Thermodynamics of Nonequilibrium Driven Diffusive Systems in Mild Contact with Boundary Reservoirs

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Abstract. We consider macroscopic systems in mild contact with boundary reservoirs and under the action of external fields. We present an explicit formula for the Hamiltonian of such systems, from which we deduce the equation of motions, the action functional, the hydrodynamic equation for the adjoint dynamics, and a formula for the quasi-potential.

We examine the case in which the external forcing depends on time and drives the system from one nonequilibrium state to another. We extend the results presented in [8] on thermodynamic transformations for systems in strong contact with boundary reservoirs to the present situation.

In particular, we propose a natural definition of renormalized work, and show that it satisfies a Clausius inequality, and that quasi-static transformations minimize the renormalized work. In addition, we connect the renormalized work to the quasi-potential describing the fluctuations in the stationary nonequilibrium ensemble.

1. Introduction

After the recent articles [16, 12], where a formula for the quasi-potential has been derived for one-dimensional exclusion processes in mild contact with reservoirs, the purpose of this article is to extend to driven diffusive systems in mild contact with boundary reservoirs the nonequilibrium thermodynamical theory developed in [8, 9, 7] for systems in strong interaction with reservoirs.

The macroscopic evolution of systems in mild contact with reservoirs differs substantially from the one observed when the system strongly interacts with the reservoirs. With strong interactions, at the level of large deviations, a density fluctuation at the boundary is too costly and not observed. In contrast, for mild boundary interactions, any smooth trajectory has a finite cost. In consequence, the associated Hamiltonian carries a term which takes into account the boundary fluctuations. We investigate in this article the consequences to the thermodynamical theory of the additional boundary Hamiltonian term.

In Section 2, we introduce a class of stochastic lattice gases, which includes exclusion, zero-range and KMP models. We define in this framework a boundary Hamiltonian, derived rigorously in [20, 12] for one-dimensional, symmetric exclusion processes in mild contact with reservoirs, and record some of its properties. For the readers convenience, these dynamics are reviewed in the appendices, where explicit formulas for the Hamiltonians and the quasi-potentials are presented. We

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also provide a microscopic dynamics not covered by this theory, as the stationary states of the boundary dynamics are different from the bulk ones.

In Section 3, supported by the models presented in the previous section, we introduce the main object of this article, a Hamiltonian composed of a bulk part and the boundary part already put forward. The bulk part coincides with the Hamiltonian of systems in strong interaction with the reservoirs, and is expressed in terms of two thermodynamics quantities, the diffusivity and the mobility. The boundary Hamiltonian, instead, the main novelty of this article, is expressed in terms of a measure which depends on the chemical potential of the reservoirs and on the density profile at the boundary. We present in Section 3 several properties of this Hamiltonian and deduce from its form the equation of motions, the action functional, the quasi-potential, the adjoint thermodynamical quantities and formulas for the currents.

In Section 4, we derive a differential equation for the quasi-potential. This equation has been obtained by Derrida, Hirschberg and Sadhu [16] for one-dimensional symmetric exclusion processes, expressing the stationary state of the system as a product of matrices. For zero-range processes it can be obtained by direct computations because the stationary state is a product measure. For KMP models, the equation is new and has not yet been derived rigorously. In this model, the boundary conditions, displayed in equations (C.4) and (C.5), do not coincide with the boundary conditions for stationary density profile (see equation (3.11)), in contrast to the case of strong boundary interactions and of exclusion and zero-range dynamics in mild interaction. See Remarks 4.1 and 4.2.

Section 5 provides a dynamic derivation of the second law of thermodynamics as expressed by a Clausius inequality for the energy exchanged between the system and the external reservoirs and fields. The results and the reasoning presented in this section and the next one follow closely [8, 9].

In Section 6, we examine transformations along equilibrium states. According to the standard thermodynamic theory, a transformation is reversible if the energy exchanged between the system and the environment is minimal. A thermodynamic principle asserts that reversible transformations are accomplished by a sequence of equilibrium states and are well approximated by quasi-static transformations in which the variations of the environment are very slow. By an explicit construction of quasi-static transformations, we show that this principle can be derived for driven diffusive systems in mild interaction with boundary reservoirs.

Fix two equilibrium states and a transformation which drives the system from the first to the second one. The *excess work* of this transformation is defined as the total work minus the minimal work needed to bring the system from the first to the second equilibrium state. We show in Section 6 that the quasi-potential coincides with the excess work of the relaxation path from the first equilibrium state to the second.

In Section 7, these results are extended to transformations along nonequilibrium states. However, nonequilibrium states are characterized by the presence of a non vanishing current in the stationary density profile. Therefore, to maintain such states one needs to dissipate a positive amount of energy per unit of time. If we consider a transformation between nonequilibrium stationary states, the energy dissipated along such transformation will necessarily include the contribution needed to maintain such states.

To take into account this amount of energy, following [25], we introduce the *renormalized work*, and extend the results of the two previous sections to transformations along nonequilibrium states. In contrast with systems in strong interaction with the reservoirs, the symmetric and the anti-symmetric currents are not orthogonal (cf. the discussion at the end of Section 3). In consequence, the definition of the renormalized work proposed here is new and involves a boundary functional which takes into account the interaction of the system with the reservoirs.

The Hamiltonian appearing in this article is the action functional of the dynamical large deviations principle (DLDP) for the empirical measure. A dynamical large deviations principle for systems in mild contact with reservoirs has only been derived rigorously for one-dimensional symmetric exclusion processes [20, 12]. We believe that a DLDP for systems in mild contact with reservoirs can also be derived for gradient exclusion processes in any dimension. For zero-range and KMP processes, however, a rigorous proof is still out of reach due to a lack of exponential moments [10].

A formula for the Hamiltonian, as explained in Section 2 (cf. equation (2.4) and (3.2)), can be easily obtained from the generator of the boundary dynamics and the stationary state of the bulk dynamics.

A large deviations principle for the empirical measure under nonequilibrium states for systems in mild contact with reservoirs is more demanding and has not yet been proved. A formula for the rate functional (the quasi-potential) for one-dimensional symmetric exclusion processes is presented in [16, 12]. For zero-range processes, as the nonequilibrium states are product measures, it is easy to derive it. For all other models, it is still an open problem.

In conclusion, in this article we extend the thermodynamic theory resulting from the Macroscopic Fluctuation Theory (MFT) to systems in mild contact with reservoirs. We introduce a Hamiltonian with an additional term coming from the mild interactions of the system with reservoirs and propose a definition of renormalized work. We prove the validity of a Clausius inequality for transformations along equilibrium and nonequilibrium states in this framework and we show that the excess of work along the relaxation path is given by the quasi-potential, for equilibrium and nonequilibrium states.

2. Microscopic dynamics

In this section, we introduce the boundary Hamiltonian from an underlying microscopic dynamics. The evolution induced by this Hamiltonian together with the bulk Hamiltonian arising from locally conservative dynamics will be examined in the next sections.

The general framework presented in this section includes the main microscopic stochastic dynamics, such as the exclusion, zero-range and KMP processes, on which the Macroscopic Fluctuation Theory (MFT) has been build. For the reader's convenience, we reviewed in the appendices the properties of these systems used below.

Let Ω be the bounded domain of $\mathbb{R}^d$ occupied by the system. Fix $N \geq 1$, and denote by $\Omega_N = \Omega \cap (\mathbb{Z}/N)^d$ its discretization. Here, $\mathbb{Z}/N = \{k/N : k \in \mathbb{Z}\}$. Elements of Ω are represented by x, y. The boundary of Ω_N, denoted by $\partial\Omega_N$, consists of points in Ω_N which have a neighbor not in Ω_N:

$$\partial\Omega_N \;=\; \big\{\, x \in \Omega_N : \exists\, y \in (\mathbb{Z}/N)^d \setminus \Omega \,, |y - x| = 1/N \,\big\}\,,$$

where $|\cdot|$ stands for the Euclidian distance.

Let $\mathcal{E}$ be a subspace of $\mathbb{R}$ which represents the possible values of the spins or occupation variables. In the case of exclusion processes, $\mathcal{E} = \{0,1\}$. For zero-range processes, $\mathcal{E} = \mathbb{N} \cup \{0\}$, and for KMP models, $\mathcal{E} = \mathbb{R}_+$. The elements of $\mathcal{E}$ are denoted by the symbols $\mathfrak{x}$, $\mathfrak{y}$.

The state space of the microscopic dynamics is represented by Σ_N: $\Sigma_N = \mathcal{E}^{\Omega_N}$ and its elements by the Greek letters $\eta = (\eta_x : x \in \Omega_N)$, ξ. Hence, η_x stands for the value of the occupation variable at $x \in \Omega_N$ for the configuration η.

The microscopic dynamics is composed of two pieces. The first one describes the evolution in the bulk, while the second one the interaction of the system with the boundary reservoirs.

We do not discuss here the bulk dynamics nor the derivation of the diffusivity and mobility. This has already been done in numerous places. We refer to [5], for example. We concentrate on the boundary dynamics.

The boundary dynamics. The system is in a mild contact with boundary reservoirs, characterized by their chemical potentials $\lambda \in \Lambda$. The boundary dynamics corresponds to a continuous-time Markov chain taking values in $\mathcal{E}$. Its generator, denoted by $\mathcal{L}_\lambda$, takes the form

$$(\mathcal{L}_\lambda f)(\mathfrak{x}) \;=\; \int_{\mathcal{E}} [f(\mathfrak{y}) \,-\, f(\mathfrak{x})]\, r_\lambda(\mathfrak{x}, d\mathfrak{y})\,, \tag{2.1}$$

where $r_\lambda(\mathfrak{x}, \cdot\,)$ are finite positive measures which represent the jump rates.

For exclusion processes, $\mathcal{E} = \{0,1\}$, $\Lambda = \mathbb{R}$, $r_\lambda(0, d\mathfrak{y}) = [\, e^\lambda/(1+e^\lambda)\,]\, \delta_1(d\mathfrak{y})$, $r_\lambda(1, d\mathfrak{y}) = [\, 1/(1+e^\lambda)\,]\, \delta_0(d\mathfrak{y})$, where $\delta_a(\cdot)$ stands for the Dirac measure concentrated at a. For zero-range processes, $\mathcal{E} = \{0\} \cup \mathbb{N}$, $\Lambda = \mathbb{R}$, the jump rates are given by $r_\lambda(\mathfrak{x}, d\mathfrak{y}) = g(\mathfrak{x})\, \delta_{\mathfrak{x}-1}(d\mathfrak{y}) \,+\, e^\lambda\, \delta_{\mathfrak{x}+1}(d\mathfrak{y})$, $\mathfrak{x} \in \mathcal{E}$. Finally, for KMP models, $\mathcal{E} = \mathbb{R}_+$, $\Lambda = (-\infty, 0)$ and $r_\lambda(\mathfrak{x}, d\mathfrak{y}) \,=\, -\,\lambda\, e^{\lambda \mathfrak{y}}\, d\mathfrak{y}$.

Of course, as boundary dynamics one could consider a Markov chain taking values on larger spaces. For example, $\mathcal{E}^\Delta$ for some finite set Δ. The theory can easily be extended to this case and this is not an important hypothesis. In Appendix D we present such a model.

Assume that for all $\lambda \in \Lambda$, the $\mathcal{E}$-valued Markov chain induced by the generator $\mathcal{L}_\lambda$ is ergodic and has a unique stationary state denoted by m_λ. Assume, furthermore, that the measures m_λ form an exponential family:

$$m_\lambda(d\mathfrak{x}) \;=\; \frac{1}{Z(\lambda)}\, e^{\lambda\, \mathfrak{x} \,-\, H(\mathfrak{x})}\, \mathfrak{n}(d\mathfrak{x}) \tag{2.2}$$

for some energy $H : \mathcal{E} \to \mathbb{R}$. In this formula, $Z(\lambda)$ is the normalization constant which turns m_λ into a probability measure, and $\mathfrak{n}$ the counting measure ($\mathfrak{n}(\mathfrak{x}) = 1$ for all $\mathfrak{x} \in \mathcal{E}$ if $\mathcal{E}$ is discrete or $\mathfrak{n}$ is the Lebesgue measure if $\mathcal{E}$ is continuous). The function $Z(\cdot)$ is called *the partition function*.

Denote by $c(\mathcal{E})$ the convex envelope of $\mathcal{E}$. Let $R : \Lambda \to c(\mathcal{E})$ be the mean of the measure m_λ:

$$R(\lambda) \;=\; \int_{\mathcal{E}} \mathfrak{x}\, m_\lambda(d\mathfrak{x})\,. \tag{2.3}$$

Clearly, by definition of the partition function, $R(\lambda) = (d/d\lambda) \log Z(\lambda)$. Taking a second derivative yields that $R'(\lambda)$ is the variance of $\mathfrak{x}$ under m_λ. In particular, $R'(\lambda)$ is strictly positive and R invertible. Let $\Xi\colon c(\mathcal{E}) \to \Lambda$ be the inverse of R:

$\Xi = R^{-1}$. We present in the appendix explicit formulas for Z, R and Ξ in each model.

The boundary Hamiltonian. Denote by $\mathcal{M}^{\mathrm{bd}}_{\lambda,\rho} : c(\mathcal{E}) \times \mathbb{R} \to \mathbb{R}$, $\lambda \in \Lambda$, $\rho \in c(\mathcal{E})$, the function given by

$$\mathcal{M}^{\mathrm{bd}}_{\lambda,\rho}(p) \;=\; \int_{\mathcal{E}} \frac{1}{U_p}\, \mathcal{L}_\lambda U_p \, dm_{\Xi(\rho)} \;, \tag{2.4}$$

where U_p is the function $U_p(\mathfrak{x}) = e^{p\,\mathfrak{x}}$. The function $\mathcal{M}^{\mathrm{bd}}_{\lambda,\rho}$ may take the value $+\infty$ for certain values of p.

In view of formula (2.1) for the generator,

$$\mathcal{M}^{\mathrm{bd}}_{\lambda,\rho}(p) \;=\; \int_{\mathcal{E}\times\mathcal{E}} m_{\Xi(\rho)}(d\mathfrak{x})\, r_\lambda(\mathfrak{x}, d\mathfrak{y}) \left[\, e^{p(\mathfrak{y}-\mathfrak{x})} - 1 \,\right] . \tag{2.5}$$

A change of variables $\mathfrak{y}' = \mathfrak{y} - \mathfrak{x}$ yields that

$$\mathcal{M}^{\mathrm{bd}}_{\lambda,\rho}(p) \;=\; \int_{\mathcal{E}} m_{\Xi(\rho)}(d\mathfrak{x}) \int_{\mathcal{E}^-} r_\lambda(\mathfrak{x}, \mathfrak{x} + d\mathfrak{y}) \left[\, e^{p\mathfrak{y}} - 1 \,\right] ,$$

provided $\mathcal{E}^- = \{\mathfrak{y} - \mathfrak{x} : \mathfrak{y}\,,\, \mathfrak{x} \in \mathcal{E}\}$. Hence, changing the order of integrations,

$$\mathcal{M}^{\mathrm{bd}}_{\lambda,\rho}(p) \;=\; = \int_{\mathcal{E}^-} \left[\, e^{p\mathfrak{y}} - 1 \,\right] m_{\lambda,\rho}(d\mathfrak{y}) \;, \tag{2.6}$$

where

$$m_{\lambda,\rho}(d\mathfrak{y}) \;=\; \int_{\mathcal{E}} m_{\Xi(\rho)}(d\mathfrak{x})\, r_\lambda(\mathfrak{x}, \mathfrak{x} + d\mathfrak{y}) \;.$$

Example 2.1. *If the generator $\mathcal{L}_\lambda$ induces a Markov chain on $\mathbb{N}_0 := \mathbb{N} \cup \{0\}$ or on $\{0, \dots, M\}$, $M \geq 1$, with nearest-neighbor jumps, (it only jumps from k to $k \pm 1$), as in the case of zero-range or exclusion processes,*

$$\mathcal{M}^{\mathrm{bd}}_{\lambda,\rho}(p) \;=\; C_\lambda(\rho)\, [e^p - 1] \;+\; A_\lambda(\rho)\, [e^{-p} - 1] \;, \tag{2.7}$$

where $C_\lambda(\rho)$, $A_\lambda(\rho)$ stand for the creation and annihilation rates, respectively:

$$C_\lambda(\rho) \;:=\; E_{m_{\Xi(\rho)}}[\, r_\lambda(k, k+1)\,] \;, \quad A_\lambda(\rho) \;:=\; E_{m_{\Xi(\rho)}}[\, r_\lambda(k, k-1)\,] \;.$$

In this formula, $r_\lambda(k, k\pm 1)$ represents for the rate at which the Markov chain jumps from k to $k \pm 1$. The variable k is integrated with respected to the measure $m_{\Xi(\rho)}$.

For the simple exclusion process, $m_{\Xi(\rho)}$ is the Bernoulli measure of parameter ρ, and $r_\lambda(0,1) = R(\lambda)$, $r_\lambda(1,0) = 1 - R(\lambda)$. Thus,

$$\mathcal{M}^{\mathrm{bd}}_{\lambda,\rho}(p) \;=\; [1-\rho]\, R(\lambda)\, [e^p - 1] \;+\; \rho\, [\, 1 - R(\lambda)\,]\, [e^{-p} - 1] \;.$$

For the zero-range dynamics, $r_\lambda(k, k+1) = e^\lambda$, $r_\lambda(k, k-1) = g(k)$. Thus,

$$\mathcal{M}^{\mathrm{bd}}_{\lambda,\rho}(p) \;=\; e^\lambda\, [e^p - 1] \;+\; \Xi(\rho)\, [e^{-p} - 1]$$

because $E_{m_{\Xi(\rho)}}[g(k)] = \Xi(\rho)$.

