# Large deviations for a stochastic model of heat flow

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Dedicated to Mitchell Feigenbaum on the Occasion of His Sixtieth Birthday

**Abstract**

We investigate a one dimensional chain of $2N$ harmonic oscillators in which neighboring sites have their energies redistributed randomly. The sites $-N$ and $N$ are in contact with thermal reservoirs at different temperature $\tau_-$ and $\tau_+$. Kipnis, Marchioro, and Presutti [18] proved that this model satisfies Fourier's law and that in the hydrodynamical scaling limit, when $N \to \infty$, the stationary state has a linear energy density profile $\bar{\theta}(u)$, $u \in [-1, 1]$. We derive the large deviation function $S(\theta(u))$ for the probability of finding, in the stationary state, a profile $\theta(u)$ different from $\bar{\theta}(u)$. The function $S(\theta)$ has striking similarities to, but also large differences from, the corresponding one of the symmetric exclusion process. Like the latter it is nonlocal and satisfies a variational equation. Unlike the latter it is not convex and the Gaussian normal fluctuations are enhanced rather than suppressed compared to the local equilibrium state. We also briefly discuss more general model and find the features common in these two and other models whose $S(\theta)$ is known.

**Keywords:** Stationary non reversible states, Large deviations, Boundary driven stochastic systems.

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# 1. Introduction

The properties of systems maintained in stationary nonequilibrium states (SNS) by contacts with very large (formally infinite) thermal reservoirs in different equilibrium states are of great theoretical and practical importance. These are arguably the simplest examples of nonequilibrium systems to which the elegant, universal, and successful formalism of equilibrium statistical mechanics might hopefully be extended. A striking universal feature of equilibrium systems is the Boltzmann–Einstein relation according to which fluctuations in macroscopic observables, arising from the grainy microscopic structure of matter, can be described fully in terms of the macroscopic thermodynamic functions (entropy, free energy) without any recourse to the microscopic theory. In trying to develop a similar formalism for SNS we have to start with the fluctuations. There has therefore been much effort devoted to developing a mathematically rigorous fluctuation theory for simple model SNS. This has led to some interesting recent results for conservative systems in contact with particle reservoirs at different chemical potentials [4–7, 10–12].

In particular it has been possible to obtain explicitly the large deviation functionals (LDF) for some one dimensional lattice systems. The internal dynamics of these systems is governed by simple exclusion processes, symmetric (SEP) or asymmetric (ASEP), while the entrance and exit of particles at the two boundaries are prescribed by the chemical potentials, $\lambda_\pm$, of the right and left reservoirs. The LDF gives the logarithm of the probabilities of finding macroscopic density profiles $\rho(u)$, where $u$ is the macroscopic space variable, different from the typical values $\bar{\rho}(u)$; namely we have $\mathrm{Prob}(\rho(u)) \sim \exp\{-N\mathcal{F}(\rho)\}$ where $N$ is the number of lattice sites.

In the symmetric case, the situation we shall be primarily concerned with here, the typical profile $\bar{\rho}(u)$ is given by the stationary solution of the diffusion equation $\partial_t \rho(t,u) = (1/2)\partial_u\big(D\partial_u\rho(t,u)\big)$, $u \in [-1,1]$ with boundary conditions $\bar{\rho}(\pm 1) = \rho_\pm$. The values $\rho_\pm$ correspond to the densities in an equilibrium system with chemical potentials $\lambda_\pm$. The latter can be obtained by setting the chemical potential of both end reservoirs equal to each other, $\lambda_+ = \lambda_-$. We note that in this equilibrium case, the function $\mathcal{F}$ is simply related to the free energy of the system. For $\rho_+ \neq \rho_-$ and constant diffusion coefficient $D$ (that is density independent and spatially uniform) the profile $\bar{\rho}(u)$ is linear; this is the only case solved so far for the SEP. The results for the LDF of the SEP for this SNS contained some surprises.

The most striking of these is non–locality: the probability of density profiles $\rho_A(u)$ and $\rho_B(u)$ in disjoint macroscopic regions $A$ and $B$ is not given by a product of the separate probabilities, i.e. the LDF is not additive. This is very different from the equilibrium case where the LDF is given (essentially) by an integral of the local free energy density for the specified profiles $\rho_A(u)$ and $\rho_B(u)$, and is thus automatically additive over macroscopic regions (even at critical points). Additivity is also true for the LDF of a system in full local thermal equilibrium (LTE), e.g. for the stationary nonequilibrium state of the zero range process. The microscopic origin of the non–locality of the LDF for the open SEP lies in the $O(N^{-1})$ corrections to LTE which extend over distances of $O(N)$; $N$ is number of lattice sites, which goes to infinity in the hydrodynamical scaling limit [1, 24]. So while the deviations from LTE vanish in this limit their contributions to the LDF, which involves summations over regions of size $N$, does not

The effect of these $O(N^{-1})$ corrections to LTE is already present at the level of Gaussian fluctuations about $\bar{\rho}(u)$. These were computed by Spohn in 1983 [24] who found that the contributions from the deviations from LTE made a finite contribution to the variance of these Gaussian fluctuations, causing them to decrease, for the SNS of the SEP from their LTE values. The reduction in the variance of Gaussian fluctuations can be recovered from the LDF by setting $\rho(u) = \bar{\rho}(u) + N^{-1/2}\phi(u)$. In fact in [5,11] it is shown that $\mathcal{F}(\rho)$ for the SEP dominates the LDF coming from the corresponding LTE state and therefore the fluctuations are suppressed.

