = 0$. The smooth function $\chi : [0,\infty) \to [0,\infty)$ is called the mobility, and we assume that for some $h : [0,\infty) \to [0,\infty)$,

$$\frac{d^2}{da^2} h(a) = \frac{1}{\chi(a)}. \tag{5.11}$$

Most results about this class of models are well known; we present them here to show that our abstract framework is consistent with 'classical' MFT.

Microscopic particle system. Although the macroscopic framework works for general mobilities, we only describe two standard microscopic particle systems that give rise to different mobilities. For independent random walkers $\chi(a) = a$, $h(a) = a\log a - a + 1$ and for the simple-exclusion process $\chi(a) = a(1-a)$, $h(a) = a\log a + (1-a)\log(1-a)$. Since these two particle systems with limit (5.10) have been extensively studied in the literature, we only present the essential features here.

For both particle systems, the particles can jump to neighbouring sites on the lattice $\mathbb{T}^d \cap (\frac{1}{n}\mathbb{Z})^d$. In order to pass to the hydrodynamic limit (5.10) and derive the corresponding large deviations, the state space will be embedded in the continuous torus. The first particle system consists of independent random walkers with drift. For any $n \in \mathbb{N}$, the corresponding empirical measure-flux pair $(\rho^{(n)}(t), W^{(n)}(t))$ is a Markov process in $\mathcal{P}(\mathbb{T}^d) \times \mathcal{M}(\mathbb{T}^d;\mathbb{R}^d)$ with generator (see [Ren18b])

$$\begin{aligned} (\mathcal{Q}^{(n)} f)(\rho, w) = n^2 \sum_{\substack{\tau\in\mathbb{Z}^d \\ |\tau|=1}} \int_{\mathbb{T}^d} & n^d \rho(dx) e^{-\left[\frac12 U(x+\frac1n\tau) - \frac12 U(x) + \frac{1}{2n}A(x)\cdot\tau\right]} \\ & \times \Big[f\big(\rho - \tfrac{1}{n^d}\delta_x + \tfrac{1}{n^d}\delta_{x+\frac1n\tau}, w + \tfrac{1}{n^{d+1}}\tau\delta_{x+\frac{1}{2n}\tau}\big) - f(\rho,w)\Big]. \end{aligned}$$

This system can also be derived as the spatial discretisation of interacting stochastic differential equations, although in such continuous-space setting it becomes less straight-forward how to define particle fluxes.

The second particle system is the weakly asymmetric simple exclusion process (WASEP) which has been extensively studied in the MFT literature (see for instance [BDSG+07, BDSG+15]). In this case the Markov process $(\rho^{(n)}(t), W^{(n)}(t))$ has generator

$$\begin{aligned} (\mathcal{Q}^{(n)} f)(\rho, w) = n^2 \sum_{\substack{\tau\in\mathbb{Z}^d \\ |\tau|=1}} \int_{\mathbb{T}^d} & n^d \rho(dx)\big(1 - n^d\rho(\{x + \tfrac1n\tau\})\big) e^{-\left[\frac12 U(x+\frac1n\tau) - \frac12 U(x) + \frac{1}{2n}A(x)\cdot\tau\right]} \\ & \times \Big[f\big(\rho - \tfrac{1}{n^d}\delta_x + \tfrac{1}{n^d}\delta_{x+\frac1n\tau}, w + \tfrac{1}{n^{d+1}}\tau\delta_{x+\frac{1}{2n}\tau}\big) - f(\rho,w)\Big]. \end{aligned}$$

Observe that in both generators, the flux w has a different scaling than the particle density ρ. This is required to ensure that the discrete-space, finite-n continuity equation converges to the continuous-space continuity equation with differential operator $-\operatorname{div}$.