The KMP model does not fall in the class described above. Here, $m_{\Xi(\rho)}$ is the exponential measure in $\mathbb{R}_+$ with density ρ, and an elementary computation yields that

$$\mathcal{M}^{\mathrm{bd}}_{\lambda,\rho}(p) \;=\; \frac{\tau}{\rho+\tau}\left(\frac{1}{1-\tau\, p} \;-\; 1\right) \;+\; \frac{\rho}{\rho+\tau}\left(\frac{1}{1+\rho\, p} \;-\; 1\right) , \;\; 0 < p < \tau^{-1} \;,$$

where $\tau = R(\lambda)$, and $\mathcal{M}^{\mathrm{bd}}_{\lambda,\rho}(p) \;=\; \infty$ if $p \notin (0, \tau^{-1})$.

Remark 2.2. *The zero-range process is usually parameterized by $\varphi = e^{\lambda}$. In the KMP model, keep in mind that the chemical potential λ, used to parametrize the exponential distributions, is negative.*

Remark 2.3. *The reader may have recognized in* (2.4) *the building block of the Donsker-Varadhan large deviations rate function:*

$$\mathcal{M}^{\mathrm{bd}}_{\lambda,\rho}(p) \;=\; \int_{\mathcal{E}} \frac{1}{U_p}\, \mathcal{L}_\lambda U_p \, dm_{\Xi(\rho)} \;\geq\; \inf_u \int_{\mathcal{E}} \frac{1}{u}\, \mathcal{L}_\lambda u \, dm_{\Xi(\rho)} \;=:\; -\, I_\lambda(m_{\Xi(\rho)})\,,$$

where the infimum is carried over all positive functions u which belong to the domain of the generator $\mathcal{L}_\lambda$. Here, I_λ stands for the Donsker-Varadhan rate functional of the large deviations principle for the empirical measure of the continuous-time Markov chain whose generator is $\mathcal{L}_\lambda$ [28].

Remark 2.4. *Let $(X_t : t \geq 0)$ be the continuous-time, $\mathcal{E}$-valued Markov chain induced by the generator $\mathcal{L}_\lambda$ introduced in* (2.1). *Assume that the process is reversible. As we learned from Donsker and Varadhan* [28]*, to prove a large deviations principle for the empirical measure $t^{-1}\int_0^t \delta_{X_s}\, ds$, the jump rates r_λ needed to be tilted by a function $F : \mathcal{E} \to \mathbb{R}$, as $r_{\lambda,F}(\mathfrak{x}, d\mathfrak{y}) = r_\lambda(\mathfrak{x}, d\mathfrak{y}) e^{-[F(\mathfrak{y})-F(\mathfrak{x})]}$. The purpose of the tilting is to change the stationary state. In fact, the equilibrium state of the Markov chain with jump rates $r_{\lambda,F}$, denoted by $m_{\lambda,F}$, is given by $m_{\lambda,F}(d\mathfrak{x}) = (1/Z_{\lambda,F})\, e^{2F(\mathfrak{x})}\, m_\lambda(d\mathfrak{x})$, where $Z_{\lambda,F}$ is a normalizing constant.*

The cost for the empirical measure $t^{-1}\int_0^t \delta_{X_s}\, ds$ to be close to the measure $m_{\lambda,F}$, denoted by $I_\lambda(m_{\lambda,F})$ in Remark 2.3, is given by the relative entropy of the perturbed dynamics with respect to the original one [28]*:*

$$I_\lambda(m_{\lambda,F}) \;=\; \lim_{t\to\infty} \frac{1}{t}\, \mathbb{E}_F\Big[\, \log \frac{d\,\mathbb{P}_F}{d\,\mathbb{P}}\,\Big|_{\mathcal{F}_t}\Big] \;=\; -\int \sqrt{\frac{dm_{\lambda,F}}{dm_\lambda}}\, \mathcal{L}_\lambda \sqrt{\frac{dm_{\lambda,F}}{dm_\lambda}}\, dm_\lambda\,. \tag{2.8}$$

In this formula, $\mathbb{P}$, $\mathbb{P}_F$ represent the distribution of the Markov chain with jump rates r_λ, $r_{\lambda,F}$, respectively, $\mathbb{E}_F$ the expectation with respect to $\mathbb{P}_F$, and $(d\mathbb{P}_F/d\mathbb{P})\,|_{\mathcal{F}_t}$ the Radon-Nikodym derivative of $\mathbb{P}_F$ with respect to $\mathbb{P}$ restricted to the σ-algebra $\mathcal{F}_t = \sigma(X(s) : 0 \leq s \leq t)$.

In the present context, only perturbations F expressed as $F(\mathfrak{x}) = p\,\mathfrak{x}$ appear. This means that only measures of the form $e^{q\,\mathfrak{x}}\, m_\lambda(d\mathfrak{x})$ are accessible. In other words, only perturbations that change the chemical potential are considered in the definition of the functional $\mathcal{M}^{\mathrm{bd}}_{\lambda,\rho}$. Moreover, and most importantly, in contrast with (2.8)*, $\log(d\mathbb{P}_F/d\mathbb{P})\,|_{\mathcal{F}_t}$ is not integrated with respect to the stationary measure induced by the perturbed dynamics associated the jump rated $r_{\lambda,F}$, that is $m_{\lambda,F}$, but with respect to the stationary state induced by the bulks dynamics. This is a consequence of the fact that the interaction with the boundaries is mild and dominated by the bulk dynamics.*

Hence, the functional $\mathcal{M}^{\mathrm{bd}}_{\lambda,\rho}$ has to be understood as follows. There is a family of boundary dynamics indexed by a chemical potential λ. The stationary state is represented by m_λ. The system is perturbed to change its chemical potential from λ to $\lambda + q$. The cost of this perturbation is not computed with respect to the new state but the one induced by the prevalent bulk dynamics (The bulk dynamics prevails over the boundary one because the interaction of the system with the reservoirs is mild). We shall refer to this cost as the bulk-cost.

Equilibrium free energy and pressure. In the present context, the equilibrium free energy takes a simple form. According to the postulates of statistical mechanics [21], since the equilibrium states are product measure, the pressure, denoted by $p(\cdot)$, and the free energy per unit of volume, denoted by $f(\cdot)$ and obtained as the Legendre transform of the pressure, are given by

$$p(\lambda) \,:=\, \log Z(\lambda)\,, \quad f(\rho) \,:=\, \sup_{\theta\in\Lambda} \big\{\theta\,\rho \,-\, p(\theta)\,\big\}\,.$$

Clearly,

$$f(\rho) \,=\, \Xi(\rho)\,\rho \,-\, p(\Xi(\rho))\,, \quad f'(\rho) \,=\, \Xi(\rho)\,. \tag{2.9}$$

Fix a reference chemical potential λ, and let

$$f_\lambda(\rho) \,:=\, \sup_{\theta\in\Lambda} \big\{\theta\,\rho \,-\, \log E_{m_\lambda}\big[\, e^{\theta\,\mathfrak{x}}\,\big]\,\big\}\,.$$

By definition of $f(\,\cdot\,)$,

$$f_\lambda(\rho) \,=\, f(\rho) \,-\, \{\lambda\,\rho \,-\, p(\lambda)\,\} \text{ and } f_\lambda''(\rho) \,=\, f''(\rho)\,. \tag{2.10}$$

It is well known that $f_\lambda(\cdot)$ is the large deviations rate functional of the sequence $N^{-1}\sum_{1\le j\le N}\mathfrak{x}_j$, where $(\mathfrak{x}_j : j\ge 1)$ are i.i.d. random variables distributed according to m_λ. The functional f_λ is called the *equilibrium free energy*. By (2.9) and (2.10),

$$f_\lambda(\rho) \,=\, \big[\,\Xi(\rho) \,-\, \lambda\,\big]\,\rho \,-\, \log\frac{Z(\Xi(\rho))}{Z(\lambda)} \quad\text{and}\quad f_\lambda'(\rho) \,=\, \Xi(\rho) \,-\, \lambda\,.$$

An identity. We turn to some properties of the functional $\mathcal{M}^{\mathrm{bd}}_{\lambda,\rho}$ needed in the next sections. We first claim that for all λ and ρ,

$$\mathcal{M}^{\mathrm{bd}}_{\lambda,\rho}(\,f'(\rho)-\lambda\,) \,=\, 0\,. \tag{2.11}$$

By (2.9), $\Xi(\rho) = f'(\rho)$. Hence, by (2.4) and (2.2),

$$\mathcal{M}^{\mathrm{bd}}_{\lambda,\rho}(p) \,=\, \frac{1}{Z(f'(\rho))}\int_{\mathcal{E}} e^{-p\,\mathfrak{x}}\,e^{f'(\rho)\,\mathfrak{x}\,-\,H(\mathfrak{x})}\,(\mathcal{L}_\lambda U_p)(\mathfrak{x})\,\mathfrak{n}(d\mathfrak{x})$$

for all p. Replacing the first p by $f'(\rho)\,-\,\lambda$, the right-hand side becomes

$$\frac{1}{Z(f'(\rho))}\int_{\mathcal{E}} e^{\lambda\,\mathfrak{x}\,-\,H(\mathfrak{x})}\,(\mathcal{L}_\lambda U_p)(\mathfrak{x})\,\mathfrak{n}(d\mathfrak{x}) \,=\, \frac{Z(\lambda)}{Z(f'(\rho))}\int_{\mathcal{E}}(\mathcal{L}_\lambda U_p)(\mathfrak{x})\,m_\lambda(d\mathfrak{x})\,.$$

The last term vanishes because m_λ is the stationary state for the dynamics induced by the generator $\mathcal{L}_\lambda$. This proves (2.11).

The functional $\mathfrak{A}_\lambda$. Let $\mathfrak{A}_\lambda$, $\lambda\in\Lambda$, be the functional given by

$$\mathfrak{A}_\lambda(\rho,p) \,:=\, \kappa\Big\{\,\mathcal{M}^{\mathrm{bd}}_{\lambda,\rho}(p) \,-\, \mathcal{M}^{\mathrm{bd}}_{\lambda,\rho}(0) \,-\, p\,(\,\mathcal{M}^{\mathrm{bd}}_{\lambda,\rho}\,)'(0)\,\Big\}\,. \tag{2.12}$$

By (2.5), the second term on the right-hand side, $\mathcal{M}^{\mathrm{bd}}_{\lambda,\rho}(0)$, vanishes. It has been included to underline that $\mathfrak{A}_\lambda(\rho,p)$ is a first order Taylor expansion. By (2.5),

$$\mathfrak{A}_\lambda(\rho,p) \,=\, \kappa\int_{\mathcal{E}\times\mathcal{E}} m_{\Xi(\rho)}(d\mathfrak{x})\,r_\lambda(\mathfrak{x},d\mathfrak{y})\,\big[\,e^{p(\mathfrak{y}-\mathfrak{x})} \,-\, 1 \,-\, p\,(\mathfrak{y}-\mathfrak{x})\,\big] \,\ge\, 0\,.$$

In particular, in the second variable, the functional $\mathfrak{A}_\lambda$ behaves quadratically close to zero:

$$\mathfrak{A}_\lambda(\rho,p) \,\approx\, p^2\,,\quad p\to 0\,,$$

for all ρ small. On the other hand, under the hypotheses of the Example 2.1, the functional $\mathfrak{A}_\lambda$ takes the form

$$\mathfrak{A}_\lambda(\rho, p) \;=\; C_\lambda(\rho)\,[e^p - 1 - p] \;+\; A_\lambda(\rho)\,[e^{-p} - 1 + p]\,,$$

Boundary condition. By (2.5),

$$(\,\mathcal{M}^{\mathrm{bd}}_{\lambda,\rho}\,)'\,(0) \;=\; \langle\, 1\,,\, \mathcal{L}_\lambda\, \mathfrak{x}\,\rangle_{m_{\Xi(\rho)}}\,, \tag{2.13}$$

where $\langle\, \cdot\,,\, \cdot\,\rangle_\nu$ represents the scalar product in $L^2(\nu)$.

The reversible case. Up to the end of this section, *assume that the operator $\mathcal{L}_\lambda$ is symmetric in $L^2(m_\lambda)$*. In other words that, for all $\lambda \in \Lambda$, the dynamics induced by the generator $\mathcal{L}_\lambda$ at the boundary is reversible for the measure m_λ. This condition is fulfilled by the simple exclusion, zero-range and KMP dynamics reviewed in the Appendices A–C, but not by the exclusion process with non-reversible boundary conditions presented in Section D.

We derive below three properties of the functional $\mathcal{M}^{\mathrm{bd}}_{\lambda,\rho}$ under this assumption. Recall the definition of $R(\lambda)$ given in (2.3) and that, by (2.9), $f'(\rho) = \Xi(\rho) = R^{-1}(\rho)$. By (2.13) and the reversibility of the measure m_λ with respect to $\mathcal{L}_\lambda$,

$$(\,\mathcal{M}^{\mathrm{bd}}_{\lambda,R(\lambda)}\,)'\,(0) \;=\; \langle\, \mathcal{L}_\lambda 1\,,\, \mathfrak{x}\,\rangle_{m_\lambda} \;=\; 0\,. \tag{2.14}$$

We turn to the reciprocal. We claim that

$$(\,\mathcal{M}^{\mathrm{bd}}_{\lambda,\rho}\,)'\,(0) \;\neq\; 0 \;\text{ if }\; f'(\rho) \;\neq\; \lambda\,. \tag{2.15}$$

Indeed, by (2.13) and (2.2), and since $\Xi(\rho) = f'(\rho)$,

$$(\,\mathcal{M}^{\mathrm{bd}}_{\lambda,\rho}\,)'\,(0) \;=\; \frac{Z(\lambda)}{Z(\Xi(\rho))}\,\langle\, e^{(f'(\rho)-\lambda)\mathfrak{x}}\,,\, \mathcal{L}_\lambda\, \mathfrak{x}\,\rangle_{m_\lambda}\,.$$

Since the measure m_λ is reversible,

$$\begin{aligned}
(\,\mathcal{M}^{\mathrm{bd}}_{\lambda,\rho}\,)'\,(0) \;&=\; -\,\frac{1}{2}\,\frac{Z(\lambda)}{Z(\Xi(\rho))}\,\int_{\mathcal{E}\times\mathcal{E}} m_\lambda(d\mathfrak{x})\, r_\lambda(\mathfrak{x}, d\mathfrak{y})\,\Big\{\, e^{(f'(\rho)-\lambda)\mathfrak{y}} \;-\; e^{(f'(\rho)-\lambda)\mathfrak{x}}\,\Big\}\,(\mathfrak{y} - \mathfrak{x}\,) \\
&=\; -\,\frac{1}{2}\,\int_{\mathcal{E}\times\mathcal{E}} m_{\Xi(\rho)}(d\mathfrak{x})\, r_\lambda(\mathfrak{x}, d\mathfrak{y})\,\Big\{\, e^{(f'(\rho)-\lambda)(\mathfrak{y}-\mathfrak{x})} \;-\; 1\,\Big\}\,(\mathfrak{y} - \mathfrak{x}\,)\,.
\end{aligned}$$

Therefore, as $z\,[e^z - 1] > 0$ for $z \neq 0$,

$$[\,f'(\rho) - \lambda\,]\,(\,\mathcal{M}^{\mathrm{bd}}_{\lambda,\rho}\,)'\,(0) \;<\; 0 \tag{2.16}$$

if $f'(\rho) \neq \lambda$. This proves (2.15).

We conclude this section proving a last relation for $\mathcal{M}_{\lambda,\rho}$. We claim that

$$\mathcal{M}_{\lambda,\rho}\big(\,f'(\rho) - f'(p)\,\big) \;=\; \mathcal{M}_{\lambda,\rho}\big(\,f'(p) - \lambda\,\big) \tag{2.17}$$

for all λ, ρ and p.

Identity (2.17) asserts that the bulk-cost (in the sense of Remark 2.4) of changing the boundary chemical potential from λ to $\lambda + 2\,[f'(\rho) - f'(p)]$ is equal to the one of changing it from λ to $2\,f'(p) - \lambda$.

We turn to the proof of (2.17). By the definition (2.4) of $\mathcal{M}_{\lambda,\rho}$ and since $\Xi(\rho) = f'(\rho)$, the left-hand side of (2.17) is equal to

$$\frac{1}{Z(f'(\rho))}\,\int_{\mathcal{E}} e^{f'(p)\,\mathfrak{x} \,-\, H(\mathfrak{x})}\,(\mathcal{L}_\lambda U_q)(\mathfrak{x})\;\mathfrak{n}(d\mathfrak{x}) \;=\; \frac{Z(\lambda)}{Z(f'(\rho))}\,\int_{\mathcal{E}} U_{q'}(\mathfrak{x})\,(\mathcal{L}_\lambda U_q)(\mathfrak{x})\;m_\lambda(d\mathfrak{x})\,,$$

where $q = f'(\rho) - f'(p)$, $q' = f'(p) - \lambda$. As the measure m_λ is reversible for the dynamics induced by $\mathcal{L}_\lambda$, the previous expression is equal to

$$\frac{Z(\lambda)}{Z(f'(\rho))} \int_{\mathcal{E}} U_q(\mathfrak{x})\, (\mathcal{L}_\lambda U_{q'})(\mathfrak{x})\, m_\lambda(d\mathfrak{x}) \;=\; \int_{\mathcal{E}} U_{q''}(\mathfrak{x})\, (\mathcal{L}_\lambda U_{q'})(\mathfrak{x})\, m_{f'(\rho)}(d\mathfrak{x})\,,$$

where $q'' = \lambda - f'(p) = -\,q'$. This completes the proof of (2.17), as $q' = f'(p) - \lambda$.

Note that (2.11) follows from (2.17), but we used here the reversibility of m_λ, while this assumption is not needed in the derivation of (2.11) presented above.

3. The Hamiltonian formalism

In this section, we present the thermodynamic description of non-equilibrium driven diffusive systems in mild contact with reservoirs. The definitions below are motivated and supported by the microscopic dynamics reviewed in Section 2 and in the appendices.

Recall that Ω stands for the bounded domain of $\mathbb{R}^d$ occupied by the system. The macroscopic state of the system is described by the local density $\rho(x)$, $x \in \Omega$. At each point x, the density $\rho(x)$ takes value in a subset $\mathcal{R}$ of $\mathbb{R}$ (the set $c(\mathcal{E})$ introduced in the previous section). The system is in a mild contact with boundary reservoirs, characterized by their chemical potentials $\lambda \in \Lambda$, and under the action of an external field $E \in \mathbb{R}^d$. The evolution is characterized by an Hamiltonian.