The above observations about the SEP raise many questions about the nature of the SNS of more realistic systems. Do their LDF and Gaussian fluctuations behave similarly to those of the SEP? In particular, to what extent do the LDF for SNS play a "similar role" to free energies in equilibrium systems? In the absence of more solved examples it is difficult to answer these questions. It is therefore useful to find and investigate the SNS of other model systems for which the LDF can be found and compare them to that of the SEP. This is what we do in the present paper and then discuss the limited universality of the results.

The SNS we consider here is a simple stochastic model of heat conduction in a crystal. It is well known, see e.g. [20,23], that harmonic chains do not obey Fourier's law of heat conduction. On the other hand, Kipnis, Marchioro, and Presutti [18] introduced a model of mechanically uncoupled harmonic oscillators in which nearest neighbor oscillators redistribute randomly their energy. This system is then coupled to thermal reservoirs at different temperatures and, thanks to the stochastic dynamics, the validity of Fourier's law is proven. In particular the stationary energy density $\bar{\theta}(u)$ is a linear profile as in the SEP. We mention that a more sophisticated stochastic model of coupled harmonic oscillators has been recently investigated. The evolution is given by superimposing the Hamiltonian dynamics with a stochastic one in which two nearest oscillators randomly exchange momenta. This model has two conservations laws (energy and total length); the hydrodynamic limit is proven in [2] for the equilibrium case and in [3] for nonequilibrium, Gaussian fluctuations are analyzed in [16].

In this paper we consider the Kipnis–Marchioro–Presutti model, our main result is the derivation of the corresponding LDF, that we denote by $S(\theta)$. It turns out that this function has both strong similarities and significant differences from that of the SEP. Like for the SEP the LDF is nonlocal and yields Gaussian fluctuations about $\bar{\theta}(u)$. Unlike the SEP, however, it is obtained by minimization, rather than maximization, of a "proto LDF" and the variance is increased compared to that obtained from LTE. Also in contrast to the SEP the LDF, $S(\theta)$, is not convex. We discuss these similarities and differences in section 7, where we also give some generalization of our and previous results to a larger class of model systems.

## 2. The model and main result

Following [18] we consider a chain of one–dimensional harmonic oscillators located at sites $x \in [-N, N] \cap \mathbb{Z} =: \Lambda_N$ and described by the canonical coordinates $(q_x, p_x)$. The oscillators are mechanically uncoupled so that the Hamiltonian of the chain is $H = \sum_{x\in\Lambda_N}(p_x^2 + q_x^2)/2$. The harmonic oscillators are however coupled by the following stochastic dynamics. Every pair of nearest neighbors sites waits an exponential time of rate one and then the corresponding oscillators exchange energy. More precisely, let $(q_y, p_y)$, $(q_{y+1}, p_{y+1})$ be the canonical coordinates at the sites $y$, $y+1$; when the exponential clock between $y$ and $y+1$ rings then the new values $(q'_y, p'_y)$, $(q'_{y+1}, p'_{y+1})$ are distributed according to the uniform distribution on the surface of constant energy

$$\frac{1}{2}\big[(q'_y)^2 + (p'_y)^2\big] + \frac{1}{2}\big[(q'_{y+1})^2 + (p'_{y+1})^2\big] = \frac{1}{2}\big[q_y^2 + p_y^2\big] + \frac{1}{2}\big[q_{y+1}^2 + p_{y+1}^2\big]$$

Moreover the boundary site $-N$, respectively $+N$, waits an exponential time of rate one and then the corresponding oscillator assume an energy distributed according to a Gibbs distribution with temperature $\tau_-$, respectively $\tau_+$. All the exponential clocks involved in the dynamics are independent.

From a mathematical point of view it is sufficient to look only at the local energy given by the random variables $\xi_x := \big(p_x^2 + q_x^2\big)/2$, for which we get a closed evolution described by the following Markov process. The state space is $\Sigma_N := \mathbb{R}_+^{\Lambda_N}$, an element of $\Sigma_N$ is denoted by $\xi := \{\xi_x \,,\, x \in \Lambda_N\}$. The infinitesimal generator of the process is the sum of a bulk generator $L_0$ plus two boundary generators $L_+$ and $L_-$

$$L_N := N^2\big[L_0 + L_- + L_+\big] \tag{2.1}$$

in which we have speeded up the time by the factor $N^2$, this corresponds to the diffusive scaling.