Passing $n \to \infty$ we arrive at the hydrodynamic limit (5.10) with $\chi(a) := a$ for the first particle system and $\chi(a) := a(1-a)$ for the second particle system. The corresponding large-deviation cost function and its dual are

$$\mathcal{L}(\rho, j) = \frac14 \|j - j^0(\rho)\|^2_{L^2(1/\chi(\rho))}, \quad \mathcal{H}(\rho,\zeta) = \|\zeta\|^2_{L^2(\chi(\rho))} + \int_{\mathbb{T}^d} \zeta(x) j^0(\rho)(x)\,dx. \tag{5.12}$$

See [Ren18b, Sec. 5] for the large-deviations of the random walkers (with $A = 0$), [KL99, Chap. 10] for exclusion process without fluxes, and [BDSG+07, Thm. 2.1] for exclusion process with fluxes (with $A = 0$).

State-flux triple and L-function. The exact form of the state-flux triple is implied by (5.12). However, as opposed to the finite-dimensional examples discussed earlier, here we are dealing infinite-dimensional spaces, which severely complicates the definition of Banach manifolds $\mathcal{Z}$, $\mathcal{W}$ and the mapping ϕ. Therefore in what follows we will only formally define these objects. The only formality will be that $\mathcal{Z}, \mathcal{W}$ are not true manifolds, in the sense that their tangent spaces $T_\rho\mathcal{Z}, T_w\mathcal{W}$ are not isometrically isomorphic to some fixed Banach space, but rather depend on the points ρ, w. This does not pose a big problem, as long as we are able to identify the local tangent and cotangent spaces $T_\rho\mathcal{Z}, T_w\mathcal{W}, T^*_\rho\mathcal{Z}, T^*_\rho\mathcal{W}$, differential $d\phi$ and its adjoint $d\phi^\mathsf{T}$ that are needed to decompose $\mathcal{L}$ locally.

For the state space we choose $\mathcal{Z} = (\mathcal{P}(\mathbb{T}^d), \mathrm{W}_2)$, the space of probability measures on the (compact) torus, endowed with the Wasserstein-2 metric W_2. For any $\rho \in \mathcal{Z}$, the corresponding cotangent and tangent spaces are

$$T^*_\rho\mathcal{Z} := \overline{\{C^\infty(\mathbb{T}^d)\}}^{\|\cdot\|_{1,\chi(\rho)}}, \quad T_\rho\mathcal{Z} = \Big\{ -\operatorname{div}(\chi(\rho)h) \text{ (in distr. sense)} : h \in \overline{\{\nabla\varphi : \varphi \in C^\infty(\mathbb{T}^d)\}}^{\|\cdot\|_{L^2(\chi(\rho))}} \Big\}.$$

with the standard (semi)norms from Wasserstein-2 geometry [Pel14, Sec. 3.4.2]

$$\|\xi\|^2_{1,\chi(\rho)} := \|\nabla\xi\|^2_{L^2(\chi(\rho))}, \qquad \|u\|^2_{-1,\chi(\rho)} := \inf_{\substack{j\in T_\rho\mathcal{W} \\ u=-\operatorname{div} j}} \|j\|^2_{L^2(1/\chi(\rho))}.$$

As in the other examples we fix a reference point $\rho^0 \in \mathcal{Z}$. For the flux space we then choose

$$\mathcal{W} = \big\{ w \in \mathcal{M}(\mathbb{T}^d; \mathbb{R}^d) : \rho^0 - \operatorname{div} w \text{ (in distr. sense)} \in \mathcal{P}(\mathbb{T}^d) \big\}$$

endowed with the metric

$$\forall w_1, w_2 \in \mathcal{W},\ d^2_{\mathcal{W}}(w_1, w_2) := \inf_{\substack{\hat w:[0,1]\to\mathcal{W} \\ \hat w(0)=w_1, \hat w(1)=w_2}} \int_0^1 \|\hat w(t)\|^2_{L^2(1/\chi(\rho_0 - \operatorname{div}\hat w(t)))}\, dt.$$

The corresponding (co-)tangent spaces are

$$T^*_\rho\mathcal{W} = L^2(\chi(\rho)), \quad T_\rho\mathcal{W} = L^2(1/\chi(\rho)),$$

which is indeed consistent with the structure of (5.12). With these definition we can now write $\langle\zeta, j\rangle = \int_{\mathbb{T}^d}\zeta(x)j(x)\,dx$ for the pairing between any $\zeta \in L^2(\chi(\rho))$ and $j \in L^2(1/\chi(\rho))$.