The boundary Hamiltonian. The boundary Hamiltonian $\mathcal{H}^{\mathrm{bd}}_\lambda$ is expressed in terms of a family $m_{\lambda,\rho}$ of finite, non-negative measures on $\mathbb{R}$, indexed by the chemical potential $\lambda \in \Lambda$ and the density $\rho \in \mathcal{R}$. Let $\mathcal{M}^{\mathrm{bd}}_{\lambda,\rho} \colon \mathbb{R} \to \overline{\mathbb{R}}$ be the functional given by

$$\mathcal{M}^{\mathrm{bd}}_{\lambda,\rho}(\,p\,) \;=\; \int_{\mathbb{R}} \big(\, e^{p\,\mathfrak{x}} \;-\; 1\,\big)\, m_{\lambda,\rho}(d\mathfrak{x})\,. \tag{3.1}$$

The boundary Hamiltonian reads

$$\mathcal{H}^{\mathrm{bd}}_\lambda\big(\,\rho\,,\,F\,\big) \;:=\; \int_{\partial\Omega} \mathcal{M}^{\mathrm{bd}}_{\lambda,\rho}(\,F\,)\;\kappa\; d\mathrm{S}\,, \tag{3.2}$$

where $\kappa : \mathbb{R}^d \to \mathbb{R}_+$ is a continuous, strictly positive function wich represents the system interaction strength with the boundary, and $d\mathrm{S}$ the surface measure. By (3.2),

$$\frac{\delta \mathcal{H}^{\mathrm{bd}}_\lambda}{\delta F}(\rho, F)(x) \;=\; \kappa\,(\mathcal{M}^{\mathrm{bd}}_{\lambda,\rho})'(F(x))\,, \quad x \,\in\, \partial\Omega\,. \tag{3.3}$$

Remark 3.1. *As κ is fixed we omit from the notation the dependence of the boundary Hamiltonian $\mathcal{H}^{\mathrm{bd}}_\lambda$ on κ.*

The Hamiltonian. The evolution of the density is described by the Hamiltonian $\mathcal{H}_{E,\lambda}$ which takes the form

$$\begin{aligned} \mathcal{H}_{E,\lambda}(\rho, F) \;&=\; \mathcal{H}^{\mathrm{bulk}}_E(\rho, F) \;+\; \mathcal{H}^{\mathrm{bd}}_\lambda(\rho, F)\,, \\ \mathcal{H}^{\mathrm{bulk}}_E(\rho, F) \;&=\; -\int_\Omega D(\rho)\,\nabla\rho\,\cdot\,\nabla F\; dx \;+\; \int_\Omega \sigma(\rho)\,\big\{\, E \,+\, \nabla F\,\big\}\,\cdot\,\nabla F\; dx\,. \end{aligned} \tag{3.4}$$

The *diffusion coefficient* $D(\rho)$ and the *mobility* $\sigma(\rho)$ are $d \times d$ positive, symmetric matrices. The transport coefficients D and σ satisfy the local Einstein relation

$$D(\rho) \;=\; \sigma(\rho)\, f''(\rho) \tag{3.5}$$

where f is the equilibrium free energy of the homogeneous system. *The pair ρ, F plays the role of position and momenta*, respectively, in the Hamiltonian formalism of classical mechanics.

Remark 3.2. *While the bulk Hamiltonian is expressed in terms of two thermodynamical features, the diffusivity D and the mobility σ, the boundary Hamiltonian is written by means of a family of measures. In all examples presented at the end of the article, D and σ are scalars.*

Denote by $J_E(\rho)$ the current of the density profile ρ, given by

$$J_E(\rho) \;=\; -\, D(\rho)\,\nabla\rho \;+\; \sigma(\rho)\,E\,, \tag{3.6}$$

Remark 3.3. *In* [7]*, the bulk Hamiltonian is defined by*

$$\mathcal{H}_E^{\mathrm{bulk}}(\rho, F) \;=\; \int_\Omega \big\{\, \nabla F \,\cdot\, \sigma(\rho)\,\nabla F \;-\; F\,\nabla\,\cdot\, J_E(\rho)\,\big\}\, dx\,, \tag{3.7}$$

Of course, one could adopt this formulation, and modify accordingly the boundary Hamiltonian to take into account the new term resulting from the integration by parts.

However, if one adopts the definition (3.7)*, the boundary Hamiltonian will contain terms with the derivative of ρ. This is not the case with the definition adopted here. The boundary Hamiltonian, given in equation* (3.2)*, only contains terms with ρ, and not its derivative.*

From a microscopic point of view, the definition (3.2) *is more natural* [20, 12]*. Moreover, in the proof of the large deviations, it is possible to show that density profiles with infinite energy can be discarded, and one can restrict the analysis to density profiles with generalized derivatives in L^2. As these profiles are Lipschitz continuous in dimension* 1*, the value of the profile at the boundary is well defined. In contrast, it is not clear how to define the value of the derivative of a profile at the boundary.*

Properties of the boundary Hamiltonian. We assume that for all λ and ρ,

$$\mathcal{M}_{\lambda,\rho}^{\mathrm{bd}}(\, f'(\rho) - \lambda\,) \;=\; 0\,. \tag{3.8}$$

This is property (2.11) of the previous section. We assume, furthermore, that

$$\begin{gathered}\frac{\delta\mathcal{H}_\lambda^{\mathrm{bd}}}{\delta\rho}(\rho,0) \;=\; 0 \;\text{ for all } \rho\,, \quad [\, f'(\rho) \,-\, \lambda\,]\,\frac{\delta\mathcal{H}_\lambda^{\mathrm{bd}}}{\delta F}(\rho,0) \;\le\; 0\,,\\ \text{and that } \;\frac{\delta\mathcal{H}_\lambda^{\mathrm{bd}}}{\delta F}(\rho,0) \;=\; 0 \;\text{ if and only if }\; f'(\rho) \;=\; \lambda\,.\end{gathered} \tag{3.9}$$

The second and third conditions correspond to (2.14), (2.15) and (2.16) since, by (3.3), $(\delta\mathcal{H}_\lambda^{\mathrm{bd}}/\delta F)(\rho,0) = \kappa\,(\mathcal{M}_{\lambda,\rho}^{\mathrm{bd}})'(0)$. Note that the inequality is strict if $f'(\rho) \neq \lambda$ in view of the last property.

We turn to the assertion in (3.9) concerning the derivative $\delta\mathcal{H}_\lambda^{\mathrm{bd}}/\delta\rho$. By the definition (3.2) of the boundary Hamiltonian, by equation (2.1) for the generator and (2.2) for the measure,

$$\frac{\delta\mathcal{H}_\lambda^{\mathrm{bd}}}{\delta\rho}(\rho, F) \;=\; \kappa\,\Xi'(\rho)\,\Big\{\, \big\langle\, \mathfrak{x}\, e^{-p\,\mathfrak{x}}\,,\, \mathcal{L}_\lambda\, e^{p\mathfrak{x}}\,\big\rangle_{m_{\Xi(\rho)}} \;-\; A(\rho)\,\big\langle\, \mathfrak{x}\, e^{-p\,\mathfrak{x}}\,,\, \mathcal{L}_\lambda\, e^{p\mathfrak{x}}\,\big\rangle_{m_{\Xi(\rho)}}\,\Big\}\,,$$

where $A(\rho) = Z'(\Xi(\rho))/Z(\Xi(\rho))$ and p has to be replaced by F at the end of the computation. Hence, at $p = F = 0$, since $\mathcal{L}_\lambda 1 = 0$, this expression vanishes, as claimed in (3.9).

Hamilton's equation of motion. The evolution of the pair (ρ, F) is described by the Hamilton's equation:

$$\partial_t \rho \;=\; \frac{\delta \mathcal{H}_{E,\lambda}}{\delta F}\;, \quad \partial_t F \;=\; -\,\frac{\delta \mathcal{H}_{E,\lambda}}{\delta \rho}\;.$$

The explicit formula for the Hamiltonian (3.4), the divergence theorem and the symmetry of the matrix D yield the pair of equations

$$\begin{cases} \partial_t u \;=\; -\,\nabla\cdot J_E(u) \;-\; 2\,\nabla\cdot\big\{\sigma(u)\,\nabla F\,\big\}\,, \\ \partial_t F \;=\; -\,\mathbf{Tr}\,\big[\,D(u)\,\mathrm{Hess}\,F\,\big] \;-\; \sigma'(u)\,\big[\,E \,+\, \nabla F\,\big]\,\cdot\,\nabla F\,. \end{cases}$$

Here, J_E is the current, introduced in (3.6), Hess F stands for the Hessian matrix of F and $\mathbf{Tr}A$ for the trace of a matrix A. These equations are complemented with the boundary conditions

$$\begin{cases} \big\{J_E(u) \;+\; 2\,\sigma(u)\,\nabla F\,\big\}\cdot \boldsymbol{n} \;=\; -\,\frac{\delta \mathcal{H}^{\mathrm{bd}}_\lambda}{\delta F}(u,F)\,, \\ D(u)\,\nabla F\cdot \boldsymbol{n} \;=\; \frac{\delta \mathcal{H}^{\mathrm{bd}}_\lambda}{\delta \rho}(u,F)\,, \end{cases}$$

where $\boldsymbol{n}$ stands for the outer normal vector to $\partial\Omega$.

These equations are derived by taking the time derivative of the equation $\mathcal{H}_{E,\lambda}(u_t, F_t) = C_0$ and integrating by parts. By (3.9), the pair $(u(t), 0)$ is a solution for Hamilton's equation of motion provided u solves the hydrodynamic equation

$$\begin{cases} \partial_t u \;+\; \nabla\cdot J_E(u) \;=\; 0\,, \\ J_E(u)\cdot \boldsymbol{n} \;=\; -\,\frac{\delta \mathcal{H}^{\mathrm{bd}}_\lambda}{\delta F}(u,0)\,\Big(\;=\; -\kappa\,(\mathcal{M}^{\mathrm{bd}}_{\lambda,u})'(0)\,\Big)\,. \end{cases} \tag{3.10}$$

The last identity follows from (3.3).

Remark 3.4. *Letting $\kappa \to 0, +\infty$ yield to Neumann boundary conditions, $J_E(u)\cdot \boldsymbol{n} = 0$, and Dirichlet boundary conditions, $(\mathcal{M}^{\mathrm{bd}}_{\lambda,u})'(0) = 0$, respectively.*

Remark 3.5. *Equation* (2.13) *provides an alternative formula for the current at the boundary for the solutions of the hydrodynamic equation* (3.10). *By* (3.3) *and* (2.13),

$$\frac{\delta \mathcal{H}^{\mathrm{bd}}_\lambda}{\delta F}(\rho,0) \;=\; \kappa\,\langle\, 1\,,\, \mathcal{L}_\lambda\,\mathfrak{x}\,\rangle_{m_{\Xi(\rho)}}\,.$$

By (3.10), *the left-hand side of this equation (with a minus sign) is equal to the value of the current at the boundary. Therefore, the current at the boundary of the solutions of the hydrodynamic equation can also be written as $-\,\kappa\,\langle\, 1\,,\, \mathcal{L}_\lambda\,\mathfrak{x}\,\rangle_{m_{\Xi(\rho)}}$.*

Assume that equation (3.10) admits a unique stationary solution, denoted by $\bar\rho_{E,\lambda}$. It solves the elliptic equation

$$\begin{cases} \nabla\cdot\, J_E(\rho) \;=\; 0\,, \\ J_E(\rho)\cdot \boldsymbol{n} \;=\; -\,\frac{\delta \mathcal{H}^{\mathrm{bd}}_\lambda}{\delta F}(\rho,0)\,. \end{cases} \tag{3.11}$$

Assume, furthermore, that $\bar\rho_{E,\lambda}$ is an attractor for the dynamical system induced by (3.10). Therefore, if $u^{(\rho)}(t)$ represents the solution of the hydrodynamic equation (3.10) with initial condition ρ, $u^{(\rho)}(0,\cdot) = \rho(\cdot)$, for every density profile γ,

$$\lim_{t\to\infty} u^{(\gamma)}(t) \;=\; \bar\rho_{E,\lambda}\,. \tag{3.12}$$

The action functional. Denote by $\mathcal{L}_{E,\lambda}$ the Lagrangian associated to the Hamiltonian $\mathcal{H}_{E,\lambda}$: For a density profile ρ and a function G,

$$\mathcal{L}_{E,\lambda}(\rho, G) \;=\; \sup_{F} \Big\{ \int_{\Omega} G\, F\, dx \;-\; \mathcal{H}_{E,\lambda}(\rho, F) \Big\}\,. \tag{3.13}$$

The action functional on an interval $[T_1, T_2]$, denoted by $I^{E,\lambda}_{[T_1,T_2]}$, is given by

$$I^{E,\lambda}_{[T_1,T_2]}(u) \;=\; \int_{T_1}^{T_2} \mathcal{L}_{E,\lambda}(u(t), \partial_t u(t))\, dt\,, \tag{3.14}$$

for a trajectory $u(t)$ (for each $t \geq 0$, $u(t)$ is a density profile). The action functional indicates the cost of a path $u(t)$ in a time interval.

The quasi-potential. The quasi-potential associated to the Hamiltonian $\mathcal{H}_{E,\lambda}$, represented by $V_{E,\lambda}$, is given by

$$V_{E,\lambda}(\gamma) \;=\; \inf_{u}\, I^{E,\lambda}_{(-\infty,0]}(u)\,, \tag{3.15}$$

where the infimum is carried over all paths $u(t)$ starting from the attractor $\bar\rho_{E,\lambda}$ and ending at γ: $\lim_{t\to-\infty} u(t) = \bar\rho_{E,\lambda}$, $u(0) = \gamma$. The quasi-potential $V_{E,\lambda}(\gamma)$ measures the minimal cost to produce a density profile γ starting from the stationary profile $\bar\rho_{E,\lambda}$.

Hamilton-Jacobi equation. Classical arguments in mechanics [1] imply that the quasi-potential $V_{E,\lambda}$ solves the Hamilton-Jacobi equation

$$\mathcal{H}_{E,\lambda}\Big(\rho\,, \frac{\delta V_{E,\lambda}}{\delta\rho}(\rho)\Big) \;=\; 0\,. \tag{3.16}$$

The equilibrium quasi-potential. A state (E,λ) is said to be an *equilibrium state* if

$$J_E(\bar\rho_{E,\lambda}) \;=\; 0\,. \tag{3.17}$$

In this case, by (3.6) and the Einstein relation (3.5), and by (3.11) and (3.9),

$$E \;=\; \nabla f'(\bar\rho_{E,\lambda}) \;\text{ on }\; \Omega \;\text{ and }\; f'(\bar\rho_{E,\lambda}) \;=\; \lambda \;\text{ on }\; \partial\Omega\,. \tag{3.18}$$

Note that the equilibrium states in the case of strong and mild interactions with the reservoirs are the same.

Remark 3.6. *By* (3.11) *and* (3.9)*, in non-equilibrium,* $f'(\bar\rho_{E,\lambda}) \neq \lambda$ *at the boundary. This is in sharp contrast with diffusive systems in strong interaction with reservoirs, where* $f'(\bar\rho_{E,\lambda}) = \lambda$ *at the boundary* [6, 8].

We claim that in equilibrium,

$$\frac{\delta V_{E,\lambda}}{\delta\rho}(\rho) \;=\; f'(\rho) \;-\; f'(\bar\rho_{E,\lambda})\,, \tag{3.19}$$

so that

$$V_{E,\lambda}(\rho) \;=\; \int_{\Omega} \big\{\, f(\rho) - f(\bar\rho_{E,\lambda}) - f'(\bar\rho_{E,\lambda})\,\big(\rho - \bar\rho_{E,\lambda}\big)\,\big\}\, dx\,. \tag{3.20}$$

We turn to the derivation of (3.19). Since $J_E(\bar\rho_{E,\lambda}) = 0$, by (3.18), we may replace on the right-hand side of (3.4) E by $\nabla f'(\bar\rho_{E,\lambda})$ to get that

$$\mathcal{H}^{\mathrm{bulk}}_E\big(\,\rho\,,\, f'(\rho) - f'(\bar\rho_{E,\lambda})\,\big) \;=\; -\int_{\Omega} D(\rho)\,\nabla\rho\cdot\nabla F\, dx \;+\; \int_{\Omega} \sigma(\rho)\,\nabla f'(\rho)\,\cdot\nabla F\, dx\,,$$

where $F = f'(\rho) - f'(\bar\rho_{E,\lambda})$. By Einstein relation (3.5), we conclude that the right-hand side vanishes.

On the other hand, by (3.18) and (3.8),

$$\mathcal{H}^{\mathrm{bd}}_\lambda\big(\,\rho\,,\,f'(\rho)-f'(\bar\rho_{E,\lambda})\,\big) \;=\; \mathcal{H}^{\mathrm{bd}}_\lambda\big(\,\rho\,,\,f'(\rho)-\lambda\,\big) \;=\; 0\,.$$

It follows from the two previous displayed equation that $f'(\rho) - f'(\bar\rho_{E,\lambda})$ solves the Hamilton-Jacobi equation, proving claim (3.19).

The adjoint Hamiltonian. The Hamiltonian introduced at the beginning of this section derives from an underlying microscopic dynamics. Denote by $\mathbb{P}^*_{\mathrm{st}}$ the probability measure describing the stationary evolution of the time-reversed process, which is still a Markovian dynamics. We refer to $\mathbb{P}^*_{\mathrm{st}}$ as the adjoint dynamics. The reader finds in section 1 of [4] a detailed description of the adjoint dynamics of a Markov process.

Assume that the empirical density of the adjoint dynamics satisfies a large deviations principle described by a Hamiltonian $\mathcal{H}^\dagger_{E,\lambda}$ of the same nature as $\mathcal{H}_{E,\lambda}$. Denote by $\mathcal{L}^\dagger_{E,\lambda}$ the Lagrangian corresponding to the Hamiltonian $\mathcal{H}^\dagger_{E,\lambda}$.