The bulk dynamics $L_0$ is defined as

$$L_0 := \sum_{x=-N}^{N-1} L_{x,x+1}$$

where

$$L_{x,x+1} f(\xi) := \int_0^1 dp\, \big[f(\xi^{(x,x+1),p}) - f(\xi)\big] \tag{2.2}$$

in which the configuration $\xi^{(x,x+1),p}$ is obtained from $\xi$ by moving a fraction $p$ of the total energy across the bond $\{x, x+1\}$ to $x$ and a fraction $1-p$ to $x+1$, i.e.

$$(\xi^{(x,x+1),p})_y := \begin{cases} \xi_y & \text{if} \quad y \neq x, x+1 \\ p\,(\xi_x + \xi_{x+1}) & \text{if} \quad y = x \\ (1-p)\,(\xi_x + \xi_{x+1}) & \text{if} \quad y = x+1 \end{cases}$$

The boundary generators $L_\pm$ are defined by a heat bath dynamics with respect to thermostats at temperatures $\tau_\pm$, i.e.

$$L_\pm f(\xi) := \int_0^\infty dr\, \frac{1}{\tau_\pm} e^{-r/\tau_\pm} \big[f(\xi^{\pm N,r}) - f(\xi)\big]$$

in which the configuration $\xi^{\pm N,r}$ is obtained from $\xi$ by setting the energy at $\pm N$ equal to $r$, i.e.

$$(\xi^{x,r})_y := \begin{cases} \xi_y & \text{if} \quad y \neq x \\ r & \text{if} \quad y = x \end{cases}$$

Note that we have set the Boltzmann constant equal to one. The process generated by (2.1), denoted by $\xi(t)$, will be called the KMP process.

We denote by $u \in [-1,1]$ the macroscopic space coordinates and introduce the space of energy profiles as $\mathcal{M} := \{\theta \in L_1([-1,1], du) \,:\, \theta(u) \geq 0\}$. We consider $\mathcal{M}$ equipped with the weak topology namely, $\theta_n \to \theta$ iff for each continuous test function $\phi$ we have $\langle \theta_n, \phi\rangle \to \langle \theta, \phi\rangle$, where $\langle \cdot, \cdot \rangle$ is the inner product in $L_2([-1,1], du)$. Given a microscopic configuration $\xi \in \Sigma_N$, we introduce the empirical energy $\pi_N(\xi)$ by mapping $\xi$ to the macroscopic profile

$$[\pi_N(\xi)]\,(u) := \sum_{x=-N}^{N} \xi_x \, 1\!\!1_{\left[\frac{x}{N} - \frac{1}{2N}, \frac{x}{N} + \frac{1}{2N}\right]}(u) \tag{2.3}$$

note that $\pi_N(\xi) \in \mathcal{M}$ is a piecewise constant function.

In the case when $\tau_- = \tau_+ = \tau$ it is easy to show that $L_N$ is reversible with respect to the product of exponential distribution with parameter $\tau$, i.e. the invariant measure is given by the equilibrium Gibbs measure at temperature $\tau$,

$$d\mu_{N,\tau}(\xi) = \prod_{x=-N}^{N} \frac{d\xi_x}{\tau}\, e^{-\xi_x/\tau} \tag{2.4}$$

When $\xi \in \Sigma_N$ is distributed according to $\mu_{N,\tau}$ then the empirical energy $\pi_N(\xi)$ concentrates, as $N \to \infty$ on the constant profile $\tau$ according to the following law of large numbers. For each $\delta > 0$ and each continuous test function $\phi = \phi(u)$

$$\lim_{N\to\infty} \mu_{N,\tau}\Big(\big|\langle \pi_N(\xi), \phi\rangle - \langle \tau, \phi\rangle\big| > \delta\Big) = 0 \tag{2.5}$$

where $\tau \in \mathcal{M}$ is the constant function with that value.

In this equilibrium case it is also easy to obtain the large deviation principle associated at the law of large numbers (2.5). More precisely, the probability that the empirical energy $\pi_N(\xi)$ is close to some profile $\theta \in \mathcal{M}$ different from $\tau$ is exponentially small in $N$ and given by a rate functional $S_0$

$$\mu_{N,\tau}\left(\pi_N(\xi) \sim \theta\right) \asymp \exp\big\{-N\, S_0(\theta)\big\} \tag{2.6}$$

where $\pi_N(\xi) \sim \theta$ means closeness in the weak topology of $\mathcal{M}$ and $\asymp$ denotes logarithmic equivalence as $N \to \infty$. The functional $S_0$ is given by

$$S_0(\theta) = \int_{-1}^{1} du\, \left[\frac{\theta(u)}{\tau} - 1 - \log\frac{\theta(u)}{\tau}\right] = \int_{-1}^{1} du\, s_0(\theta(u), \bar\theta_0) \tag{2.7}$$

where $\bar\theta_0 = \tau$ is the constant energy density profile for $\tau_+ = \tau_- = \tau$. The above functional can in fact be obtained as the Legendre transform of the pressure $G_0(h)$

$$S_0(\theta) = \sup_h \big[\langle \theta, h\rangle - G_0(h)\big]$$

where $G_0$ is defined as

$$G_0(h) := \lim_{N\to\infty} \frac{1}{N} \log \mathbb{E}_{\mu_{N,\tau}}\Big(e^{N\langle h, \pi_N(\xi)\rangle}\Big) = -\int_{-1}^{1} du\, \log[1 - \tau\, h(u)] \tag{2.8}$$

in which $\mathbb{E}_{\mu_{N,\tau}}$ denotes the expectation with respect to $\mu_{N,\tau}$.