Finally we define $\phi : \mathcal{W} \to \mathcal{Z}$ as

$$\phi(w) := \rho^0 - \operatorname{div} w,$$

and therefore $d\phi_\rho = -\operatorname{div} : T_\rho\mathcal{W} \to T_\rho\mathcal{Z}$ is indeed a bounded linear operator with bounded linear adjoint $d\phi^\mathsf{T}_\rho = \nabla : T^*_\rho\mathcal{Z} \to T^*_\rho\mathcal{W}$.

Note that this setup is slightly different from the standard Wasserstein geometry, where the fluxes are defined so as to satisfy $\dot\rho = \operatorname{div}(\rho j)$, while in our context the fluxes satisfy $\dot\rho = \operatorname{div} j$. This difference is merely a convention, and we will see below that the contraction onto $\mathcal{Z}$ with $\chi(\rho) = \rho$ leads to the classical Wasserstein setting via the EDI.

Quasipotential. The quasipotential $\mathcal{V} : \mathcal{Z} \to \mathbb{R}$ is defined as, recalling (5.11),

$$\mathcal{V}(\rho) = \int_{\mathbb{T}^d} \big[h(\rho(x)) + U(x)\rho(x)\big]\,dx,$$

Note that $\mathcal{V}(\rho)$ is well-defined for $\rho \in \mathcal{Z}$ which are absolutely continuous with respect to the uniform measure on the torus, i.e. $\rho(dx) = \rho(x)dx$. Using

$$d\mathcal{V}(\rho) = h'(\rho) + U, \quad \nabla d\mathcal{V}(\rho) = (\chi(\rho))^{-1}\nabla\rho + \nabla U,$$

its easy to verify that $\mathcal{H}(\rho, d\phi^\mathsf{T}_\rho d\mathcal{V}(\rho)) = 0$ and therefore $\mathcal{V}$ is indeed a quasipotential in the sense of Definition 2.5. Note that in the case $\chi(a) = a$, $\mathcal{V}$ is the relative entropy with respect to the Gibbs-Boltzmann measure $\mu(dx) = Z^{-1}e^{-U(x)}\,dx$.

Dissipation potential, forces and orthogonality. Using Definition (2.8) the driving force is

$$F(\rho) = \frac{1}{2}(\chi(\rho))^{-1}j^0(\rho), \quad \mathrm{Dom}(F) = \big\{\rho \in \mathcal{Z} : \ \rho(dx) = \rho(x)dx, \ \chi(\rho(x)) > 0 \text{ almost everywhere}\big\}.$$

The dissipation potential and its dual are

$$\Phi^*(\rho,\zeta) = \|\zeta\|^2_{L^2(\chi(\rho))} + \langle \zeta, j^0(\rho) - 2\chi(\rho)F(\rho)\rangle = \|\zeta\|^2_{L^2(\chi(\rho))}, \quad \Phi(\rho, j) = \frac{1}{4}\|j\|^2_{L^2(1/\chi(\rho))}.$$

Observe that $\mathrm{Dom}_{\mathrm{symdiss}}(F) = \mathrm{Dom}(F)$, i.e. the dissipation potential is symmetric. Following Corollary 2.19, the symmetric and antisymmetric forces are

$$F^{\mathrm{sym}}(\rho) = -\frac{1}{2}d\phi_\rho^\mathsf{T} d\mathcal{V}(\rho) = -\frac{1}{2}\big[(\chi(\rho))^{-1}\nabla\rho + \nabla U\big], \quad F^{\mathrm{asym}}(\rho) = F(\rho) - F^{\mathrm{sym}}(\rho) = -\frac{1}{2}A,$$

with $\mathrm{Dom}(F^{\mathrm{sym}}) = \mathrm{Dom}(F)$. Note that the antisymmetric force F^{asym} is independent of ρ.