Fix $T>0$ and a trajectory $u(t)$, $0\le t\le T$. Let $v(t) = u(-t)$. By equation (2.2) in [4],

$$V_{E,\lambda}(u(0)) + \int_0^T \mathcal{L}^\dagger_{E,\lambda}(\,u(t)\,,\,\partial_t u(t)\,)\,dt \;=\; V_{E,\lambda}(u(T)) + \int_{-T}^0 \mathcal{L}_{E,\lambda}(\,v(t)\,,\,\partial_t v(t)\,)\,dt\,.$$

Dividing this identity by T and letting $T\to 0$ yields that

$$\mathcal{L}^\dagger_{E,\lambda}(\,u(0)\,,\,\partial_t u(0)\,) \;=\; \mathcal{L}_{E,\lambda}(\,v(0)\,,\,\partial_t v(0)\,) \;+\; \frac{\delta V_{E,\lambda}}{\delta\rho}(u(0))\,\partial_t u(0)\,.$$

Since $v(0) = u(0)$ and $\partial_t v(0) = -\,\partial_t u(0)$, for all ρ, γ,

$$\mathcal{L}^\dagger_{E,\lambda}(\,\rho,\gamma\,) \;=\; \mathcal{L}_{E,\lambda}(\,\rho,-\gamma\,) \;+\; \frac{\delta V_{E,\lambda}}{\delta\rho}(\rho)\,\gamma\,. \tag{3.21}$$

As the Hamiltonian is the convex conjugate of the Lagrangian, an elementary computation yields that

$$\mathcal{H}^\dagger_{E,\lambda}(\,\rho,F\,) \;=\; \mathcal{H}_{E,\lambda}\Big(\,\rho\,,\,\frac{\delta V_{E,\lambda}}{\delta\rho}(\rho) \,-\, F\,\Big)\,. \tag{3.22}$$

This formula coincides with equation (4.15) presented in [7] for the adjoint Hamiltonian in the case of strong boundary interactions.

The adjoint Hamiltonian $\mathcal{H}^\dagger_{E,\lambda}$ plays a central role in the macroscopic fluctuation theory. It is shown in [12] that the solution of the variational problem (3.15), which defines the quasi-potential, is the time-reversed trajectory of the Hamilton's equation of motion induced by the adjoint Hamiltonian.

Set $\mathcal{H}^{\dagger,\mathrm{bulk}}_{E,\lambda}(\,\rho,F\,) \;=\; \mathcal{H}^{\mathrm{bulk}}_E(\,\rho\,,\,\mathcal{V}(\rho) \,-\, F\,)$, where $\mathcal{V}(\rho) = (\delta V_{E,\lambda}/\delta\rho)(\rho)$ and define $\mathcal{H}^{\dagger,\mathrm{bd}}_{E,\lambda}$ in a similar way. Note that $\mathcal{H}^{\dagger,\mathrm{bulk}}_{E,\lambda}$ depends on the chemical potential λ because so does the quasi-potential $V_{E,\lambda}$.

The adjoint current. In view of the definition (3.6) of the current, the bulk Hamiltonian $\mathcal{H}^{\mathrm{bulk}}_E$ can be expressed as

$$\mathcal{H}^{\mathrm{bulk}}_E(\rho,F) \;=\; \int_\Omega J_E(\rho)\,\cdot\,\nabla F\,dx \;+\; \int_\Omega \nabla F\,\cdot\,\sigma(\rho)\,\nabla F\,dx\,. \tag{3.23}$$

By (3.22), with the bulk Hamiltonian instead of the full one,

$$\mathcal{H}^{\dagger,\mathrm{bulk}}_{E,\lambda}(\,\rho, F\,) \;=\; \int_\Omega J^\dagger_{E,\lambda}(\rho)\,\cdot\,\nabla F\,dx \;+\; \int_\Omega \nabla F\,\cdot\,\sigma(\rho)\,\nabla F\,dx \\ +\; \int_\Omega \Big\{\, J_E(\rho) \,+\, \sigma(\rho)\,\nabla\,\frac{\delta V_{E,\lambda}}{\delta\rho}\,(\rho)\,\Big\}\cdot\nabla\,\frac{\delta V_{E,\lambda}}{\delta\rho}\,(\rho)\,dx\;,$$

provided we set

$$J^\dagger_{E,\lambda}(\rho) \;=\; -\,J_E(\rho) \;-\; 2\,\sigma(\rho)\,\nabla\,\frac{\delta V_{E,\lambda}}{\delta\rho}\,(\rho)\,\cdot \tag{3.24}$$

Hence, as a function of the second variable, up to an additive constant, the adjoint bulk Hamiltonian has the same structure as the original one, provided we replace the current $J_E(\rho)$ by $J^\dagger_{E,\lambda}(\rho)$. As observed before, $J^\dagger_{E,\lambda}$ depends on λ because so does the quasi-potential $V_{E,\lambda}$.

The adjoint hydrodynamic equation. Computing the derivatives of the adjoint Hamiltonian yields that $(u(t),0)$ is a solution of the adjoint Hamilton's equations provided $u(t)$ solves the equation

$$\begin{cases} \partial_t u \;+\; \nabla\cdot J^\dagger_{E,\lambda}(u) \;=\; 0\;, \\ J^\dagger_{E,\lambda}(u)\cdot\boldsymbol{n} \;=\; \dfrac{\delta\mathcal{H}^{\mathrm{bd}}_\lambda}{\delta F}\Big(\,u, \dfrac{\delta V_{E,\lambda}}{\delta\rho}\,(u)\,\Big)\;, \end{cases} \tag{3.25}$$

called, hereafter, the adjoint hydrodynamic equation.

Currents. In view of (3.24), it is natural to define the symmetric and anti-symmetric currents, denoted by $J^s_{E,\lambda}(\rho)$, $J^a_{E,\lambda}(\rho)$, respectively, as

$$J^s_{E,\lambda}(\rho) \;=\; -\,\sigma(\rho)\,\nabla\frac{\delta V_{E,\lambda}}{\delta\rho}(\rho)\;,\quad J^a_{E,\lambda}(\rho) \;=\; (1/2)\,\big\{\,J_E(\rho) \;-\; J^\dagger_{E,\lambda}(\rho)\,\big\}\;. \tag{3.26}$$

The Hamilton-Jacobi equation provides an orthogonality relation between the symmetric and anti-symmetric currents. In equation (3.23), replace F by $\delta V_{E,\lambda}/\delta\rho$ and recall the definition of the symmetric current to express the second term on the right-hand side of (3.23) as a function of $J^s_{E,\lambda}(\rho)$. As $J_E(\rho) = J^s_{E,\lambda}(\rho) + J^a_{E,\lambda}(\rho)$,

$$\mathcal{H}^{\mathrm{bulk}}_E\big(\,\rho\,,\,\frac{\delta V_{E,\lambda}}{\delta\rho}(\rho)\,\big) \;=\; -\int_\Omega J^a_{E,\lambda}(\rho)\cdot\frac{1}{\sigma(\rho)}\,J^s_{E,\lambda}(\rho)\,dx\;.$$

In particular, the Hamilton-Jacobi equation (3.16) becomes an orthogonality relation between the anti-symmetric and the symmetric currents:

$$\int_\Omega J^a_{E,\lambda}(\rho)\cdot\frac{1}{\sigma(\rho)}\,J^s_{E,\lambda}(\rho)\,dx \;=\; \mathcal{H}^{\mathrm{bd}}_\lambda\big(\,\rho\,,\,\frac{\delta V_{E,\lambda}}{\delta\rho}(\rho)\,\big) \;=\int_{\partial\Omega}\mathcal{M}^{\mathrm{bd}}_{\lambda,\rho}\big(\,\frac{\delta V_{E,\lambda}}{\delta\rho}(\rho)\,\big)\;\kappa\;dS\;. \tag{3.27}$$

Remark 3.7. *In the case of strong boundary interactions, it has been shown that the symmetric and the asymmetric currents satisfy an orthogonality relation (see equation (4.5) in* [8] *and equation (2.22) in* [7]*). This orthogonality relation is fundamental in the proof of the Clausius inequality for the renormalized work in* [7].

It would be interesting to obtain a similar relation in the present context. In order to achieve this, one would need to write the right-hand side of (3.27) *as the scalar product of the symmetric boundary current with the anti-symmetric one.*

This would permit to interpret equation (3.27) *as an orthogonality relation between the symmetric and the anti-symmetric current. We were not able to.*

4. A formula for the quasi-potential

In few cases, it is possible to derive an explicit formula for the quasi-potential. Assume that $d = 1$ and that there is no external field, $E = 0$. Then, for each density ρ,

$$\frac{\delta V_{E,\lambda}}{\delta \rho} \;=\; f'(\rho) \;-\; f'(F) \tag{4.1}$$

is a solution of the Hamilton-Jacobi equation provided F solves the equation

$$\begin{cases} \Delta f'(F) \;+\; \dfrac{\sigma(\rho) - \sigma(F)}{d(\rho) - d(F)} \, |\, \nabla f'(F)\, |^2 \;=\; 0\,, \\ [\, d(\rho) - d(F)\,]\, \nabla f'(F) \cdot \boldsymbol{n} \;=\; \kappa\, \mathcal{M}^{\mathrm{bd}}_{\lambda,\rho}\big(\, f'(\rho) \;-\; f'(F)\,\big)\,. \end{cases} \tag{4.2}$$

In this formula, d is the primitive of D: $d'(\rho) = D(\rho)$.

The proof of this claim is similar to the one presented in [4]. Let $\Gamma = f'(\rho) - f'(F)$, recall the definition of the bulk Hamiltonian and the Einstein relation (3.5) to get that

$$\begin{aligned} \mathcal{H}^{\mathrm{bulk}}_E\big(\,\rho\,,\,\Gamma\,\big) \;&=\; \int_\Omega \sigma(\rho)\, \nabla\Gamma \cdot \nabla\Gamma \; dx \;-\; \int_\Omega \sigma(\rho) \nabla f'(\rho) \;\cdot\; \nabla\Gamma \; dx \\ &=\; -\int_\Omega \sigma(\rho)\, \nabla f'(\rho) \cdot \nabla f'(F) \; dx \;+\; \int_\Omega \sigma(\rho)\, |\, \nabla f'(F)\, |^2 \; dx\,. \end{aligned}$$

By Einstein relation (3.5), and since d is a primitive of D, $\sigma(\rho)\, \nabla f'(\rho) = D(\rho)\, \nabla\rho = \nabla d(\rho)$. Therefore, the first term on the right-hand side can be written as

$$-\int_\Omega \big[\, \nabla d(\rho) \;-\; \nabla d(F)\,\big] \cdot \nabla f'(F) \; dx \;-\; \int_\Omega \nabla d(F) \cdot \nabla f'(F) \; dx\,.$$

By the divergence theorem and since $\nabla d(F) \;=\; \sigma(F)\, \nabla f'(F)$, this expression is equal to

$$\int_\Omega \big[\, d(\rho) - d(F)\,\big]\, \Delta f'(F) \; dx - \int_{\partial\Omega} \big[\, d(\rho) - d(F)\,\big]\, \nabla f'(F) \cdot \boldsymbol{n} \; dS - \int_\Omega \sigma(F)\, |\, \nabla f'(F)\, |^2 \; dx\,.$$

By (3.2) and (4.2), the expression appearing in second integral is equal to $\mathcal{H}^{\mathrm{bd}}_\lambda(\,\rho\,,\, f'(\rho) - f'(F))$

Up to this point, we proved that

$$\mathcal{H}_{E,\lambda}\big(\,\rho\,,\,\Gamma\,\big) \;=\; \int_\Omega \big[\, d(\rho) \;-\; d(F)\,\big]\, \Delta f'(F) \; dx \;+\; \int_\Omega \big[\, \sigma(\rho) \;-\; \sigma(F)\,\big]\, |\, \nabla f'(F)\, |^2 \; dx\,.$$

On the left-hand side, the bulk Hamiltonian appearing at the beginning of the computation has been replaced by the full one in view of the last observation of the previous paragraph. The right-hand side vanishes in view of the first equation in (4.2). This completes the proof of the claim.

It has been proved in [12] that for symmetric exclusion processes in mild contact with reservoirs the quasi-potential is given by (4.1). For zero-range models, this is also easy to check since in this case even in nonequilibrium the stationary states are product measures. Actually, when σ is constant (as in Ginzburg-Landau dynamics) or $\sigma = d$ (as in zero-range dynamics), the first equation in (4.2) becomes autonomous in F.

Remark 4.1. *For the one-dimensional exclusion process and the zero-range dynamics, the boundary conditions of equation* (4.2) *coincide with the ones of equation* (3.11)*. That is, the boundary conditions for the stationary density profile in equation* (3.11) *and the ones for the auxiliary function F in equation* (4.2) *coincide. This is the also case for interacting particle systems in strong interaction with the boundary reservoirs, where the boundary conditions are of Dirichlet type* [17, 4].

To derive the identity of the boundary conditions, observe that by the Einstein relation and since $J_E(F) = -D(F)\nabla F$, the boundary condition in (4.2) *can be restated as*

$$J(F)\cdot \boldsymbol{n} \;=\; -\,\kappa\,\frac{\sigma(F)}{d(\rho)-d(F)}\;\mathcal{M}^{\mathrm{bd}}_{\lambda,\rho}\big(\,f'(\rho)\;-\;f'(F)\,\big)\;.$$

For zero-range and exclusion dynamics, a computation, presented at the appendix, yields that for all μ, ϱ and p

$$\frac{\sigma(p)}{d(\varrho)-d(p)}\;\mathcal{M}^{\mathrm{bd}}_{\mu,\varrho}\big(\,f'(\varrho)\;-\;f'(p)\,\big)\;=\;\big(\,\mathcal{M}^{\mathrm{bd}}_{\mu,p}\,\big)'(0)\;. \tag{4.3}$$

This proves that the boundary condition in (4.2) *and* (3.11) *coincide in view of* (3.3)*. Therefore, in these examples equation* (4.2) *becomes*

$$\begin{cases} \Delta f'(F)\;+\;\dfrac{\sigma(\rho)-\sigma(F)}{d(\rho)-d(F)}\,|\,\nabla f'(F)\,|^2\;=\;0\;, \\ J(F)\cdot\boldsymbol{n}\;=\;-\,\kappa\,(\mathcal{M}^{\mathrm{bd}}_{\lambda,F})'(0)\;. \end{cases} \tag{4.4}$$

Note that the left-hand side of (4.3) *depends on ϱ, while the right-hand side does not.*

Remark 4.2. *Contrarily, for the KMP model, the boundary conditions of equation* (4.2) *are different from the ones of equation* (3.11)*. The equation for the auxiliary function is presented in* (C.4)*. This is in sharp contrast with the case of strong interaction with the boundary, where the boundary conditions coincide.*

Remark 4.3. *Equation* (2.17) *provides an identity for the term $\mathcal{M}^{\mathrm{bd}}_{\mu,\varrho}(\,f'(\varrho)\;-\;f'(p)\,)$ which holds under the general hypotheses of Section 2.*

Remark 4.4 (Boundary conditions for the quasi-potential)**.** *When the system interacts strongly with the boundary reservoirs, the boundary equations for the hydrodynamic equation and for the adjoint hydrodynamic equation are of Dirichlet type. For this reason, one may restrict the investigation of the quasi-potential to density profiles which satisfy Dirichlet boundary conditions. Since the boundary conditions for the auxiliary function F, introduced in* (4.1)*, are also of Dirichlet type, in view of* (4.1)*, one concludes that the functional derivative of the quasi-potential vanishes at the boundary when computed at a density profile.*

For systems in mild interaction with the boundary, the situation is completely different. The boundary conditions for the hydrodynamic and the adjoint hydrodynamic equations, equations (3.10) *and* (3.25)*, respectively, are different. There are no reasons to restrict the attention to particular density profiles. But even considering profiles which satisfy the Robin boundary conditions appearing in* (3.10) *and* (3.11)*, we were not able to derive boundary conditions for the functional derivative of the quasi-potential computed at fixed density profiles. We did not push this investigation too much as we did not need an equation for the boundary condition of the functional derivative of the quasi-potential in our analysis.*

In terms of the auxiliary function F, the currents take the form

$$J^s_{0,\lambda}(\rho) \;=\; J(\rho) \;+\; \sigma(\rho)\,\nabla f'(F)\,, \quad J^a_{0,\lambda}(\rho) \;=\; -\,\sigma(\rho)\,\nabla f'(F)\,,$$
$$J^\dagger_{0,\lambda}(\rho) \;=\; J(\rho) \;+\; 2\,\sigma(\rho)\,\nabla f'(F)\,.$$

Orthogonal relation for the currents. Assume that the matrix $D(\rho)$ is a scalar and that the external field E vanishes. We keep E in the notation though it vanishes. Recall the representation (4.1) for the quasi-potential. By the Einstein relation (3.5),

$$J^s_{E,\lambda}(\rho) \;=\; -\,D(\rho)\,\nabla\rho \;+\; \sigma(\rho)\,\nabla f'(F) \;=\; J_E(\rho) \;+\; \sigma(\rho)\,\nabla f'(F)\,.$$

Therefore, $J^a_{E,\lambda}(\rho) \;=\; -\,\sigma(\rho)\,\nabla f'(F)$. Keep in mind that $E=0$ although it remains in the notation. By this formula for the anti-symmetric current and the second equation in (4.2) the orthogonality relation (3.27) can be written as

$$\int_\Omega J^a_{E,\lambda}(\rho)\cdot\frac{1}{\sigma(\rho)}\,J^s_{E,\lambda}(\rho)\,dx \;+\; \int_{\partial\Omega}\frac{d(\rho)-d(F)}{\sigma(\rho)}\,J^a_{E,\lambda}(\rho)\cdot\boldsymbol{n}\,dS \;=\; 0\,. \tag{4.5}$$

5. A Clausius inequality

Fix a time-dependent chemical potential $\lambda(t,x)$ and external field $E(t,x)$. For a density profile ρ, let $u(t,x)$ be the solution of

$$\begin{cases} \partial_t u \;+\; \nabla\cdot J_{E(t)}(u) \;=\; 0\,, \\ J_{E(t)}(u)\cdot\boldsymbol{n} \;=\; -\,\dfrac{\delta\mathcal{H}^{\mathrm{bd}}_{\lambda(t)}}{\delta F}(u,0)\,, \\ u(0,\cdot) \;=\; \rho(\cdot)\,, \end{cases} \tag{5.1}$$

where $J_{E(t)}(u)$ is given by (3.6) with $u(t)$, $E(t)$ replacing ρ, E, respectively.