If $\tau_- \neq \tau_+$ the process generated by $L_N$ is no longer reversible and its invariant measure $\mu_{N,\tau_\pm}$ is not explicitly known. Theorem 4.2 in [18] implies however the following law of large numbers. For each $\delta > 0$ and each continuous $\phi$

$$\lim_{N\to\infty} \mu_{N,\tau_\pm}\Big(\big|\langle \pi_N(\xi), \phi\rangle - \langle \bar\theta, \phi\rangle\big| > \delta\Big) = 0 \tag{2.9}$$

where $\bar\theta$ is the linear profile interpolating $\tau_-$ and $\tau_+$, i.e.

$$\bar\theta(u) = \tau_-\, \frac{1-u}{2} + \tau_+\, \frac{1+u}{2} \tag{2.10}$$

It is natural to look for the large deviations asymptotic for $\mu_{N,\tau_\pm}$. In the case of the symmetric simple exclusion process (SEP) this program has been carried out in [5,6,10,11]. The main result of this paper is an expression for the large deviation rate functional for $\mu_{N,\tau_\pm}$ analogous to the one for the SEP. The functional we obtain is nonlocal, as is the one for the SEP, but it turns out to be nonconvex while the one for SEP is convex. We mention that non convexity of the rate functional also occurs for the asymmetric exclusion process [12].

Without loss of generality we assume $\tau_- < \tau_+$ and introduce the set $\mathcal{T}_{\tau_\pm} := \{\tau \in C^1([-1,1]) \,:\, \tau'(u) > 0\,,\ \tau(\pm 1) = \tau_\pm\}$, here $\tau'$ is the derivative of $\tau$. Given $\theta \in \mathcal{M}$ and $\tau \in \mathcal{T}_{\tau_\pm}$ we introduce the trial functional

$$\mathcal{G}(\theta, \tau) := \int_{-1}^{1} du\, \Big[\frac{\theta(u)}{\tau(u)} - 1 - \log\frac{\theta(u)}{\tau(u)} - \log\frac{\tau'(u)}{[\tau_+ - \tau_-]/2}\Big] \tag{2.11}$$

In this paper we show that the empirical energy for $\mu_{N,\tau_\pm}$ satisfies the large deviation principle with a nonlocal, nonconvex rate functional $S(\theta)$ given by

$$S(\theta) = \inf_{\tau \in \mathcal{T}_{\tau_\pm}} \mathcal{G}(\theta, \tau) \tag{2.12}$$

that is we have

$$\mu_{N,\tau_\pm}\left(\pi_N(\xi)\sim\theta\right)\asymp\exp\big\{-N\,S(\theta)\big\}\tag{2.13}$$

We note there is a very close similarity between (2.12) and the analogous result for the SEP, we emphasize however that in (2.12) we minimize over the auxiliary profile $\tau$, while in SEP one needs to maximize. This is, of course, related to the non convexity of our $S$ versus the convexity of the rate functional for SEP. It would be very interesting to understand this basic difference also in terms of the combinatorial methods in [10–12] besides the dynamical approach presented here.

Given $\theta\in\mathcal{M}$, we show that the minimizer in (2.12) is uniquely attained for some profile $\tau(u)=\tau[\theta](u)$; therefore $S(\theta)=\mathcal{G}(\theta,\tau[\theta])$. Moreover $\tau[\theta](u)$ is the unique strictly increasing solution of the boundary value problem

$$\begin{cases}\tau^2\dfrac{\tau''}{(\tau')^2}+\theta-\tau=0\\ \tau(\pm1)=\tau_\pm\end{cases}\tag{2.14}$$

which is the Euler–Lagrange equation $\delta\mathcal{G}/\delta\tau=0$ when $\theta$ is kept fixed.

We note that for $\theta=\bar\theta$ the solution of (2.14) is given by $\tau[\bar\theta]=\bar\theta$ therefore $S(\bar\theta)=\mathcal{G}(\bar\theta,\bar\theta)=0$. On the other hand, by the convexity of the real functions $\mathbb{R}_+\ni x\mapsto x-1-\log x$ and $\mathbb{R}_+\ni x\mapsto-\log x$, for each $\theta\in\mathcal{M}$ and $\tau\in\mathcal{T}_{\tau_\pm}$ we have $\mathcal{G}(\theta,\tau)\ge0$ hence $S(\theta)\ge0$. By the same argument we also get that $S(\theta)=0$ if and only if $\theta=\bar\theta$. This shows that the large deviation principle (2.13) implies the law of large numbers (2.9) and gives an exponential estimate as $N\to\infty$. We finally remark that the reversible case (2.7) is recovered from (2.11)–(2.13) in the limit $\tau_+-\tau_-\to0$ which impose $\tau(u)$ constant.

*Outline of the following sections.*

Our derivation of the rate functional $S$ follows the dynamical/variational approach introduced in [4, 5]. We look first, in Section 3, at the dynamical behavior in the diffusive scaling limit in a bounded time interval $[0,T]$. In particular, we obtain a dynamical large deviation principle which gives the exponential asymptotic for the event in which the empirical energy follows a prescribed space–time path.