The generalised orthogonality relations in Proposition 2.24 apply with

$$\Phi^*_{\zeta^2}(\rho,\zeta^1) = \|\zeta^1\|^2_{L^2(\chi(\rho))}, \quad \theta_\rho(\zeta^1,\zeta^2) = 2(\zeta^1,\zeta^2)_{L^2(\chi(\rho))},$$

where $(\cdot,\cdot)_{L^2(\chi(\rho))}$ is the $\chi(\rho)$-weighted L^2 norm. This shows that for quadratic dissipation potentials, the generalised expansion of Proposition 2.24 indeed collapses to the usual expansion of squares, i.e.:

$$\begin{aligned}\Phi^*(\rho,\zeta^1+\zeta^2) &= \|\zeta^1+\zeta^2\|^2_{L^2(\chi(\rho))} = \|\zeta^1\|^2_{L^2(\chi(\rho))} + 2(\zeta^1,\zeta^2)_{L^2(\chi(\rho))} + \|\zeta^2\|^2_{L^2(\chi(\rho))}\\ &= \Phi^*(\rho,\zeta^1) + \theta_\rho(\zeta^2,\zeta^1) + \Phi^*_{\zeta^1}(\rho,\zeta^2).\end{aligned}$$

Decomposition of the Lagrangian. The decompositions in Theorem 2.27 hold with the L-functions

$$\begin{aligned}\mathcal{L}_{2\lambda F}(\rho,j) &= \frac{1}{4}\|j - 4\lambda\chi(\rho)F(\rho)\|^2_{L^2(1/\chi(\rho))},\\ \mathcal{L}_{F-2\lambda F^{\mathrm{sym}}}(\rho,j) &= \frac{1}{4}\|j - 2\chi(\rho)F^{\mathrm{asym}} - 2(1-2\lambda)\chi(\rho)F^{\mathrm{sym}}(\rho)\|^2_{L^2(1/\chi(\rho))}, &(5.13)\\ \mathcal{L}_{F-2\lambda F^{\mathrm{asym}}}(\rho,j) &= \frac{1}{4}\|j - 2(1-2\lambda)\chi(\rho)F^{\mathrm{asym}} - 2\chi(\rho)F^{\mathrm{sym}}(\rho)\|^2_{L^2(1/\chi(\rho))}, &(5.14)\end{aligned}$$

and the corresponding Fisher informations

$$\begin{aligned}\mathcal{R}^\lambda_F(\rho) &= \mathcal{H}(\rho,-2\lambda F(\rho)) = \lambda(1-\lambda)\,\|{-2}F(\rho)\|^2_{L^2(\chi(\rho))}\,,\\ \mathcal{R}^\lambda_{F^{\mathrm{sym}}}(\rho) &= \mathcal{H}(\rho,-2\lambda F^{\mathrm{sym}}(\rho)) = \lambda(1-\lambda)\,\|{-2}F^{\mathrm{sym}}(\rho)\|^2_{L^2(\chi(\rho))}\,,\\ \mathcal{R}^\lambda_{F^{\mathrm{asym}}}(\rho) &= \mathcal{H}(\rho,-2\lambda F^{\mathrm{asym}}) = \lambda(1-\lambda)\,\|{-2}F^{\mathrm{asym}}\|^2_{L^2(\chi(\rho))}\,.\end{aligned}$$

The positivity of these Fisher informations is obvious from the definition. In this setting, the decompositions in Theorem 2.27 can be derived simply by expanding the squares in the the L-function.

Repeating the calculations in Corollary 2.32 for $\chi(a) = a$, we arrive at the local FIR equality for diffusion processes (with u as a placeholder for $\dot\rho$) [HPST20, Eq. (14)]

$$\langle d\,\mathrm{RelEnt}(\rho|\mu), u\rangle + \left\|\nabla\log\frac{\rho}{\mu}\right\|_{L^2(\rho)} \le \hat{\mathcal{L}}(\rho,j),$$

where the contracted L-function $\hat{\mathcal{L}}$ is defined in (2.38), the relative entropy with respect to μ is defined as $\mathrm{RelEnt}(\cdot|\mu) := \mathcal{V}(\cdot)$.