The energy exchanged between the system and the external reservoirs and fields in the time interval $[0,T]$ is given by

$$W_{[0,T]}(\lambda(\cdot),E(\cdot),\rho)$$
$$:=\; \int_0^T\Big\{-\int_{\partial\Omega}\lambda(t,x)\,j(t,x)\cdot\boldsymbol{n}(x)\,d\mathrm{S}(x) \;+\; \int_\Omega j(t,x)\cdot E(t,x)\,dx\Big\}\,dt\,,$$

where $j(t,x) \;=\; J_{E(t)}(u(t))\,(x)$ is the current of profile $u(t,\cdot)$. The first term on the right-hand side is the energy provided by the reservoirs while the second is the energy provided by the external field. We claim that

$$W_{[0,T]}(\lambda(\cdot),E(\cdot),\rho) \;\geq\; F(u(T)) \;-\; F(\rho)\,, \tag{5.2}$$

where F is the equilibrium free energy functional defined by

$$F(\rho) \;:=\; \int_\Omega f(\rho(x))\,dx\,. \tag{5.3}$$

Indeed, dropping from the notation the dependence on x, adding and subtracting $f'(u(t))$ in the boundary term, rewrite the energy exchanged as

$$W_{[0,T]}(\lambda(\cdot),E(\cdot),\rho) \;=\; -\int_0^T dt\int_{\partial\Omega}[\lambda(t)-f'(u(t))]\,j(t)\cdot\boldsymbol{n}\,dS$$
$$+\int_0^T dt\Big\{-\int_{\partial\Omega}f'(u(t))\,j(t)\cdot\boldsymbol{n}\,dS \;+\; \int_\Omega j(t)\cdot E(t)\,dx\Big\}\,.$$

By the divergence theorem, the right-hand side is equal to

$$\begin{aligned} & - \int_0^T dt \int_{\partial\Omega} [\lambda(t) - f'(u(t))]\; j(t) \cdot \boldsymbol{n}\; dS \\ & \quad + \int_0^T dt \int_\Omega \big\{ - \nabla \cdot \big[f'(u(t))\, j(t) \big] + j(t) \cdot E(t) \big\}\; dx \;. \end{aligned} \tag{5.4}$$

Recall from (2.12) the definition of the functional $\mathfrak{A}_\lambda(\rho, \cdot\,)$, copied here for the reader's convenience:

$$\mathfrak{A}_\lambda(\rho, p) \;=\; \kappa \Big\{ \mathcal{M}^{\mathrm{bd}}_{\lambda,\rho}(p) \;-\; \mathcal{M}^{\mathrm{bd}}_{\lambda,\rho}(0) \;-\; p\, (\, \mathcal{M}^{\mathrm{bd}}_{\lambda,\rho}\,)'(0) \Big\} \;. \tag{5.5}$$

It has been shown in Section 2 that $\mathfrak{A}_\lambda$ is positive and that close to zero it behaves quadratically in the second variable:

$$\mathfrak{A}_\lambda(\rho, p) \;\geq\; 0 \;, \quad \mathfrak{A}_\lambda(\rho, p) \;\approx\; p^2 \;,\;\; p \to 0 \;, \tag{5.6}$$

for all ρ.

By the boundary conditions in (5.1) and (3.3),

$$-\, [\, \lambda(t) \;-\; f'(u(t))\,]\; j(t) \cdot \boldsymbol{n} \;=\; \kappa\, [\, \lambda(t) \;-\; f'(u(t))\,]\, (\, \mathcal{M}^{\mathrm{bd}}_{\lambda(t),u(t)}\,)'(0) \;.$$

Since $\mathcal{M}^{\mathrm{bd}}_{\lambda,\rho}(0) = 0$ and, by (3.8), $\mathcal{M}^{\mathrm{bd}}_{\lambda,\rho}(\, f'(\rho) \;-\; \lambda\,) = 0$ this expression is equal to

$$\kappa \Big\{ \mathcal{M}^{\mathrm{bd}}_{\lambda(t),u(t)}(p) \;-\; \mathcal{M}^{\mathrm{bd}}_{\lambda(t),u(t)}(0) \;-\; p\, (\, \mathcal{M}^{\mathrm{bd}}_{\lambda(t),u(t)}\,)'(0) \Big\} \;=\; \mathfrak{A}_{\lambda(t)}(u(t), p) \;,$$

for $p = f'(u(t)) \;-\; \lambda(t)$. Therefore, the first term in (5.4) can be written as

$$\int_0^T dt \int_{\partial\Omega} \mathfrak{A}_{\lambda(t)}(\, u(t)\,,\, f'(u(t)) - \lambda(t)\,)\; dS \;.$$

By (5.6), this expression is positive. On the other hand, the second term of (5.4) is equal to

$$\begin{aligned} & \int_0^T dt \int_\Omega \big[\; - f'(u(t))\, \nabla \cdot j(t) \;-\; f''(u(t))\, \nabla u(t) \cdot j(t) \;+\; j(t) \cdot E(t) \,\big]\; dx \\ & \quad = \; \int_0^T dt\, \frac{d}{dt} \int_\Omega f(u(t))\; dx \;+\; \int_0^T dt \int_\Omega j(t) \cdot \sigma(u(t))^{-1} j(t)\; dx \;, \end{aligned}$$

where we used the Einstein relation (3.5), and the definition (3.6) of the current $j(t) = J_{E(t)}(u(t))$. In conclusion, we proved that

$$\begin{aligned} W_{[0,T]}(\lambda(\cdot), E(\cdot), \rho) \;&=\; F(u(T)) - F(\rho) \;+\; \int_0^T dt \int_\Omega j(t) \cdot \sigma(u(t))^{-1} j(t)\; dx \\ & \quad + \; \int_0^T dt \int_{\partial\Omega} \mathfrak{A}_{\lambda(t)}(\, u(t)\,,\, f'(u(t)) - \lambda(t)\,)\; dS \;. \end{aligned} \tag{5.7}$$

Since the last two term are positive, inequality (5.2) follows.

This argument provides a dynamic derivation of the second law of thermodynamics as expressed by the Clausius inequality (5.2). The key ingredients have been the assumption of local equilibrium together with the local Einstein relationship (3.5).

6. Transformation along equilibrium states

In this section, we examine transformations along equilibrium states. Recall from (3.17) that equilibrium states are characterized by the absence of current at stationarity: $J(\bar\rho_{E,\lambda}) = 0$.

Reversible and quasi static transformations. Fix $T > 0$, and two equilibrium states (E_0, λ_0), (E_1, λ_1) so that

$$J(\bar\rho_{E_0,\lambda_0}) \;=\; J(\bar\rho_{E_1,\lambda_1}) \;=\; 0\,. \tag{6.1}$$

Consider a system initially in the state $\bar\rho_0 = \bar\rho_{E_0,\lambda_0}$ which is driven to a new state $\bar\rho_1 = \bar\rho_{E_1,\lambda_1}$ by changing the chemical potential and the external field in time in a way that $(E(t),\lambda(t)) = (E_0,\lambda_0)$ for $t \le 0$ and $(E(t),\lambda(t)) = (E_1,\lambda_1)$ for $t \ge T$. This transformation from $\bar\rho_0$ to $\bar\rho_1$ is called *reversible* if the energy exchanged with the reservoirs is minimal. A basic thermodynamic principle asserts that reversible transformation are accomplished by a sequence of equilibrium states and are well approximated by *quasistatic* transformations, transformations in which the variation of the thermodynamical variables is very slow so that the density profile at time $u(t)$ is very close to the stationary profile $\bar\rho_{E(t),\lambda(t)}$.

Let $u(t,x)$, $t \ge 0$, $x \in \Omega$, be the solution of (5.1) with initial condition $\rho = \bar\rho_0$. Recall that we denote by $j(t)$ the current at time t of the density profile $u(t)$: $j(t) = J_{E(t)}(u(t))$. Since the thermodynamical variables are equal to (E_1,λ_1) for $t \ge T$, as $t \to \infty$, $u(t)$ and the current $j(t)$ relax exponentially fast to $\bar\rho_1$ and $J_{E_1}(\bar\rho_1)$, respectively. By (6.1), $J_{E_1}(\bar\rho_1) = 0$, and, by (3.18) and (5.5), $\mathfrak{A}_{\lambda_1}(\,\bar\rho_1\,,\, f'(\bar\rho_1) - \lambda_1\,) = \mathfrak{A}_{\lambda_1}(\,\bar\rho_1\,,\,0\,) = 0$. Therefore, the integrals in (5.7) are finite as $T \to \infty$ and

$$\begin{aligned} W(\lambda(\cdot), E(\cdot), \bar\rho_0) \;&=\; F(\bar\rho_1) \;-\; F(\bar\rho_0) \;+\; \int_0^\infty dt \int_\Omega j(t)\cdot\sigma(u(t))^{-1} j(t)\, dx \\ &\quad +\; \int_0^\infty dt \int_{\partial\Omega} \mathfrak{A}_{\lambda(t)}(\,u(t)\,,\, f'(u(t)) - \lambda(t)\,)\, dS \\ &\quad \ge\; F(\bar\rho_1) \;-\; F(\bar\rho_0)\,. \end{aligned} \tag{6.2}$$

Last inequality follows from (5.6). Note that we did not assume any regularity of the thermodynamical variables in time so that they can also be discontinuous.

It remains to show that in the quasistatic limit equality is achieved in (6.2). That is the thermodynamic relation

$$W = \Delta F \tag{6.3}$$

holds, where $\Delta F = F(\bar\rho_1) - F(\bar\rho_0)$ is the variation of the free energy. If this is the case, by running the transformation backward in time, we can return to the original state exchanging the energy $-\Delta F$. For this reason the transformations for which (6.2) becomes an equality are called reversible.

However, for any fixed transformation the inequality in (6.2) is strict because the last two terms on the right-hand side of the identity in (6.2) are strictly positive. The second one is strictly positive in view of the last assertion of (3.9). Hence, reversible transformations cannot be achieved exactly. We can however exhibit a sequence of transformations for which these strictly positive terms can be made arbitrarily small. This sequence of transformations is what is called quasistatic transformations.

Fix smooth functions $\lambda(t)$, $E(t)$ such that $(\lambda(0),E(0)) = (\lambda_0,E_0)$, $(\lambda(t),E(t)) = (\lambda_1,E_1)$ for $t \ge T$. Assume that $(\lambda(t),E(t))$ are equilibrium states for all $t \ge 0$. This means that $J(\bar\rho_{\lambda(t),E(t)}) = 0$ for all $t \ge 0$. Given $\delta > 0$, set $\lambda_\delta(t) = \lambda(\delta t)$, $E_\delta(t) = E(\delta t)$. The sum of the last two terms on the right-hand side of (6.2) is

given by

$$\int_0^\infty dt \int_\Omega \{ \nabla f'(u_\delta(t)) \, - \, E_\delta(t) \} \cdot \sigma(u_\delta(t)) \{ \nabla f'(u_\delta(t)) \, - \, E_\delta(t) \} \, dx + \int_0^\infty dt \int_{\partial\Omega} \mathfrak{A}_{\lambda_\delta(t)}(u_\delta(t) \, , \, f'(u_\delta(t)) - \lambda_\delta(t)) \, dS \, ,$$

where u_δ is the solution to (5.1) with initial condition $\bar\rho_0$ and parameters $\lambda_\delta(t)$, $E_\delta(t)$.

Recall that $\bar\rho_{\lambda_\delta(t),E_\delta(t)}$ is the equilibrium state associated to the thermodynamical variables $\lambda_\delta(t)$, $E_\delta(t)$. Since $J(\bar\rho_{\lambda(t),E(t)}) = 0$, $E_\delta(t) = \nabla f'(\bar\rho_{\lambda_\delta(t),E_\delta(t)})$. Therefore, the previous expression is equal to

$$\int_0^\infty dt \int_\Omega \{ \nabla f'(u_\delta(t)) \, - \, \nabla f'(\bar\rho_{\lambda_\delta(t),E_\delta(t)}) \} \cdot \sigma(u_\delta(t)) \{ \nabla f'(u_\delta(t)) \, - \, \nabla f'(\bar\rho_{\lambda_\delta(t),E_\delta(t)}) \} \, dx + \int_0^\infty dt \int_{\partial\Omega} \mathfrak{A}_{\lambda_\delta(t)}(u_\delta(t) \, , \, f'(u_\delta(t)) - \lambda_\delta(t)) \, dS \, ,$$

The difference between the solution of the hydrodynamic equation $u_\delta(t)$ and the stationary profile $\bar\rho_{\lambda_\delta(t),E_\delta(t)}$ is of order δ uniformly in time, and so is the differences $f'(u_\delta(t)) - f'(\bar\rho_{\lambda_\delta(t),E_\delta(t)})$. As the integration over time essentially extends over an interval of length δ^{-1}, the first term of the previous expression vanishes for $\delta \to 0$. Similarly, by (5.6), $\mathfrak{A}_{\lambda_\delta(t)}(u_\delta(t) \, , \, f'(u_\delta(t)) - \lambda_\delta(t))$ is bounded by $C_0[f'(u_\delta(t)) - \lambda_\delta(t)]^2 = C_0[f'(u_\delta(t)) - f'(\bar\rho_{\lambda_\delta(t),E_\delta(t)})]^2$. Hence, the second term of the previous expression also vanishes as $\delta \to 0$.

This implies that equality in (6.2) is achieved in the limit $\delta \to 0$. Note that in the previous argument we did not use any special property of the path $\lambda(t)$ besides its smoothness in time. Otherwise, the trajectory $(E(t), \lambda(t))$ from (E_0, λ_0) to (E_1, λ_1) can be arbitrary along equilibrium states.

Excess work. Consider a transformation $(E(t), \lambda(t))$, $t \ge 0$, and an initial density profile ρ. Assume that $(E(t), \lambda(t)) \to (E_1, \lambda_1)$, as $t \to +\infty$ fast enough, where (E_1, λ_1) defines an equilibrium state (that is $J(\bar\rho_{E_1,\lambda_1}) = 0$). The *excess work* $W_{\mathrm{ex}} = W_{\mathrm{ex}}(\lambda(\cdot), E(\cdot), \rho)$ is defined as the difference between the energy exchanged between the system and the external driving and the work involved in a reversible transformation from ρ to $\bar\rho_1$, namely

$$\begin{aligned} W_{\mathrm{ex}} \, = \, W \, - \, \min W \, &= \, \int_0^\infty dt \int_\Omega j(t) \cdot \sigma(u(t))^{-1} j(t) \, dx \\ &+ \, \int_0^\infty dt \int_{\partial\Omega} \mathfrak{A}_{\lambda(t)}(u(t) \, , \, f'(u(t)) - \lambda(t)) \, dS \, , \end{aligned} \tag{6.4}$$

where we used (6.2) as well as the fact that the minimum of W is given by the right-hand side of (6.3). Observe that W_{ex} is a positive functional of the transformation $(E(t), \lambda(t))$ and the initial condition ρ. Of course, by taking a sequence of quasi-static transformations W_{ex} can be made arbitrarily small.

Relaxation path and availability. Consider an equilibrium system in the state $\bar\rho_0$, characterized by a chemical potential λ_0 and an external field E_0. This system is put in contact with reservoirs at constant chemical potential λ_1 and an external field E_1, different from the chemical potential λ_0 and the external field E_0 associated to $\bar\rho_0$. Assume that (E_1, λ_1) is an equilibrium state. For $t > 0$ the system thus evolves

according to the hydrodynamic equation (5.1) with initial condition $\bar\rho_0$, external field E_1, and boundary condition λ_1.

When $t \to +\infty$ the system relaxes to the equilibrium state $\bar\rho_1$. As the path $(E(\cdot), \lambda(\cdot))$ is constant in time, the excess work is a function of (E_1, λ_1) and $\bar\rho_0$ and we denote $W_{\mathrm{ex}}(E(\cdot), \lambda(\cdot), \bar\rho_0)$ simply by $W_{\mathrm{ex}}(E_1, \lambda_1, \bar\rho_0)$.

In view of (6.4), the constitutive equation (3.6) and (6.2), the excess work along such a path is given by

$$\begin{aligned} W_{\mathrm{ex}}(E_1, \lambda_1, \bar\rho_0) = & - \int_0^\infty dt \int_\Omega \big[\nabla f'(u(t)) - E_1\big] \cdot j(t)\, dx \\ & + \int_0^\infty dt \int_{\partial\Omega} \mathfrak{A}_{\lambda_1}(\, u(t)\,,\, f'(u(t)) - \lambda_1\,)\, dS\,. \end{aligned}$$

Since (E_1, λ_1) is an equilibrium state, $J(\bar\rho_1) = 0$, so that $\nabla f'(\bar\rho_1) = E_1$. We may thus replace E_1 by $\nabla f'(\bar\rho_1)$ in the previous equation. After an integration by parts, since $f'(\bar\rho_1) = \lambda_1$, in view of the boundary conditions of (5.1) and the definition (5.5) of $\mathfrak{A}_\lambda$, the right-hand side becomes

$$\int_0^\infty dt \int_\Omega \big[\, f'(u(t)) \,-\, f'(\bar\rho_1)\,\big]\, \nabla \cdot j(t)\, dx\,.$$

By (5.1) this expression is equal to

$$-\int_0^\infty dt \int_\Omega \big[f'(u(t)) - f'(\bar\rho_1)\big]\, \partial_t u(t)\, dx\,.$$

We have therefore shown that

$$W_{\mathrm{ex}}(E_1, \lambda_1, \bar\rho_0) = \int_\Omega \big[f(\bar\rho_0) - f(\bar\rho_1) - f'(\bar\rho_1)\big(\bar\rho_0 - \bar\rho_1\big)\big]\, dx \;=\; V_{E_1,\lambda_1}(\bar\rho_0)\,, \quad (6.5)$$

where the last identity follows from (3.20).