In Section 4 we introduce the quasi potential, it is defined by the minimal cost, as measured by the dynamical rate functional, to produce an energy fluctuation $\theta$ starting from the typical profile $\bar\theta$. By the arguments in [4, 5], the quasi potential equals the rate functional $S(\theta)$ of the invariant measure $\mu_{N,\tau_\pm}$. A mathematical rigorous proof of this statement for the SEP is given in [7]. As discussed in [4, 5], the quasi potential is the appropriate solution of a Hamilton–Jacobi equation which involves the transport coefficients of the macroscopic dynamics. The derivation of the functional $S$ is then completed by showing that (2.12) is the appropriate solution of this Hamilton–Jacobi equation. As in the case of the SEP we are also able, by following this dynamical/variational approach, to characterize the minimizer for the variational problem defining the quasi potential; this path is the one followed by the process, with probability going to one as $N\to\infty$, in the spontaneous creation of the fluctuation $\theta$. In Section 4 we also show that the functional $S$ is not convex, obtain its expression for constant profiles $\theta$, and derive an *additivity principle* analogous to the one for simple exclusion processes obtained in [11, 12].

In the remaining part of the paper we discuss some extensions of the previous results. In particular, in Section 5 we discuss the KMP process in higher space dimension, $d\ge1$, and obtain an upper bound for the quasi potential in terms of the local equilibrium one. We note that for the SEP it is possible to prove [5, 6] an analogous *lower bound*. We also discuss the Gaussian fluctuations around the stationary profile $\bar\theta$; as for the SEP [5, 9–11, 24] the correction due to nonequilibrium is given by the Green function of the Dirichlet Laplacian. In particular, this correction is non local; as in the case of the SEP, this is due to the long range correlations [18]. However, for the KMP process, the nonequilibrium enhances the Gaussian fluctuations while in the SEP it decreases them. As the covariance of the Gaussian fluctuations equals the inverse of the second derivative of $S(\theta)$ at $\bar\theta$, the enhancement of Gaussian fluctuations corresponds to the upper bound of $S(\theta)$ in terms of the local equilibrium functional. In the analysis in [18] a crucial role is played by a process, in *duality* with respect to the KMP process, in which the local variable at the site $x$ takes integral values. In Section 6 we discuss briefly the large deviations properties of this dual model and obtain the expression for the large deviation functional. Finally in Section 7 we discuss the derivation of the large deviation functional for generic one–dimensional nonequilibrium symmetric models with a single conservation law. We obtain a simple condition, which is satisfied by the zero range process, the Ginzburg–Landau dynamics, the SEP, the KMP process and its dual, that allows the derivation of the large deviation function by means of a suitable trial functional. Even when this condition fails to hold, it yields a simple criterion to predict the enhancement/supression of the Gaussian fluctuation in the stationary nonequilibrium state with respect to the full local thermal equilibrium.

The discussion in this paper will be kept at the physicists level of mathematical rigor. However, for the more mathematically inclined reader, we shall point out the main differences and technical difficulties with respect to the case of the SEP, which has been analyzed in full mathematical rigor [6].

## 3. Macroscopic dynamical behavior

In this Section we consider the KMP process in a bounded time interval $[0,T]$ under the diffusive scaling limit. We discuss the law of large numbers (hydrodynamic limit) and the associated dynamical large deviations principle for the empirical energy (2.3).

Given a continuous strictly positive energy profile $\theta \in C([-1,1];\mathbb{R}_+)$, we denote by $\nu^N_\theta$ the probability on $\Sigma_N$ corresponding to a local equilibrium distribution (LTE) with an energy profile given by $\theta$. It is defined as

$$d\nu^N_\theta(\xi) := \prod_{x=-N}^{N} d\nu^N_{\theta,x}(\xi_x)$$

where

$$d\nu^N_{\theta,x} := \frac{d\xi_x}{\theta(x/N)} \exp\Big\{ -\frac{\xi_x}{\theta(x/N)}\Big\}$$

Given two probability measures $\nu,\mu$ on $\Sigma_N$ we denote by $h(\nu|\mu)$ the relative entropy of $\nu$ with respect to $\mu$, it is defined as

$$h(\nu|\mu) := \int d\mu(\xi)\, \frac{d\nu(\xi)}{d\mu(\xi)} \log \frac{d\nu(\xi)}{d\mu(\xi)}$$

We shall consider the KMP process with initial condition distributed according to the product measure $\nu^N_{\theta_0}$ for some energy profile $\theta_0$. A straightforward computation then shows there exists a constant $C$ (depending on $\theta_0$) such that for any $N$ we have the relative entropy bound

$$h(\nu^N_{\theta_0}|\nu^N_{\bar\theta}) \le CN \tag{3.1}$$

where $\bar\theta$ is the stationary energy profile (2.10). By the weak law of large numbers for independent variables we also have that $\nu^N_{\theta_0}$ is associated to the energy profile

$\theta_0$ in the following sense. For each $\delta > 0$ and each continuous $\phi$

$$\lim_{N\to\infty} \nu^N_{\theta_0}\Big(\big|\langle \pi_N(\xi), \phi\rangle - \langle \theta_0, \phi\rangle\big| > \delta\Big) = 0 \tag{3.2}$$

We remark that for the SEP it is possible (and convenient, see [6]) to consider deterministic initial conditions. For the KMP process, as the "single spin space" $\mathbb{R}_+$ is not discrete, such initial conditions do not satisfy the entropy bound (3.1), which is required in the standard derivation, see e.g. [17,25], of the hydrodynamic limit. For this reason we have chosen the initial condition distributed according to the product measure $\nu^N_{\theta_0}$. On the other hand, by the method developed in [21], it should be also possible to consider deterministic initial configurations.