We now briefly comment on the symmetric and antisymmetric L-functions. Substituting $\lambda = \frac{1}{2}$ in (5.14) and expanding the square we find

$$\begin{aligned}\mathcal{L}_{F^{\mathrm{sym}}}(\rho,j) &= \frac{1}{4}\|j\|^2_{L^2(1/\chi(\rho))} + \frac{1}{4}\|-2\chi(\rho)F^{\mathrm{sym}}(\rho)\|^2_{L^2(1/\chi(\rho))} - \frac{1}{2}\langle j, -2F^{\mathrm{sym}}(\rho)\rangle\\ &= \frac{1}{4}\|j\|^2_{L^2(1/\chi(\rho))} + \frac{1}{4}\|\nabla d\mathcal{V}(\rho)\|^2_{L^2(\chi(\rho))} - \frac{1}{2}\langle \mathrm{div}\, j, d\mathcal{V}(\rho)\rangle,\end{aligned}$$

where we have used $-2F^{\mathrm{asym}}(\rho) = \nabla d\mathcal{V}(\rho)$ and the definition of $\|\cdot\|_{-1,\chi(\rho)}$. Using this decomposition of $\mathcal{L}_{F^{\mathrm{sym}}}$, the contracted symmetric L-function

$$\hat{\mathcal{L}}_{F^{\mathrm{sym}}}(\rho, u) := \inf_{j\in T_\rho\mathcal{W}:\, u=-\operatorname{div} j} \mathcal{L}_{F^{\mathrm{sym}}}(\rho, j),$$

admits the decomposition

$$\hat{\mathcal{L}}_{F^{\mathrm{sym}}}(\rho, u) = \Psi(\rho, u) + \Psi^*(\rho, -\tfrac{1}{2}d\mathcal{V}(\rho)) + \frac{1}{2}\langle d\mathcal{V}(\rho), u\rangle, \tag{5.15}$$

where the contracted dissipation potential $\Psi(\rho, u) = \frac{1}{4}\|u\|^2_{-1,\chi(\rho)}$ and its dual $\Psi^*(\rho, s) = \|s\|^2_{1,\chi(\rho)}$ (recall abstract definition in (2.40)). The decomposition (5.15) is the standard Wasserstein-based EDI for the drift-diffusion equation (5.10) (see for instance [MPR14, Sec. 4.2]).

Similarly, the purely antisymmetric L-function and its contraction read

$$\mathcal{L}_{F^{\mathrm{asym}}}(\rho, j) = \frac{1}{4}\|j + \chi(\rho)A\|^2_{L^2(1/\chi(\rho))}, \quad \hat{\mathcal{L}}_{F^{\mathrm{asym}}}(\rho, u) = \frac{1}{4}\|u + \operatorname{div}(\chi(\rho)A)\|^2_{-1,\chi(\rho)},$$

with zero-cost velocity $u^0(\rho) = -\operatorname{div}(\chi(\rho)A) = -\nabla(\chi(\rho))\cdot A$. While the corresponding evolution equation $\dot\rho(t) = \operatorname{div}(\chi(\rho)A)$ preserves the energy

$$\mathcal{E} : \mathcal{Z} \to \mathbb{R}, \quad \mathcal{E}(\rho) := \int_{\mathbb{T}^d} U(x)\, d\rho(x),$$

it is not clear if we can define an operator $\mathbb{J}$ such that Conjecture 2.36 holds. However in the case $A = J\nabla U$ where $J \in \mathbb{R}^{d\times d}$ is a constant skew-symmetric matrix, we define the operator

$$\mathbb{J} : \mathcal{Z} \to (T^*_\rho\mathcal{Z} \to T_\rho\mathcal{Z}), \quad \mathbb{J}(\rho)(\zeta) := \operatorname{div}(\rho J\nabla\zeta).$$

Using the antisymmetry of J it follows that

$$\langle\zeta^1, \mathbb{J}(\rho)\zeta^2\rangle = \int_{\mathbb{T}^d} \zeta^1 \operatorname{div}(\rho J\nabla\zeta^2) = -\int_{\mathbb{T}^d} \nabla\zeta^1 \cdot J\nabla\zeta^2\rho = -\langle\mathbb{J}(\rho)\zeta^1, \zeta^2\rangle,$$

i.e. $\mathbb{J}$ is a skew-symmetric operator. Furthermore $\mathbb{J}$ satisfies the Jacobi identity by an elementary but tedious calculation which we skip. Therefore the antisymmetric zero-cost velocity indeed evolves according to the standard Hamiltonian system (see for instance [DPZ13, Section 3.2]) with energy $\mathcal{E}$ and Poisson structure $\mathbb{J}$.