Note that the excess work W_{ex} is not the difference of a thermodynamic potential between the states $\bar\rho_0$ and $\bar\rho_1$. We refer to [8] and [26, Ch. 7] for a connection of this result with *availability* and the maximal useful work that can be extracted from the system.

7. Transformation along nonequilibrium states

Nonequilibrium states are characterized by the presence of a non vanishing current in the stationary density profile. Therefore, to maintain such states one needs to dissipate a positive amount of energy per unit of time. If we consider a transformation between nonequilibrium stationary states, the energy dissipated along such transformation will necessarily include the contribution needed to maintain such states. The arguments of the previous section have therefore to be modified in order to take into account this amount of energy. This issue, first raised in [25], has been more recently considered e.g. in [2, 11, 23, 24, 8, 9].

The appropriate definition of thermodynamic functionals for nonequilibrium systems is a central but difficult topic. Our starting point is the formula (5.7) for the energy exchanged in the time interval $[0, T]$ between the system and the external reservoirs and fields.

Towards a definition. Fix $T > 0$ and a nonequilibrium state (E, λ) so that $J_E(\bar\rho_{E,\lambda}) \neq 0$ and $f'(\bar\rho_{E,\lambda}) \neq \lambda$. Let $(E(t), \lambda(t)) = (E, \lambda)$, $0 \le t \le T$. By (5.7),

$$\begin{aligned} W_{[0,T]}(\lambda(\cdot), E(\cdot), \bar\rho_{E,\lambda}) \;&=\; T \int_\Omega J_E(\bar\rho_{E,\lambda}) \cdot \sigma(\bar\rho_{E,\lambda})^{-1} J_E(\bar\rho_{E,\lambda})\, dx \\ &\quad + \, T \int_{\partial\Omega} \mathfrak{A}_\lambda(\, \bar\rho_{E,\lambda}\,,\, f'(\bar\rho_{E,\lambda}) \,-\, \lambda\,)\, dS\,. \end{aligned}$$

Note that both terms on the right-hand side are strictly positive. The second one is strictly positive in view of the last assertion of (3.9) and because $f'(\bar\rho_{E,\lambda}) \neq \lambda$ at the boundary in nonequilibrium states.

To justify the definition of renormalized work proposed below, we turn back to formula (5.7) for the work. Assume that the transformation is performed along equilibrium states: $J_{E(t)}(\bar\rho_{E(t),\lambda(t)}) = 0$ for all $0 \le t \le T$.

Since, in equilibrium, the current is equal to its symmetric part, in (5.7), $j(t) = J_{E(t)}(u(t)) = J^s_{E(t),\lambda(t)}(u(t))$. On the other hand, in equilibrium, by equation (3.19), $(\delta V_{E,\lambda}/\delta\rho)(\rho) = f'(\rho) - \lambda$. Therefore, for transformations along equilibrium states, we may rewrite the work as

$$\begin{aligned} &F(u(T)) \;-\; F(\rho) \;+\; \int_0^T dt \int_\Omega J^s_{E(t),\lambda(t)}(u(t)) \cdot \sigma(u(t))^{-1} J^s_{E(t),\lambda(t)}(u(t))\, dx \\ &+ \int_0^T dt \int_{\partial\Omega} \mathfrak{A}_{\lambda(t)}\Big(\, u(t)\,,\, \frac{\delta V_{E(t),\lambda(t)}}{\delta\rho}(u(t))\,\Big)\, dS\,. \end{aligned} \tag{7.1}$$

Fix an equilibrium state (E, λ) and consider a constant transformation $(E(t), \lambda(t)) = (E, \lambda)$, $0 \le t \le T$, starting from the density profile $\bar\rho_{E,\lambda}$. Since $\bar\rho_{E,\lambda}$ minimizes the quasi-potential $V_{E,\lambda}$, $(\delta V_{E,\lambda}/\delta\rho)(\bar\rho_{E,\lambda}) = 0$. Hence, by the definition (5.5) of $\mathfrak{A}_\lambda$, $\mathfrak{A}_\lambda(\, \bar\rho_{E,\lambda}\,,\, (\delta V_{E,\lambda}/\delta\rho)\,(\bar\rho_{E,\lambda})\,) \,=\, \mathfrak{H}^{(3)}_\lambda(\, \bar\rho_{E,\lambda}\,,\, 0\,) \,=\, 0$. On the other hand, by (3.26), $J^s_{E,\lambda}(\bar\rho_{E,\lambda}) = 0$. This shows that both integrals in the previous displayed equation vanish.

This property extends to non-equilibrium states (E, λ). Indeed, since the quasi-potential $V_{E,\lambda}$ is minimal at the stationary profile, $(\delta V_{E,\lambda}/\delta\rho)\ (\bar\rho_{E,\lambda}) = 0$. Hence, by (3.26), $J^s_{E,\lambda}(\bar\rho_{E,\lambda}) = 0$, and by the reasons presented in the previous paragraph, $\mathfrak{A}_\lambda(\, \bar\rho_{E,\lambda}\,,\, 0\,) \,=\, 0$.

Renormalized work. The previous arguments support the following definition or renormalized work. Fix $T > 0$, a density profile ρ, and space-time dependent chemical potentials $\lambda(t) = \lambda(t, x)$ and external field $E(t) = E(t, x)$, $0 \le t \le T$, $x \in \Omega$. Let $u(t) = u(t, x)$, $j(t) = J_{E(t)}(u(t, x))$, $t \ge 0$, $x \in \Omega$, be the solution of the hydrodynamic equation (5.1) with initial condition ρ. Define the renormalized work $W^{\mathrm{ren}}_{[0,T]} = W^{\mathrm{ren}}_{[0,T]}(E(\cdot), \lambda(\cdot), \rho)$ performed by the reservoirs and the external field in the time interval $[0, T]$ as

$$\begin{aligned} W^{\mathrm{ren}}_{[0,T]} \;&:=\; F(u(T)) \;-\; F(\rho) \\ &\quad + \int_0^T dt \int_\Omega J^s_{E(t),\lambda(t)}(u(t)) \cdot \sigma(u(t))^{-1} J^s_{E(t),\lambda(t)}(u(t))\, dx \\ &\quad + \int_0^T dt \int_{\partial\Omega} \mathfrak{A}_{\lambda(t)}\Big(\, u(t)\,,\, \frac{\delta V_{E(t),\lambda(t)}}{\delta\rho}(u(t))\,\Big)\, dS\,. \end{aligned} \tag{7.2}$$

Remark 7.1. *In* [8]*, the renormalized work is defined by subtracting some quantities from the work. Then, taking advantage of the orthogonality between the symmetric and the anti-symmetric currents, a formula for the renormalized work similar to* (7.2) *is derived.*

Here, instead of subtracting a quantity we rather replaced in the formula of the work the equilibrium quasi-potential by the nonequilibrium one and the current by the symmetric current.

As observed in the previous subsection, the above definition of renormalized work coincides with the one of work when the states $(E(t), \lambda(t))$*,* $0 \le t \le T$*, are all equilibrium states.*

Assume that $\lambda(t), E(t)$ converge to λ_1, E_1 as $t \to +\infty$ fast enough. Let $\bar\rho_1 = \bar\rho_{E_1,\lambda_1}$ be the stationary profile associated to the pair (E_1, λ_1). Since $u(T)$ converges to $\bar\rho_1$, the symmetric part of the current, $J^s_{E(T),\lambda(T)}(u(T))$, relaxes as $T \to \infty$ to $J^s_{E_1,\lambda_1}(\bar\rho_1) = 0$ fast enough. Similarly, $[\,\delta V_{E(T),\lambda(T)}/\delta\rho\,](u(T))$ converges to $[\,\delta V_{E_1,\lambda_1}/\delta\rho\,](\bar\rho_1) = 0$. Hence, since, by (5.6), $\mathfrak{A}_\lambda$ is quadratic in the second variable, $\mathfrak{A}_{\lambda(T)}(\,u(T)\,,\,[\,\delta V_{E(T),\lambda(T)}/\delta\rho\,](u(T))\,)$ relaxes quickly to $\mathfrak{A}_{\lambda_1}(\,u(T),\,[\,\delta V_{E_1,\lambda_1}/\delta\rho\,](\bar\rho_1)\,) = \mathfrak{A}_{\lambda_1}(\,u(T)\,,\,0\,) = 0$.

Therefore, the two integrals in the previous formula are convergent as $T \to \infty$ and

$$W^{\mathrm{ren}}_{[0,T]} \;=\; F(\bar\rho_1) \;-\; F(\rho) \;+\; \int_0^\infty dt \int_{\partial\Omega} \mathfrak{A}_{\lambda(t)}\Big(\,u(t)\,,\,\frac{\delta V_{E(t),\lambda(t)}}{\delta\rho}(u(t))\,\Big)\,dS$$
$$+\;\int_0^\infty dt \int_\Omega J^s_{E(t),\lambda(t)}(u(t))\cdot\sigma(u(t))^{-1} J^s_{E(t),\lambda(t)}(u(t))\,dx\,. \tag{7.3}$$

Since, by (5.6), $\mathfrak{A}_\lambda(a,p) \ge 0$,

$$W^{\mathrm{ren}}(\,E(\cdot)\,,\,\lambda(\cdot)\,,\,\rho\,) \;\ge\; F(\bar\rho_1) \;-\; F(\rho)\,. \tag{7.4}$$

The previous equation states that the Clausius inequality holds for the renormalized work, see [23, 8].

Quasi-static transformations. As for transformations of equilibrium states, we show that, given two nonequilibrium states, there exists a sequence of transformations from the first to the second for which the last two terms on the right-hand of (7.3) can be made arbitrarily small.

Fix (E_0, λ_0) and assume that the initial profile ρ is the stationary profile associated to this pair: $\rho = \bar\rho_{E_0,\lambda_0}$. Fix $T > 0$ and choose smooth functions $\lambda(t), E(t)$, $0 \le t \le T$, such that $(E(0), \lambda(0)) = (E_0, \lambda_0)$, $(E(T), \lambda(T)) = (E_1, \lambda_1)$. For $\delta > 0$, let $(E_\delta(t), \lambda_\delta(t)) = (E(\delta t), \lambda(\delta t))$, and $u_\delta(t)$ be the solution of (5.1) with initial condition $\bar\rho_0 = \bar\rho_{E_0,\lambda_0}$, external field $E_\delta(t)$, and chemical potential $\lambda_\delta(t)$. Set $j_\delta(t) = J_{E_\delta(t)}(u_\delta(t))$. The last term on the right-hand side of (7.3) is given by

$$\int_0^\infty dt \int_\Omega J^s_{E_\delta(t),\lambda_\delta(t)}(u_\delta(t))\cdot\sigma(u_\delta(t))^{-1} J^s_{E_\delta(t),\lambda_\delta(t)}(u_\delta(t))\,dx\,.$$

For each fixed t, let $\bar\rho_\delta(t) = \bar\rho_{E_\delta(t),\lambda_\delta(t)}$ be the stationary profile associated to the driving $E_\delta(t), \lambda_\delta(t)$ with frozen t. Since $J^s_{E_\delta(t),\lambda_\delta(t)}(\bar\rho_\delta(t)) = 0$, we can rewrite the previous integral as

$$\int_0^\infty dt \int_\Omega \widehat{J}_\delta(t)\cdot\sigma(u_\delta(t))^{-1}\widehat{J}_\delta(t)\,dx\,,$$

where $\widehat{J}_\delta(t) = J^s_{E_\delta(t),\lambda_\delta(t)}(u_\delta(t)) - J^s_{E_\delta(t),\lambda_\delta(t)}(\bar\rho_\delta(t))$.

The difference between the solution of the hydrodynamic equation $u_\delta(t)$ and the stationary profile $\bar\rho_\delta(t)$ is of order δ uniformly in time, and so is the difference $J^s_{E_\delta(t),\lambda_\delta(t)}(u_\delta(t)) - J^s_{E_\delta(t),\lambda_\delta(t)}(\bar\rho_\delta(t))$. As the integration over time essentially extends over an interval of length δ^{-1}, the previous expression vanishes for $\delta \to 0$.

A similar argument can be carried out to the first integral in (7.3) because $u_\delta(t)$ is close to $\bar\rho_\delta(t)$, $[\,\delta V_{E_\delta(t),\lambda_\delta(t)}/\delta\rho\,](\bar\rho_\delta(t)) = 0$, $\mathfrak{A}_{\lambda_\delta(t)}(\,u_\delta(t)\,,\,0\,) = 0$, and $\mathfrak{A}_\lambda$ is quadratic in the second variable. This implies that equality in (7.4) is achieved in the limit $\delta \to 0$. In this argument we did not use any special property of the path $(E(t),\lambda(t))$ besides its smoothness in time, the trajectory $(E(t),\lambda(t))$ from (E_0,λ_0) to (E_1,λ_1) can be otherwise arbitrary.

Quasi static transformations thus minimize asymptotically the renormalized work and in the limit $\delta \to 0$ we obtain the nonequilibrium version of the thermodynamic relation (6.3), that is

$$W^{\mathrm{ren}} \;=\; \Delta F\,, \tag{7.5}$$

where ΔF represents the variation of the equilibrium free energy functional, $\Delta F = F(\bar\rho_1) - F(\bar\rho_0)$.

It is remarkable that the Clausius inequality and the optimality of quasi-static transformations, basic laws of equilibrium thermodynamics, admit exactly the same formulation for nonequilibrium states with the definition proposed in (7.2). By Remark 7.1, (7.4), (7.5) contain the equilibrium situations as a particular case.

Relaxation path: excess work and quasi potential. Consider at time $t = 0$ a stationary nonequilibrium profile $\bar\rho_0$ corresponding to some driving (E_0,λ_0). This system is put in contact with new reservoirs at chemical potential λ_1 and a new external field E_1. For $t > 0$ the system evolves according to the hydrodynamic equation (5.1) with initial condition $\bar\rho_0$, time independent boundary condition λ_1 and external field E_1. In particular, as $t \to \infty$ the system relaxes to $\bar\rho_1$.

Along such a path, in view of the orthogonality relation (3.27), writing J^s as $J - J^a$, the excess work is given by

$$\begin{aligned} W_{\mathrm{ex}}(E_1,\lambda_1,\bar\rho_0) \;:=\; & \int_0^\infty dt \int_{\partial\Omega} \mathfrak{A}_{\lambda_1}\Big(\,u(t)\,,\,\frac{\delta V_{E_1,\lambda_1}}{\delta\rho}(u(t))\,\Big)\,dS \\ & + \int_0^\infty dt \int_\Omega J_{E_1}(u(t))\cdot\sigma(u(t))^{-1} J^s_{E_1,\lambda_1}(u(t))\,dx \\ & - \int_0^\infty dt \int_{\partial\Omega} \mathcal{M}^{\mathrm{bd}}_{\lambda_1,u(t)}\big(\,\frac{\delta V_{E_1,\lambda_1}}{\delta\rho}(u(t))\,\big)\,\kappa\,d\mathrm{S}\,. \end{aligned}$$

By definition (3.26) of the symmetric part of the current, by an integration by parts, and by (5.1), (3.3), the second term on the right-hand side is equal to

$$\begin{aligned} & \int_0^\infty dt \int_\Omega \nabla\cdot J_{E_1}(u(t))\,\frac{\delta V_{E_1,\lambda_1}}{\delta\rho}(u(t))\,dx \\ & + \int_0^\infty dt \int_{\partial\Omega} \frac{\delta V_{E_1,\lambda_1}}{\delta\rho}(u(t))\,(\mathcal{M}^{\mathrm{bd}}_{\lambda_1,u(t)})'(0)\,\kappa\,dS\,. \end{aligned}$$

By (5.1),

$$\int_0^\infty dt \int_\Omega \nabla\cdot J_{E_1}(u(t))\,\frac{\delta V_{E_1,\lambda_1}}{\delta\rho}(u(t))\,dx \;=\; -\int_0^\infty dt \int_\Omega \partial_t u(t)\,\frac{\delta V_{E_1,\lambda_1}}{\delta\rho}(u(t))\,dx\,.$$

The right-hand side is equal to $V_{E_1,\lambda_1}(\bar\rho_0) - V_{E_1,\lambda_1}(\bar\rho_1) = V_{E_1,\lambda_1}(\bar\rho_0)$.

In conclusion, as $\mathfrak{M}^{\mathrm{bd}}_{\lambda_1,u(t)}(0) = 0$, in view of the definition (5.5) of $\mathfrak{A}_{\lambda_1}$,

$$W_{\mathrm{ex}}(E_1,\lambda_1,\bar\rho_0) \;=\; V_{E_1,\lambda_1}(\bar\rho_0) \;+\; \int_0^\infty dt \int_{\partial\Omega} \mathfrak{A}_{\lambda_1}\Big(u(t)\,,\, \frac{\delta V_{E_1,\lambda_1}}{\delta\rho}(u(t))\Big)\, dS \\ -\; \int_0^\infty dt \int_{\partial\Omega} \mathfrak{A}_{\lambda_1}\big(u(t)\,,\, \frac{\delta V_{E_1,\lambda_1}}{\delta\rho}(u(t))\big)\, d\mathrm{S}\,, \tag{7.6}$$

so that

$$W_{\mathrm{ex}}(E_1,\lambda_1,\bar\rho_0) \;=\; V_{E_1,\lambda_1}(\bar\rho_0)\,.$$

This identity extends to nonequilibrium states the relation (6.5) between the excess work and the quasi potential.

Remark 7.2. *As observed in* [8]*, the previous identity provides a characterization of the quasi-potential which does not involve large deviations.*

Appendix A. Zero range dynamics

Recall the notation introduced in Section 2. In this section, $\mathcal{E} = \mathbb{N}\cup\{0\}$ so that $c(\mathcal{E}) = [0,\infty)$. The dynamics can be informally described as follows. At each site, independently from the others, particles wait exponential times, whose parameter depends only on the number of particles at that site, and then jumps to a nearest neighboring site according to the transition probability of some random walk on Ω_N. Superimposed to this bulk dynamics, to model the effect of the reservoirs, we have creation and annihilation of particles, according to some birth and death process, at the boundary of Ω_N.