We denote by $\mathbb{P}_{\nu^N_{\theta_0}}$ the distribution of the KMP process when the initial condition is distributed according to $\nu^N_{\theta_0}$. The measure $\mathbb{P}_{\nu^N_{\theta_0}}$ is a probability on the space $D([0,T];\Sigma_N)$ of right continuous with left limit paths from $[0,T]$ to $\Sigma_N$. The expectation with respect to $\mathbb{P}_{\nu^N_{\theta_0}}$ is denoted by $\mathbb{E}_{\nu^N_{\theta_0}}$.

3.1. **Hydrodynamic limit.** Equation (3.2) is the law of large number for the empirical energy at time $t = 0$; the hydrodynamic limit states that for each macroscopic time $t \in [0,T]$ there exists an energy profile $\theta(t)$ such we have the same law of large numbers

$$\lim_{N\to\infty} \mathbb{P}_{\nu^N_{\theta_0}}\Big(\big|\langle \pi_N(\xi(t)), \phi\rangle - \langle \theta(t), \phi\rangle\big| > \delta\Big) = 0 \tag{3.3}$$

Furthermore, we can obtain the energy profile $\theta(t)$ by solving the hydrodynamic equation. For the KMP process (as for the SEP) this is simply the the linear heat equation with boundary conditions $\tau_\pm$, i.e. $\theta(t) = \theta(t,u)$ solves

$$\begin{cases} \partial_t \theta(t) &=& \frac{1}{2}\Delta\theta(t) \\ \theta(t,\pm 1) &=& \tau_\pm \\ \theta(0,u) &=& \theta_0(u) \end{cases} \tag{3.4}$$

where $\Delta$ is the Laplacian. Note that the stationary profile $\bar\theta$ in (2.10) is the unique stationary solution of (3.4).

We give below a brief heuristic derivation, which is particularly simple for the KMP process, of the hydrodynamic limit. We refer to [14,15] for a rigorous proof in the case of the so called gradient nonequilibrium models with finite single spin state space; the extension to the KPM process should not present additional problems.

Let $\phi$ be a smooth function whose support is a subset of $(-1,1)$; from the general theory of Markov processes, we have that

$$\frac{d}{dt}\mathbb{E}_{\nu^N_{\theta_0}}\big(\langle \pi_N(\xi(t)), \phi\rangle\big) = \mathbb{E}_{\nu^N_{\theta_0}}\big(L_N\langle \pi_N(\xi(t)), \phi\rangle\big) \tag{3.5}$$

Since the support of $\phi$ is a strict subset of $[-1,1]$, only $N^2 L_0$ contributes to $L_N\langle \pi_N(\xi(t)), \phi\rangle$. A simple computation shows that, when $y \neq \pm N$,

$$L_0 \xi_y = \frac{1}{2}\big[\xi_{y-1} + \xi_{y+1} - 2\xi_y\big] \tag{3.6}$$

we thus get

$$\begin{aligned} L_N\langle \pi_N(\xi(t)), \phi\rangle &= \frac{N^2}{2}\sum_{x\in\Lambda_N}\big[\xi_{x-1}(t) + \xi_{x+1}(t) - 2\xi_x(t)\big]\int_{x/N-1/(2N)}^{x/N+1/(2N)} du\, \phi(u) \\ &\approx \frac{1}{2N}\sum_{x\in\Lambda_N} \Delta_N\phi(x/N)\, \xi_x(t) \approx \frac{1}{2}\langle \pi_N(\xi(t)), \Delta\phi\rangle \end{aligned}$$

here $\Delta_N \phi(x/N) := N^2\big[\phi((x-1)/N) + \phi((x+1)/N) - 2\phi(x/N)\big]$ is the discrete Laplacian. The first step above comes from (3.6) and (2.3), the second step from discrete integration by parts and last step from the regularity of $\phi$.

We have thus obtained the weak formulation of (3.4); it remains to show that also the boundary condition $\theta(t,\pm 1) = \tau_\pm$ is satisfied. For this we need to use the boundary generators $N^2 L_\pm$. These are Glauber like dynamics accelerated by $N^2$ so that the energy has well thermalized to its equilibrium value. We get

$$\mathbb{E}_{\nu^N_{\theta_0}}\left(\xi_{\pm N}(t)\right) \approx \tau_\pm \tag{3.7}$$

A standard martingale computation shows that, with a negligible error as $N \to \infty$, $\pi_N(\xi(t))$ becomes non random. We can then remove the expectation value in the previous equations and get (3.3).

3.2. **Dynamic large deviations.** We want next to obtain the large deviation principle associated to the law of large number (3.3); more precisely we want to estimate the probability that the empirical energy $\pi_N(\xi(t))$ does not follow the solution of (3.4) but remains close to some prescribed path $\pi = \pi(t,u)$. This probability will be exponentially small in $N$ and we look for the exponential rate. We follow the classic procedure in large deviation theory: we perturb the dynamics in such a way that the path $\pi$ becomes typical and compute the cost of such a perturbation.