6 Conclusion and discussion

In this paper we have presented an abstract macroscopic framework, which, for a given flux-density L-function, provides its decomposition into dissipative and non-dissipative components and a generalised notion of orthogonality between them. This decomposition provides a natural generalisation of the gradient-flow framework to systems with non-dissipative effects. Specifically we prove that the symmetric component of the L-function corresponds to a purely dissipative system and conjecture that the antisymmetric component corresponds to a Hamiltonian system, which has been verified in several examples. We then apply this framework to various examples, both with quadratic and non-quadratic L-functions.

We now comment on several related issues and open questions.

Why does the density-flux description work? While at the level of the evolution equations which are of continuity-type, the density-flux description does not offer any advantage (recall (1.1)), at the level of the cost functions it allows us to naturally encode divergence-free effects. This is clearly visible for instance in Theorem 2.27, where the evolutions corresponding to $\mathcal{L}_{F^{\mathrm{sym}}}$, $\mathcal{L}_{F^{\mathrm{asym}}}$ are dissipative and energy-preserving respectively, while the zero of the full L-function characterises the macroscopic evolution. A simple contraction argument allows us to retrieve the classical gradient-flow structure as well as the FIR inequalities in a fairly general setting, which further reveals the power of this description.

Antisymmetric force and L-function. While in the abstract framework the antisymmetric force $F^{\mathrm{asym}} = F^{\mathrm{asym}}(\rho)$ is a function of $\rho \in \mathrm{Dom}(F^{\mathrm{asym}})$, in all the concrete examples studied in this paper, F^{asym} is independent of ρ. It is not clear to us if this is a general property of the antisymmetric force or a special characteristic of the examples studied in this paper.

In Section 2.6 we conjectured that the zero-velocity flux for the contracted antisymmetric L-function admits a Hamiltonian structure, which was concretely proved for IPFG and zero-range process in Proposition 4.2, 5.3 respectively. While this gives insight into the associated zero-flows, it is not clear if $\mathcal{L}_{F^{\mathrm{asym}}}$ admits a variational formulation akin to the gradient-flow structure for $\mathcal{L}_{F^{\mathrm{sym}}}$ discussed in Corollory 2.34.

Chemical-reaction networks. Complex balance (5.8) has been assumed in the literature to ensure the existence of an invariant measure in the chemical-reaction network (see for instance [ACK10, Thm. 3.3]). However the proof of Proposition 5.4, which states that the relative entropy is the quasipotential, uses a weaker assumption than complex balance (see footnote 4). An important open question is whether this weaker assumption is a substantial relaxation of the complex balance assumption and whether it is sufficient to prove the existence of an invariant measure.

Furthermore, the Hamiltonian structure of the zero-velocity for $\mathcal{L}_{F^{\mathrm{asym}}}$ in the chemical-reaction setting is open. As pointed out in Section 5.2, the non-locality of the jump rates for chemical-reaction networks offers a challenge as opposed to the local jump rates for IPFG and zero-range process.

Generalised orthogonality. The notion of generalised orthogonality as introduced in Section 2.4 allows us to decompose the L-function as in Theorem 2.27 for the special case $\lambda = \frac{1}{2}$. However a natural question is whether this notion of orthogonality encoded via θ_ρ can be generalised to allow for any $\lambda \in [0, 1]$. This would provide a deeper understanding of our main decomposition Theorem 2.27 as well as a clear interpretation of the Fisher information in terms of a modified dissipation potential.