Fix a time-dependent external field $E\colon \mathbb{R}_+\times\Omega\to\mathbb{R}^d$ and chemical potential $\lambda\colon \mathbb{R}_+\times\partial\Omega\to\mathbb{R}_+$. The generator $L_{t,N}$ of the zero range process is given by

$$L_t \;=\; L^{\mathrm{bulk}}_{t,N} \;+\; L^{\mathrm{bd}}_{t,N}\,,$$

where $L^{\mathrm{bulk}}_{t,N}$ describes the bulk dynamics and $L^{\mathrm{bd}}_{t,N}$ the boundary dynamics at time t. The generator of the bulk dynamics is given by

$$(L^{\mathrm{bulk}}_{t,N} f)(\eta) \;=\; N^2 \sum_{x\in\Omega_N} \sum_{\substack{y\in\Omega_N\\ |y-x|=\varepsilon_N}} g(\eta_x)\, e^{(1/2)E(t,x)\cdot(y-x)}\, \big[\, f(\sigma^{x,y}\eta) - f(\eta)\,\big]\,.$$

In this formula, $\varepsilon_N = 1/N$ and $\sigma^{x,y}\eta$ is the configuration obtained from η by moving a particle from x to y:

$$(\sigma^{x,y}\eta)_z \;=\; \begin{cases} \eta_z & \text{if} \quad z\neq x,y \\ \eta_z - 1 & \text{if} \quad z = x \\ \eta_z + 1 & \text{if} \quad z = y\,. \end{cases} \tag{A.1}$$

The generator of the boundary dynamics is given by

$$(L^{\mathrm{bd}}_{t,N} f)(\eta) \;=\; N \sum_{x\in\Omega_N} \sum_{\substack{y\notin\Omega_N\\ |y-x|=\varepsilon_N}} g(\eta_x)\, e^{(1/2)E(t,x)\cdot(y-x)}\, \big[\, f(\sigma^{x,-}\eta) - f(\eta)\,\big] \\ +\; N \sum_{x\in\Omega_N} \sum_{\substack{y\notin\Omega_N\\ |y-x|=\varepsilon_N}} e^{\lambda(t,y)}\, e^{(1/2)E(t,y)\cdot(x-y)}\, \big[\, f(\sigma^{x,+}\eta) - f(\eta)\,\big]\,.$$

In this formula, $\sigma^{x,+}\eta$, $\sigma^{x,-}\eta$ are the configurations obtained from η by removing, adding a particle at x, respectively:

$$(\sigma^{x,\pm}\eta)_z \begin{cases} \eta_z & \text{if} \quad z \neq x \\ \eta_z \pm 1 & \text{if} \quad z = x\,. \end{cases} \tag{A.2}$$

Note that the bulk dynamics has been speeded-up by N^2, while the boundary dynamics by N. Denote by $\eta^N(t)$ the continuous-time Markov chain on Ω_N induced by the generator $L_{t,N}$ and by $\mathbb{P}_\eta^{\lambda,E}$, $\eta \in \Omega_N$, the distribution of the process $\eta^N(\cdot)$ when its initial state is η.

Stationary states. Consider the case in which the driving (λ, E) does not depend on time. As the Markov chain is irreducible, there exists a unique invariant measure, denoted by $\mu_N^{\lambda,E}$. It is remarkable that such invariant measure can be constructed explicitly and it is product, see [13] for the one dimensional case.

Denote by $\lambda_c \in \overline{\mathbb{R}}$ the radius of convergence of the series

$$Z(\lambda) \;=\; 1 \;+\; \sum_{k\geq 1} \frac{e^{\lambda k}}{g(1)\cdots g(k)} \tag{A.3}$$

For $\lambda < \lambda_c$, let m_λ be the probability measure on $\mathbb{N}$ given by

$$m_\lambda(k) \;=\; \frac{1}{Z(\lambda)}\, \frac{e^{\lambda k}}{g(1)\cdots g(k)}\,, \quad k \in \mathbb{N}\cup\{0\}\,. \tag{A.4}$$

Let $\phi_N = \phi_N^{\lambda,E} : \Omega_N \to \mathbb{R}_+$ be the unique solution of the elliptic equation

$$\begin{aligned} &N^2 \sum_{\substack{y\in\Omega_N \\ |y-x|=\varepsilon_N}} \Big\{ \phi_N(y)\, e^{(1/2)E(y)\cdot(x-y)} \;-\; \phi_N(x)\, e^{(1/2)E(x)\cdot(y-x)} \Big\} \\ &+ N \sum_{\substack{y\notin\Omega_N \\ |y-x|=\varepsilon_N}} \Big\{ \phi_N(y)\, e^{(1/2)E(y)\cdot(x-y)} \;-\; \phi_N(x)\, e^{(1/2)E(x)\cdot(y-x)} \Big\} \;=\; 0\,, \quad x\in\Omega_N\,, \end{aligned}$$

$$\phi_N(z) \;=\; e^{\lambda(z)}\,, \quad z \notin \Omega_N\,.$$

The stationary state $\mu_N^{\lambda,E}$ is the product measure on Ω_N whose marginals are given by

$$\mu_N^{\lambda,E}\{\eta : \eta_x = k\} \;=\; m_{\lambda_N(x)}(k)\,, \quad x\in\Omega_N\,,\; k\geq 0\,, \;\text{ where }\; \lambda_N(x) \;=\; \log \phi_N(x)\,.$$

In the homogeneous equilibrium state, $E = 0$ and λ constant, the solution of the elliptic equation is given by $\phi_N = \exp\{\lambda\}$ so that the invariant measure is Gibbs with Hamiltonian

$$H_N(\eta) = \sum_{x\in\Omega_N} \sum_{k=1}^{\eta_x} \log g(k)\,.$$

Bulk Hamiltonian. Recall the definition of the function R its inverse $\Xi = R^{-1}$, and the equilibrium free energy, introduced in (2.3) and below. By [5], the diffusivity and the mobility are respectively given by

$$D(\rho) \;=\; \Phi'(\rho)\,, \quad \sigma(\rho) \;=\; \Phi(\rho)\,, \;\text{ where }\; \Phi(\rho) \;=\; e^{\Xi(\rho)}\,.$$

An elementary computation yields that the Einstein relation (3.5) is fulfilled and that $f'(\rho) = \log \Phi(\rho)$. By (3.4), the bulk Hamiltonian is given by

$$\mathcal{H}_E^{\mathrm{bulk}}(\rho, F) \;=\; -\int_\Omega \Phi'(\rho)\, \nabla\rho \cdot \nabla F \, dx \;+\; \int_\Omega \Phi(\rho) \left\{ E \,+\, \nabla F \right\} \cdot \nabla F \, dx \;, \quad \text{(A.5)}$$

Boundary Hamiltonian. In view of the definition of the generator $L_{t,N}^{\mathrm{bd}}$, in the context of the zero-range process, the boundary generator $\mathcal{L}_\lambda$, $\lambda < \lambda_c$, introduced in (2.1), is given by

$$(\mathcal{L}_\lambda f)(\mathfrak{x}) \;=\; g(\mathfrak{x})\, [\, f(\mathfrak{x}-1) \,-\, f(\mathfrak{x})\,] \;+\; e^{\lambda}\, [\, f(\mathfrak{x}+1) \,-\, f(\mathfrak{x})\,] \,.$$

The boundary Hamiltonian, $\mathcal{M}_\lambda^{\mathrm{bd}} \colon (0,\infty) \times \mathbb{R} \to \mathbb{R}$, introduced in (2.4), is given by

$$\mathcal{M}_{\lambda,a}^{\mathrm{bd}}(p) \;=\; e^{\lambda}\, [e^{p} - 1] \;+\; e^{\Xi(a)}\, [e^{-p} - 1] \,. \quad \text{(A.6)}$$

Quasi-potential. Assume that the external field vanishes and fix a chemical potential λ. Recall the definition of the variable $d(\cdot)$ introduced below (4.2). In the context of zero-range processes, $d(\rho) = \Phi(\rho) = \sigma(\rho)$.

We claim that

$$\frac{\delta V_{0,\lambda}}{\delta \rho}(\rho) \;=\; f'(\rho) \;-\; f'(\bar\rho_{0,\lambda}) \,, \quad \text{(A.7)}$$

where $\bar\rho_{0,\lambda}$ the solution of (3.11). In particular, for zero-range processes, the quasi-potential has an explicit formula.

To prove (A.7), we first claim that identity (4.3) holds for zero-range processes. Since $d(\rho) = \sigma(\rho) = \Phi(\rho)$, and $f'(\rho) = \log \Phi(\rho)$, the left-hand side of (4.3) can be written as

$$\frac{\Phi(\rho)}{\Phi(\rho) - \Phi(F)} \left\{ e^{\lambda} \left[\frac{\Phi(\rho)}{\Phi(F)} \,-\, 1 \right] \,+\, \Phi(\rho) \left[\frac{\Phi(F)}{\Phi(\rho)} \,-\, 1 \right] \right\} \;=\; e^{\lambda} \,-\, \Phi(F) \,.$$

The right-hand side is equal to $(\mathcal{M}_{\lambda,F}^{\mathrm{bd}})'(0)$, proving (4.3).

Since $d(\rho) = \sigma(\rho)$, by Remark 4.1 and (4.4), in the context of zero-range processes, equation (4.2) becomes

$$\begin{cases} \Delta f'(F) \;+\; \|\nabla f'(F)\,\|^2 \;=\; 0 \,, \\ J(F)\cdot \boldsymbol{n} \;=\; -\kappa\, (\mathcal{M}_{\lambda,F}^{\mathrm{bd}})'(0) \,. \end{cases}$$

A simple algebra based on Einstein relation and the relations between mobility, diffusivity and Φ permits to rewrite the previous equation as

$$\begin{cases} \nabla \cdot J(F) \;=\; 0 \,, \\ J(F)\cdot \boldsymbol{n} \;=\; -\kappa\, (\mathcal{M}_{\lambda,F}^{\mathrm{bd}})'(0) \,. \end{cases} \quad \text{(A.8)}$$

This equation corresponds to the stationary equation (3.11). Hence, by (4.1), for zero-range dynamics, the quasi-potential is given by (A.7).

Appendix B. Exclusion processes

Recall the notation introduced in Section 2. In the context of exclusion processes, $\mathcal{E} = \{0,1\}$ so that $c(\mathcal{E}) = [0,1]$. The dynamics can be informally described as follows. Particles are distributed on Ω_N in such a way that, at each site, there is at most one particle. Each particle, independently from the others, wait a mean-one exponential random time, and then jumps to a nearest neighboring site according to the transition probability of some random walk on Ω_N. If the chosen site is

occupied by another particle, the jumps is suppressed. Superimposed to this bulk dynamics, to model the effect of the reservoir, at the boundary of Ω_N, particles are created and annihilated according to some birth and death process.

Fix a time-dependent external field $E\colon \mathbb{R}_+ \times \Omega \to \mathbb{R}^d$ and chemical potential $\lambda\colon \mathbb{R}_+ \times \partial\Omega \to \mathbb{R}_+$. The generator $L_{t,N}$ of the exclusion process is given by

$$L_{t,N} \;=\; L_{t,N}^{\mathrm{bulk}} \;+\; L_{t,N}^{\mathrm{bd}}\,, \tag{B.1}$$

where $L_{t,N}^{\mathrm{bulk}}$ describes the bulk dynamics and $L_{t,N}^{\mathrm{bd}}$ the boundary dynamics at time t. The generator of the bulk dynamics is given by

$$(L_{t,N}^{\mathrm{bulk}} f)(\eta) \;=\; N^2 \sum_{x\in\Omega_N} \sum_{\substack{y\in\Omega_N \\ |y-x|=\varepsilon_N}} \eta_x\,[\,1-\eta_y\,]\, e^{(1/2)E(t,x)\cdot(y-x)}\,\big[\, f(\sigma^{x,y}\eta) - f(\eta)\,\big]\,,$$

where $\varepsilon_N = 1/N$ and $\sigma^{x,y}\eta$ have been introduced in (A.1).

The generator of the boundary dynamics is given by

$$\begin{aligned}(L_{t,N}^{\mathrm{bd}} f)(\eta) \;=\; & N \sum_{x\in\Omega_N} \sum_{\substack{y\notin\Omega_N \\ |y-x|=\varepsilon_N}} \eta_x\, \frac{1}{1+e^{\lambda(t,y)}}\, e^{(1/2)E(t,x)\cdot(y-x)}\,\big[\, f(\sigma^{x,-}\eta) - f(\eta)\,\big] \\ & +\; N \sum_{x\in\Omega_N} \sum_{\substack{y\notin\Omega_N \\ |y-x|=\varepsilon_N}} [\,1-\eta_x\,]\, \frac{e^{\lambda(t,y)}}{1+e^{\lambda(t,y)}}\, e^{(1/2)E(t,y)\cdot(x-y)}\,\big[\, f(\sigma^{x,+}\eta) - f(\eta)\,\big]\,,\end{aligned}$$

where the configuration $\sigma^{x,\pm}\eta$ has been introduced in (A.2).

Note that the bulk dynamics has been speeded-up by N^2, while the boundary dynamics by N. Denote by $\eta^N(t)$ the continuous-time Markov chain on Ω_N induced by the generator $L_{t,N}$ and by $\mathbb{P}_\eta^{\lambda,E}$, $\eta\in\Omega_N$, the distribution of the process $\eta^N(\cdot)$ when its initial state is η.

Stationary states. Consider the case in which the driving (λ, E) does not depend on time. As the Markov chain is irreducible, there exists a unique invariant measure, denoted by $\mu_N^{\lambda,E}$. In contrast with the zero-range process, beyond the equilibrium case where the current vanishes, the stationary state $\mu_N^{\lambda,E}$ is not a product measure and exhibits long range correlations [27]. In the special case $E=0$, λ, the measure $\mu_N^{\lambda,E}$ is the product measure with Bernoulli marginals of density $e^\lambda/(1+e^\lambda)$.

Bulk Hamiltonian. By [5], the diffusivity and the mobility are respectively given by

$$D(\rho) \;=\; 1\,, \quad \sigma(\rho) \;=\; \rho\,(1-\rho)\,.$$

An elementary computation yields that the Einstein relation (3.5) is fulfilled. By (3.4), the bulk Hamiltonian is given by

$$\mathcal{H}_E^{\mathrm{bulk}}(\rho, F) \;=\; -\int_\Omega \nabla\rho\cdot\nabla F\,dx \;+\; \int_\Omega \rho\,(1-\rho)\,\big\{\, E \,+\, \nabla F\,\big\}\cdot\nabla F\,dx\,, \tag{B.2}$$

Boundary Hamiltonian. In view of the definition of the generator $L_{t,N}^{\mathrm{bd}}$, in the context of the exclusion process, the boundary generator $\mathcal{L}_\lambda$, introduced in (2.1), is given by

$$(\mathcal{L}_\lambda f)(0) \;=\; \frac{e^\lambda}{1+e^\lambda}\,[\,f(1) \,-\, f(0)\,]\,, \quad (\mathcal{L}_\lambda f)(1) \;=\; \frac{1}{1+e^\lambda}\,[\,f(0) \,-\, f(1)\,]\,.$$

The boundary Hamiltonian, $\mathcal{M}_\lambda^{\mathrm{bd}}\colon [0,1]\times\mathbb{R}\to\mathbb{R}$, introduced in (2.4), is given by

$$\mathcal{M}_{\lambda,\rho}^{\mathrm{bd}}(p) \;=\; [1-\rho]\, R(\lambda)\, [e^p-1] \;+\; \rho\, [\, 1-R(\lambda)\,]\, [e^{-p}-1]\,, \tag{B.3}$$

where $R(\lambda)$ is the mean of the measure m_λ and has been introduced in (2.3).

Quasi-potential. Assume that $d=1$, $\Omega=(0,1)$, and recall the definition of the function $d(\cdot)$ introduced below (4.2). For exclusion processes, $d(\rho)=\rho$, $f'(\rho)=\log[\rho/(1-\rho)]$. By (B.3), equation (4.3) is satisfied, and equation (4.4) takes the form

$$\begin{cases} \Delta F \;=\; (\,\rho\,-\,F\,)\,\dfrac{(\,\nabla F\,)^2}{F\,(1-F)}\,, \\ F'\cdot \boldsymbol{n} \;=\; \kappa\,[\,\varrho(\lambda)-F\,] \;\text{ at }\; x=0\,,\;\; x=1\,, \end{cases} \tag{B.4}$$

where $\varrho(\lambda)=e^\lambda/(1+e^\lambda)$. It has been shown in [12] that equation (B.4) has a unique solution. Hence, by (4.1), in dimension 1 with no external field,

$$\frac{\delta V_{0,\lambda}}{\delta\rho}(\rho) \;=\; f'(\rho) \;-\; f'(F)\,.$$

Appendix C. KMP model

Recall the notation introduced in Section 2. This time $\mathcal{E}=c(\mathcal{E})=\mathbb{R}_+$, and η_x, $x\in\Omega_N$, represents the energy at site x for the configuration η. The bulk dynamics can be informally described as follows. At each bond (x,y) in Ω_N, at exponential times, the energy of the two vertices is added and then redistributed according to a uniform measure.