Let $H = H(t,u)$ be a smooth function vanishing at the boundary, i.e. $H(t,\pm 1) = 0$. We then consider the following time dependent perturbations of the generators $L_{x,x+1}$ in (2.2)

$$L^H_{x,x+1} f(\xi) := \int_0^1 dp\, e^{[H(t,x/N)-H(t,(x+1)/N)][p\xi_{x+1}-(1-p)\xi_x]}\big[f(\xi^{(x,x+1),p}) - f(\xi)\big]$$

Note that we have essentially just added a small drift $N^{-1}\nabla H(t,x/N)$ in the energy exchange across the bond $\{x,x+1\}$. We denote by $\mathbb{P}^H_{\nu^N_{\theta_0}}$ the distribution on the path space $D([0,T];\Sigma_N)$ of this perturbed KMP process. As before $\mathbb{E}^H_{\nu^N_{\theta_0}}$ is the expectation with respect to $\mathbb{P}^H_{\nu^N_{\theta_0}}$.

The first step to obtain the dynamic large deviations is to derive the hydrodynamic equation for the perturbed KMP process. We claim that for each $t \in [0,T]$, each continuous $\phi$, and each $\delta > 0$ we have

$$\lim_{N\to\infty} \mathbb{P}^H_{\nu^N_{\theta_0}}\Big(\big|\langle \pi_N(\xi(t)), \phi\rangle - \langle \theta(t), \phi\rangle\big| > \delta\Big) = 0 \tag{3.8}$$

where $\theta(t) = \theta(t,u)$ solves

$$\begin{cases} \partial_t \theta(t) &= \dfrac{1}{2}\Delta\theta(t) - \nabla\big(\theta(t)^2 \nabla H(t)\big) \\ \theta(t,\pm 1) &= \tau_\pm \\ \theta(0,u) &= \theta_0(u) \end{cases} \tag{3.9}$$

The argument to justify (3.9) is similar to the previous one. Including the effect of the perturbation, the computation following (3.6) now becomes (as before $y \neq \pm N$)

$$
\begin{aligned}
L_0^H \xi_y &= \int_0^1 dp\, e^{[H(t,(y-1)/N)-H(t,y/N)][p\xi_y-(1-p)\xi_{y-1}]}\big[(1-p)(\xi_y+\xi_{y-1})-\xi_y\big] \\
&\quad + \int_0^1 dp\, e^{[H(t,y/N)-H(t,(y+1)/N)][p\xi_{y+1}-(1-p)\xi_y]}\big[p\,(\xi_{y+1}+\xi_y)-\xi_y\big] \\
&\approx \frac{\xi_{y-1}+\xi_{y+1}-2\xi_y}{2} + \big[H(t,(y-1)/N)-H(t,y/N)\big]\frac{\xi_y\xi_{y-1}-\xi_y^2-\xi_{y-1}^2}{3} \\
&\quad + \big[H(t,y/N)-H(t,(y+1)/N)\big]\frac{-\xi_y\xi_{y+1}+\xi_y^2+\xi_{y+1}^2}{3}
\end{aligned}
$$

As before, we consider a smooth function $\phi$ whose support is a strict subset of $(-1,1)$; then only $N^2 L_0^H$ contributes to $L_N^H\langle \pi_N(\xi(t)),\phi\rangle$ and we get

$$
\begin{aligned}
L_N^H\langle \pi_N(\xi(t)),\phi\rangle &\approx \frac{1}{N}\sum_x N^2\phi(x/N)\bigg\{\frac{\xi_{x-1}(t)+\xi_{x+1}(t)-2\xi_x(t)}{2} \\
&\quad + \big[H(t,(x-1)/N)-H(t,x/N)\big]\frac{\xi_x(t)\xi_{x-1}(t)-\xi_x(t)^2-\xi_{x-1}(t)^2}{3} \\
&\quad + \big[H(t,x/N)-H(t,(x+1)/N)\big]\frac{-\xi_x(t)\xi_{x+1}(t)+\xi_x(t)^2+\xi_{x+1}(t)^2}{3}\bigg\} \\
&\approx \frac{1}{N}\sum_x \xi_x(t)\Delta_N\phi(x/N) \\
&\quad + \frac{1}{N}\sum_x \frac{-\xi_x(t)\xi_{x+1}(t)+\xi_x(t)^2+\xi_{x+1}(t)^2}{3}\,\nabla_N H(t,x/N)\,\nabla_N\phi(x/N)
\end{aligned}
$$

where $\nabla_N f(x/N) := N[f((x+1)/N) - f(x/N)]$ is the discrete gradient. In the above computations we just used Taylor expansions and discrete integrations by parts. With respect to the very simple case discussed before, we face now the main problem in establishing the hydrodynamic limit: the above equation is not closed in $\pi_N(\xi(t))$, i.e. its right hand side is not a function of $\pi_N(\xi(t))$. In order to derive the hydrodynamic equation (3.9), we need to express $-\xi_x\xi_{x+1}+\xi_x^2+\xi_{x+1}^2$ in terms of the empirical energy $\pi_N(\xi)$. This will be done by assuming a "local equilibrium" state, we refer to [6,14,15,17,25] for a rigorous justification in the context of conservative interacting particle systems.