Quasipotentials for multiple invariant measures. In Remark 3.8 we discussed the possibility of having multiple quasipotentials. On a macroscopic level, forcing uniqueness for non-quadratic Hamilton-Jacobi equations is generally challenging. This is not merely a technical issue, since even on a microscopic level there may be multiple invariant measures; we have not pursued this possibility any further.

Global-in-time decompositions. In this paper we have focussed on the local-in-time description of the L-function as opposed to working with time-dependent trajectories. While it is not obvious how to generalise the various abstract results to allow for global-in-time descriptions, we expect that it can be worked out case by case for the examples presented in this paper. The main difficulty here is that the time-dependent trajectories are allowed to explore the boundary of the domain where the forces are not well-defined, and therefore an appropriate regularisation procedure is required to extend the domain of definition of these forces.

Acknowledgements. The authors are grateful to Alexander Mielke who provided the proof of the Hamiltonian structure for linear antisymmetric flows discussed in Appendix A. The authors thank Jin Feng, Davide Gabrielli, Mark Peletier, Richard Kraaij and Péter Koltai for insightful discussions. US thanks Julien Reygner who first pointed out the possibility of a connection between FIR inequalities and MFT. This work was presented at the MFO Workshop 2038 'Variational Methods for Evolution' and the authors would like to thank the participants for stimulating interactions. The work of RP and MR has been funded by the Deutsche Forschungsgemeinschaft (DFG) through grant CRC 1114 "Scaling Cascades in Complex Systems", Project C08. The work of US was supported by the Alexander von Humboldt foundation and the DFG under Germany's Excellence Strategy–MATH+: The Berlin Mathematics Research Center (EXC-2046/1)-project ID:390685689 (subproject EF4-4).

Appendices

A Hamiltonian structure for linear antisymmetric flow

For the ease of notation, throughout this appendix we will use $\langle\cdot,\cdot\rangle$ to denote the standard inner product of vectors in $\mathbb{R}^d$. We study the linear ODEs of the form

$$\dot{\omega} = \frac{1}{2}A\omega \in \mathbb{R}^d \quad \text{with} \quad A^\mathsf{T}\omega_* = A\omega_* = 0 \text{ for some } \omega_* \neq 0. \tag{A.1}$$

In Theorem A.2 we provide a complete characterisation of a natural Hamiltonian structure for these ODEs. In contrast to the typical settings of Hamiltonian systems, where $A \in \mathbb{R}^{d\times d}$ is assumed to be skew-symmetric, here we assume the existence of an invariant vector ω_* for the dynamics. The zero-cost antisymmetric flux for the IPFG system discussed in Section 4 is of the form (A.1).

The following lemma provides a useful alternate characterisation of the Jacobi identity for Poisson structures which will be used to prove Theorem A.2 below.

Lemma A.1. *For any $x \in \mathbb{R}^d$, define $\{\cdot,\cdot\} : \mathbb{R}^d \times \mathbb{R}^d \to \mathbb{R}$ by*

$$\{\mathcal{G}_1(x), \mathcal{G}_2(x)\} := \langle D\mathcal{G}_1, \widetilde{\mathbb{J}} D\mathcal{G}_2\rangle, \tag{A.2}$$

where $\mathcal{G}_1, \mathcal{G}_2 : \mathbb{R}^d \to \mathbb{R}$ are C^2-mappings, D is the Jacobian, and the C^1 matrix-valued function $x \to \widetilde{\mathbb{J}}(x) \in \mathbb{R}^{d\times d}$ is antisymmetric, i.e. $\widetilde{\mathbb{J}}^\mathsf{T} = -\widetilde{\mathbb{J}}$. The bracket (A.2) *satisfies the Jacobi identity if and only if for any smooth $\mathcal{G}_1, \mathcal{G}_2, \mathcal{G}_3 : \mathbb{R}^d \to \mathbb{R}$ we have*

$$\langle \mathcal{G}_1, D\widetilde{\mathbb{J}}[\widetilde{\mathbb{J}}\mathcal{G}_2]\mathcal{G}_3\rangle + \langle \mathcal{G}_2, D\widetilde{\mathbb{J}}[\widetilde{\mathbb{J}}\mathcal{G}_3]\mathcal{G}_1\rangle + \langle \mathcal{G}_3, D\widetilde{\mathbb{J}}[\widetilde{\mathbb{J}}\mathcal{G}_1]\mathcal{G}_2\rangle = 0, \tag{A.3}$$

where $Df[v]$ is the directional derivative of f along the vector v and the identity holds for every $x \in \mathbb{R}^d$.