Fix a time-dependent chemical potential $\lambda\colon \mathbb{R}_+\times\mathbb{R}^d\to\mathbb{R}_-$. *Note that λ takes negative values.* We adopted this convention, which might be slightly confusing, to uniformize the notation of all three models. Moreover, there is no external field. The generator $L_{t,N}$ of the KMP process is given by

$$L_t \;=\; L_{t,N}^{\mathrm{bulk}} \;+\; L_{t,N}^{\mathrm{bd}}\,,$$

where $L_{t,N}^{\mathrm{bulk}}$ describes the bulk dynamics and $L_{t,N}^{\mathrm{bd}}$ the boundary dynamics at time t. The generator of the bulk dynamics is given by

$$(L_{t,N}^{\mathrm{bulk}} f)(\eta) \;=\; N^2 \sum_{(x,y)\in\Omega_N} \int_0^1 \big[\, f(\sigma_r^{x,y}\eta) - f(\eta)\,\big]\, dr\,.$$

In this formula, the sum is performed over all unordered edges of Ω_N and $\sigma_r^{x,y}\eta$ is the configuration obtained from η by replacing η_x, η_y by $r(\eta_x+\eta_y)$, $(1-r)(\eta_x+\eta_y)$, respectively:

$$(\sigma_r^{x,y}\eta)_z \;=\; \begin{cases} \eta_z & \text{if} \quad z\neq x,y \\ r(\eta_x+\eta_y) & \text{if} \quad z=x \\ (1-r)(\eta_x+\eta_y) & \text{if} \quad z=y\,. \end{cases}$$

The generator at the boundary is given by

$$(L_{t,N}^{\mathrm{bd}} f)(\eta) \;=\; N \sum_{x\in\Omega_N} \sum_{\substack{y\notin\Omega_N \\ |y-x|=\varepsilon_N}} \int_0^\infty -\lambda(t,y)\, e^{\lambda(t,y)r}\big[\, f(\sigma_r^x\eta) - f(\eta)\,\big]\, dr\,,$$

where $\sigma_r^x\eta$ is the configuration obtained from η by replacing η_x by r:

$$(\sigma_r^x\eta)_z \;=\; \begin{cases} \eta_z & \text{if} \quad z\neq x \\ r & \text{if} \quad z=x\,. \end{cases}$$

The stationary states. Denote by m_λ, $\lambda < 0$, the distribution of an exponential random variable with mean $\tau(\lambda) = -\lambda^{-1}$. Denote by μ_N^λ the product measure on Σ_N whose marginals are given by

$$\int_{\Sigma_N} F(\eta_x)\, \mu_N^\lambda(d\eta) \;=\; \int_{\mathbb{R}_+} F(\mathfrak{x})\, m_\lambda(d\mathfrak{x})\,, \quad x \in \Omega_N\,, \quad F \in C_b(\mathbb{R})\,.$$

An elementary computation shows that μ_N^λ is a stationary state (actually, reversible) for the KMP dynamics when $\lambda(t,x)$ is constant and equal to λ. Ergodicity yields that it is the unique one.

Bulk Hamiltonian. By [5], the diffusivity and the mobility of the KMP models are given by

$$D(\rho) \;=\; 1\,, \quad \sigma(\rho) \;=\; \rho^2\,. \tag{C.1}$$

Therefore, by (3.4), the bulk Hamiltonian is given by

$$\mathcal{H}^{\mathrm{bulk}}(\rho, F) \;=\; -\int_\Omega \nabla\rho \cdot \nabla F\, dx \;+\; \int_\Omega \rho^2\, \nabla F \cdot \nabla F\, dx\,. \tag{C.2}$$

Boundary Hamiltonian. For KMP dynamics, the boundary generator $\mathcal{L}_\lambda$, $\lambda < 0$, introduced in (2.1), is given by

$$(\mathcal{L}_\lambda f)(\mathfrak{x}) \;=\; (-\lambda) \int_{\mathbb{R}_+} [\, f(\mathfrak{y}) \,-\, f(\mathfrak{x})\,]\, e^{\lambda \mathfrak{y}}\, d\mathfrak{y}\,.$$

The boundary Hamiltonian, $\mathfrak{M}^{\mathrm{bd}}_{\lambda,\rho}\colon (0, \tau^{-1}) \to \mathbb{R}$, introduced in (2.4), is given by

$$\mathfrak{M}^{\mathrm{bd}}_{\lambda,\rho}(p) \;=\; \frac{\tau}{\rho+\tau}\Big(\frac{1}{1-\tau\, p} \,-\, 1\Big) \;+\; \frac{\rho}{\rho+\tau}\Big(\frac{1}{1+\rho\, p} \,-\, 1\Big)\,. \tag{C.3}$$

Quasi-potential. Assume that $d = 1$, $\Omega = (0,1)$, and recall the definition of the function $d(\cdot)$ introduced below (4.2). For KMP dynamics, $d(\rho) = \rho$, $f'(\rho) = -(1/\rho)$, and equation (4.2) takes the form

$$\begin{cases} \Delta F \;+\; (\,\rho \,-\, F\,)\, \dfrac{(\nabla F)^2}{F^2} \;=\; 0\,, \\ \nabla F \cdot \boldsymbol{n} \;=\; \kappa\, F^2\, \dfrac{\tau - F}{\rho F - \tau\rho + \tau F}\,. \end{cases} \tag{C.4}$$

In terms of the variables $G = f'(F)$, $\gamma = f'(\rho)$, $\lambda = f'(\tau)$, the equation reads

$$\begin{cases} \Delta G \;-\; \Big(\dfrac{1}{\gamma} + \dfrac{1}{G}\Big)\, (\nabla G)^2 \;=\; 0\,, \\ \nabla G \cdot \boldsymbol{n} \;=\; \kappa\, \gamma\, \dfrac{G - \lambda}{G - \lambda - \gamma}\,. \end{cases} \tag{C.5}$$

Uniqueness of solutions of equation (C.4) has still to be proven. It has been done in [10] if the boundary conditions are replaced by Dirichlet ones. If uniqueness holds, by (4.1), the quasi-potential of the KMP model is given by

$$\frac{\delta V_{0,\lambda}}{\delta\rho}(\rho) \;=\; f'(\rho) \;-\; f'(F) \;=\; \frac{1}{F} \;-\; \frac{1}{\rho}\,.$$

Appendix D. Exclusion process with non-reversible boundary conditions

Inspired by the model introduced in [14, 15], and the works [19, 18], in this section, we present a model which do not satisfy (3.8), (3.9). This is a consequence from the fact that the stationary state induced by the boundary dynamics does not coincide with the one induced by the bulk dynamics. To concentrate on the source of the differences, we assume that there is no external field and we set $d = 1$.

Let $\Omega = (0,1)$ so that $\Omega_N = \{\epsilon_N, \dots, 1-\epsilon_N\}$, where, recall, $\epsilon_N = 1/N$. The state space and the bulk dynamics are the ones introduced in Section B with $\Omega = (0,1)$ and $E = 0$. To define the boundary dynamics we introduce a set of jump rates. Fix $\ell \geq 1$, and let $c_j^R \colon \{0,1\}^{\{-\ell,\dots,-1\}} \to \mathbb{R}_+$, $c_j^L \colon \{0,1\}^{\{1,\dots,\ell\}} \to \mathbb{R}_+$, $1 \leq j \leq \ell$ be nonnegative functions.

The generator of the boundary dynamics is given by

$$(L_{t,N}^{\mathrm{bd}} f)(\eta) \;=\; N \sum_{j=1}^{\ell} c_j^R(\tau_N \eta) \left[f(\sigma^{N-j}\eta) - f(\eta) \right] \;+\; N \sum_{j=1}^{\ell} c_j^L(\eta) \left[f(\sigma^{j}\eta) - f(\eta) \right] .$$

In this formula, $\tau_N \eta$ is the configuration η translated by N so that $(\tau_N \eta)_j = \eta_{N+j}$, $j \in \mathbb{Z}$. Moreover, the configuration $\sigma^k \eta$ stands for

$$(\sigma^k \eta)_j \begin{cases} \eta_j & \text{if} \quad j \neq k \\ 1 - \eta_k & \text{if} \quad j = k \, . \end{cases}$$

The generator L_N of the dynamics is given by (B.1), and does not depend on time.

The model introduced above embraces the exclusion process introduced in Section B with no external field (to incorporate the chemical potential, it is enough to let the jump rates $c_j^{R,L}$ to depend on λ). It also encompasses the current reservoir model considered by De Masi et al. [14, 15] and the exclusion models with nonreversible boundary dynamics examined in [19, 18].

Bulk $\times$ Boundary dynamics. In contrast with the previous models, here particles are created and annihilated at more than one site in the bulk of Ω_N, and according to different rates which depend on the environment. For this reason, the boundary dynamics can not be represented by a one-site dynamics as in (2.1). The state space is here $\{0,1\}^{\{1,\dots,\ell\}}$ instead of $\{0,1\}$ as in the exclusion dynamics of Section B.

Consider a neighborhood $\{N-k, \dots, N-1\}$ of the right boundary. The stationary state of the bulk dynamics restricted to this set (we forbid exchange of particles between $N-k-1$ an $N-k$) is the uniform measure over all configurations with a fixed number of particles. For k large, by the equivalence of ensembles, locally this measure is close to a Bernoulli product measure with some fixed density.

Unless in very special cases, the stationary state on $\{N-\ell, \dots, N-1\}$ induced by the generator $L_{t,N}^{\mathrm{bd}}$ introduced above is not a Bernoulli product measure. When this does not happen, there is a conflict between the bulk dynamics, which drives the system towards a Bernoulli product measure, and the bulk dynamics, which propels the system to another stationary state. As the bulk dynamics is accelerated by N^2, while the boundary dynamics is speeded-up by N, the bulk dynamics wins and the state of the system at the boundary is close the a Bernoulli product measure. In particular, local equilibrium occurs and the entropy method to derive the hydrodynamic behavior can be applied [18].

One can also, up to technical obstacles, prove a large deviations principle and derive a formula for the Hamiltonian. A rigorous proof of this statement is not yet available.

Stationary states. Assume that the Markov chain induced by the generator L_N is irreducible. This is the case, for example, if one of the jump rates of each side of the set Ω_N is strictly positive. In this case, there exists a unique invariant measure, denoted by μ_N. Except in exceptional cases, the stationary state is not a product measure and not known explicitly.

Bulk Hamiltonian. The bulk Hamiltonian is the one presented in (B.2).

Boundary Hamiltonian. Since the boundary of Ω consists of two points, $\partial\Omega = \{0,1\}$, the surface integral becomes a sum and the boundary Hamiltonian reads

$$\mathcal{H}^{\mathrm{bd}}\big(\,\rho\,,\,F\,\big) \;:=\; \mathcal{M}_\rho^{\mathrm{bd},0}(\,F\,)\,\kappa(0) \;+\; \mathcal{M}_\rho^{\mathrm{bd},1}(\,F\,)\,\kappa(1)\,,$$

where

$$\mathcal{M}_\rho^{\mathrm{bd},1}(p) \;=\; \sum_{j=1}^{\ell} E_{\nu_\rho}\Big[\, c_j^R(\eta)\;\big[\, e^{p(1-2\eta_{-j})}-1\,\big]\,\Big]\,,$$

$$\mathcal{M}_\rho^{\mathrm{bd},0}(p) \;=\; \sum_{j=1}^{\ell} E_{\nu_\rho}\Big[\, c_j^L(\eta)\;\big[\, e^{p(1-2\eta_{j})}-1\,\big]\,\Big]\,.$$

In this formula, ν_ρ represents the Bernoulli product measure with density ρ. These expressions can be written as in (B.3). For $k = 0,\, 1$,

$$\mathcal{M}_\rho^{\mathrm{bd,k}}(p) \;=\; [1-\rho]\,R_k^+(\rho)\,[e^p-1] \;+\; \rho\,R_k^-(\rho)\,[e^{-p}-1]\,, \tag{D.1}$$

where

$$R_1^+(\rho) \;=\; \sum_{j=1}^{\ell} E_{\nu_\rho}\big[\, c_{+,j}^R(\eta)\,\big]\,, \quad R_1^-(\rho) \;=\; \sum_{j=1}^{\ell} E_{\nu_\rho}\big[\, c_{-,j}^R(\eta)\,\big]\,.$$

Here, $c_{\pm,j}^R(\eta) = c_j^R(\eta^{\pm,-j})$, and $\eta^{\pm,-j}$ is the configuration which coincides with η at all sites but $-j$, and at $-j$ takes the value $[1-(\pm 1)]/2$: $(\eta^{-,-j})_{-j} = 1$ and $(\eta^{+,-j})_{-j} = 0$. A similar formula holds for $R_0^\pm(\rho)$.

What does not hold for this model. The proof of (3.8) presented in Section 2 requires the boundary dynamics to be stationary with respect the measure induced by the bulk dynamics, a property which does not hold here. In consequence, the arguments presented in Section 3 to show that in equilibrium the boundary density satisfies the identity $f'(\rho) = \lambda$ do not apply. Relation (3.8) is also used below (5.6) to rewrite the boundary term in (5.4) as an integral of the functional $\mathfrak{A}_\lambda$. In particular, the proof of Clausius inequality does not apply to this model.

This means that few assertions made in this article remain valid for this model which deserves further investigations.

Quasi-potential. An explicit formula for the quasi-potential, similar to (B.4), is an open problem for this model.

Remark D.1. *The equilibrium stationary states of the microscopic dynamics presented in these appendices are all product measures. It should be possible to extend this theory to one-dimensional Ising models under the Kawasaki dynamics in mild contact with boundary reservoirs. The technical difficulty lies in the fact that these models are non-gradient* [22, Chapter 7].

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References

[1] V. I. Arnol'd: *Mathematical methods of classical mechanics*, second edition, Springer-Verlag, New York, 1989.
[2] M. Baiesi, C. Maes, B. Wynants: Fluctuations and response of nonequilibrium states. Phys. Rev. Lett. **103**, 010602 (2009).
[3] R. Baldasso, O. Menezes, A. Neumann, R. R. Souza: Exclusion process with slow boundary. J. Stat. Phys. **167**, 1112–1142 (2017).
[4] L. Bertini, A. De Sole, D. Gabrielli, G. Jona-Lasinio, and C. Landim, Macroscopic fluctuation theory for stationary non equilibrium state, J. Statist. Phys. **107**, 635–675 (2002).
[5] L. Bertini, A. De Sole, D. Gabrielli, G. Jona-Lasinio, C. Landim; Large deviation approach to non equilibrium processes in stochastic lattice gases. Bol. Soc. Brasil. Mat. (N.S.) **37**, 611 –643 (2006).
[6] L. Bertini, A. De Sole, D. Gabrielli, G. Jona-Lasinio, C. Landim; Towards a nonequilibrium thermodynamics: a self-contained macroscopic description of driven diffusive systems. J. Stat. Phys. **135**, 857–872 (2009).
[7] L. Bertini, A. De Sole, D. Gabrielli, G. Jona-Lasinio, C. Landim; Macroscopic fluctuation theory. Rev. Modern Phys. **87**, 593–636 (2015).
[8] L. Bertini, D. Gabrielli, G. Jona-Lasinio, and C. Landim: Thermodynamic transformations of nonequilibrium states. J. Statist. Phys. **149**, 773–802 (2012).
[9] L. Bertini, D. Gabrielli, G. Jona-Lasinio, C. Landim; Clausius inequality and optimality of quasi static transformations for nonequilibrium stationary states. Phys. Rev. Lett. **110**, 020601 (2013)
[10] L. Bertini, D. Gabrielli, J. L. Lebowitz: Large deviations for a stochastic model of heat flow. J. Statist. Phys. **121**, 843–885, (2005).
[11] E. Boksenbojm, C. Maes, K. Netočný, J. Pešek: Heat capacity in nonequilibrium steady states. Europhys. Lett. EPL **96**, 40001 (2011).
[12] A. Bouley, C. Erignoux, C. Landim: Steady state large deviations for one-dimensional, symmetric exclusion processes in weak contact with reservoirs. arXiv:2107.06606 (2021)
[13] De Masi A., Ferrari P.; A remark on the hydrodynamics of the zero-range processes. J. Stat. Phys. **36**, 81–87 (1984).
[14] A. De Masi, E. Presutti, D. Tsagkarogiannis, M. E. Vares: Current Reservoirs in the Simple Exclusion Process. J Stat Phys **144**, 1151–1170 (2011).
[15] A. De Masi, E. Presutti, D. Tsagkarogiannis, M. E. Vares: Non-equilibrium Stationary States in the Symmetric Simple Exclusion with Births and Deaths. J Stat Phys **147**, 519–528 (2012). https://doi.org/10.1007/s10955-012-0481-2
[16] B. Derrida, O. Hirschberg, T Sadhu: Large deviations in the symmetric simple exclusion process with slow boundaries. J. Stat. Phys. (2021) doi.org/10.1007/s10955-020-02680-3
[17] B. Derrida, J. L. Lebowitz, E. R. Speer: Large deviation of the density profile in the steady state of the open symmetric simple exclusion process. J. Stat. Phys. **107**, 599–634 (2002).

[18] C. Erignoux, P. Gonçalves, G. Nahum: Hydrodynamics for SSEP with non-reversible slow boundary dynamics: Part I, the critical regime and beyond. J Stat Phys **181**, 1433–1469 (2020). https://doi.org/10.1007/s10955-020-02633-w
[19] C. Erignoux, C. Landim, T. Xu: Stationary states of boundary driven exclusion processes with nonreversible boundary dynamics. J. Stat. Phys. **171**, 599–631 (2018).
[20] T. Franco, P. Gonçalves, C. Landim, A. Neumann: Dynamical large deviations for boundary driven symmetric exclusion processes in weak contact with reservoirs. arXiv:2203.14417 (2022)
[21] S. Friedli, Y. Velenik: *Statistical Mechanics of Lattice Systems: A Concrete Mathematical Introduction* Cambridge University Press, 2017.
[22] C. Kipnis, C. Landim *Scaling limits of interacting particle systems.* Springer-Verlag, Berlin, 1999.
[23] T. Komatsu, N. Nakagawa: Expression for the stationary distribution in nonequilibrium steady states. Phys. Rev. Lett. **100**, 030601 (2008).
[24] T. Komatsu, N. Nakagawa, S. Sasa, H. Tasaki: Entropy and nonlinear nonequilibrium thermodynamic relation for heat conducting steady states. J. Stat. Phys. **142**, 127–153 (2011).
[25] Y. Oono, M. Paniconi: Steady state thermodynamics. Dynamic organization of fluctuations (Nishinomiya, 1997). Progr. Theoret. Phys. Suppl. **130**, 29–44 (1998).
[26] A. B.Pippard: *Elements of classical thermodynamics for advanced students of physics.* Cambridge University Press, New York 1957.
[27] H. Spohn: Long range correlations for stochastic lattice gases in a nonequilibrium steady state. J. Phys. A **16**, 4275–4291 (1983).
[28] S. R. S. Varadhan: *Large deviations and applications.* Society for Industrial and Applied Mathematics, 1984.

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