The proof follows by straightforward manipulation of the Jacobi identity. We now present the Hamiltonian structure for (A.1).

Theorem A.2. *The linear ODE* (A.1) *admits the Hamiltonian system $(\mathbb{R}^d, \tilde{\mathcal{E}}, \widetilde{\mathbb{J}})$ with the linear energy and the linear Poisson structure*

$$\tilde{\mathcal{E}}(\omega) = c - \langle\omega_*, \omega\rangle, \quad \widetilde{\mathbb{J}}(\omega) = \frac{1}{2|\omega_*|^2}\Big(\omega_* \otimes (A\omega) - (A\omega)\otimes\omega_*\Big),$$

for any $c \in \mathbb{R}$. Consequently $\dot{\omega} = \widetilde{\mathbb{J}}(\omega)D\tilde{\mathcal{E}}(\omega)$.

Proof. For any $b \in \mathbb{R}^d$ we have

$$\widetilde{\mathbb{J}}(\omega)b = \frac{1}{2|\omega_*|^2}\left(\langle A\omega, b\rangle\omega_* - \langle\omega_*, b\rangle A\omega\right) = \frac{1}{2|\omega_*|^2}\Big(\langle\omega, A^\mathsf{T}b\rangle\omega_* - \langle\omega_*, b\rangle A\omega\Big)$$

and inserting $b = \omega_*$ in this relation and using $A^\mathsf{T}\omega_* = 0$ it follows that $\frac{1}{2}A\omega = -\widetilde{\mathbb{J}}(\omega)\omega_* = \widetilde{\mathbb{J}}(\omega)D\tilde{\mathcal{E}}(\omega)$. Since $\widetilde{\mathbb{J}}(\omega)^\mathsf{T} = -\widetilde{\mathbb{J}}(\omega)$ be definition, we only need to prove the Jacobi identity (A.3) to prove this result. Using the linearity of $\widetilde{\mathbb{J}}$ we find $D\widetilde{\mathbb{J}}(\omega)[v] = \widetilde{\mathbb{J}}(v)$, and therefore for any $\mathcal{G} \in \mathbb{R}^d$ we have

$$D\widetilde{\mathbb{J}}(\omega)[\widetilde{\mathbb{J}}(\omega)\mathcal{G}] = \widetilde{\mathbb{J}}(\widetilde{\mathbb{J}}(\omega)\mathcal{G}) = \frac{1}{2|\omega_*|^2}\Big(\omega_* \otimes \Big(A\widetilde{\mathbb{J}}(\omega)\mathcal{G}\Big) - \Big(A\widetilde{\mathbb{J}}(\omega)\mathcal{G}\Big)\otimes\omega_*\Big).$$

Using $A\omega_* = 0$ we find

$$A\widetilde{\mathbb{J}}(\omega)\mathcal{G} = -\frac{1}{2|\omega_*|^2}\langle\mathcal{G}, \omega_*\rangle A^2\omega.$$

Using the above two relations we arrive at

$$\langle\mathcal{G}_1, D\widetilde{\mathbb{J}}(\omega)[\widetilde{\mathbb{J}}(\omega)\mathcal{G}_2]\mathcal{G}_3\rangle = \frac{1}{4|\omega_*|^4}\Big(\langle\mathcal{G}_1, A^2\omega\rangle\langle\mathcal{G}_2, \omega_*\rangle\langle\omega_*, \mathcal{G}_3\rangle - \langle\mathcal{G}_1, \omega_*\rangle\langle\mathcal{G}_2, \omega_*\rangle\langle A^2\omega, \mathcal{G}_3\rangle\Big).$$

Similarly computing the remaining two terms in the left hand side of (A.3) and adding we have the required result. ◻

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