Let us consider a microscopic site $x$ which is far from the boundary and introduce a volume $V$, centered at $x$, which is very large in microscopic units, but still infinitesimal at the macroscopic level. The time evolution in $V$ is essentially given only by the bulk dynamics $N^2 L_0^H$; since the total amount of energy in $V$ changes only via boundary effects and we are looking at what happens after $O(N^2)$ microscopic time units, we expect that the system in $V$ has relaxed to the micro–canonical state corresponding to the local empirical energy $\pi_N(\xi(t))(x/N)$. To compute this state let us construct first the canonical measure in $V$ with constant temperature $\tau > 0$, namely the product measure $d\nu_{V,\tau}(\xi) := \prod_{x\in V}\tau^{-1}\,d\xi_x\, e^{-\xi_x/\tau}$. Let now $m_{V,\theta}$ be the associated micro–canonical measure with energy density $\theta$, i.e.

$$
m_{V,\theta}(d\xi) := \nu_{V,\tau}\Big(d\xi\,\Big|\,\sum_{x\in V}\xi_x = \theta|V|\Big)
$$

We introduce the function $\sigma(\theta)$ defined by

$$
\sigma(\theta) := \lim_{V\uparrow\mathbb{Z}}\ \mathbb{E}_{m_{V,\theta}}\big(-\xi_x\xi_{x+1}+\xi_x^2+\xi_{x+1}^2\big) \tag{3.10}
$$

where we recall that $\mathbb{E}_{m_{V,\theta}}$ denotes the expectation with respect to the probability $m_{V,\theta}$. By the equivalence of ensemble we can compute $\sigma(\theta)$ also as

$$\sigma(\theta) = \mathbb{E}_{\nu_{V,\theta}}\big( - \xi_x \xi_{x+1} + \xi_x^2 + \xi_{x+1}^2 \big) = 3\,\theta^2$$

According to the previous discussion, the system in the volume $V$ is well approximated by a micro–canonical state with energy density $\pi_N(\xi(t))(x/N)$. As it is shown by the standard proofs in hydrodynamic limits, see e.g. [17, 25], we can thus replace, for $N$ large, $-\xi_x(t)\xi_{x+1}(t) + \xi_x(t)^2 + \xi_{x+1}(t)^2$ with $3[\pi_N(\xi(t))(x/N)]^2$. We then obtain

$$\frac{d}{dt}\mathbb{E}_{\nu^N_{\theta_0}}\big(\langle \pi_N(\xi(t)), \phi\rangle\big) \approx \frac{1}{2}\langle \pi_N(\xi(t)), \Delta\phi\rangle + \langle \pi_N(\xi(t))^2 \nabla H, \nabla\phi\rangle \tag{3.11}$$

which is the weak formulation of (3.9). The arguments to show that the boundary conditions $\theta(t, \pm 1) = \tau_\pm$ are satisfied and to remove the expectation value are the same ones as in the derivation of (3.4).

Let $\pi = \pi(t, u)$, $(t, u) \in [0, T] \times [-1, 1]$ be a given path. We recall that our task is to estimate the probability that the empirical energy $\pi_N(\xi(t))$ is close to $\pi(t)$ (short for $\pi(t, u)$). We write this probability in terms of the perturbed KMP process, namely

$$\mathbb{P}_{\nu^N_{\theta_0}}\big(\pi_N(\xi(t)) \sim \pi(t), t \in [0, T]\big) = \mathbb{E}^H_{\nu^N_{\theta_0}}\left(\frac{d\mathbb{P}_{\nu^N_{\theta_0}}}{d\mathbb{P}^H_{\nu^N_{\theta_0}}}\, \mathbb{I}_{\{\pi_N(\xi(t))\sim\pi(t)\}}\right) \tag{3.12}$$

Equation (3.9) tells us for which $H$ the path $\pi$ becomes typical for the perturbed KMP process. We thus choose $H(t, u)$ so that

$$\begin{cases} \nabla\big(\pi(t)^2 \nabla H(t)\big) = -\partial_t \pi(t) + \dfrac{1}{2}\Delta\pi(t) \\ H(t, \pm 1) = 0 \end{cases} \tag{3.13}$$

which is essentially a Poisson equation for $H$ (recall that $\pi$ is fixed). With this choice we have, for $N$ large, $\mathbb{P}^H_{\nu^N_{\theta_0}}\big(\pi_N(\xi(t)) \sim \pi(t)\big) \approx 1$ and to derive the dynamical large deviation principle we only need to compute the Radon–Nykodim derivative $d\mathbb{P}_{\nu^N_{\theta_0}}/d\mathbb{P}^H_{\nu^N_{\theta_0}}$.

We consider first the case of a deterministic initial configuration $\xi_0 \in \Sigma_N$. In this case, by a standard computation in the theory of jump Markov processes, see e.g. [17, Appendix 1.7] or [5, Appendix A]), we have

$$\frac{d\mathbb{P}_{\xi_0}}{d\mathbb{P}^H_{\xi_0}}(\xi) = \exp\big\{ - N \mathcal{J}^N_{[0,T]}(\xi, H)\big\}$$

where

$$\begin{aligned} \mathcal{J}^N_{[0,T]}(\xi, H) := {}& \langle \pi_N(\xi(T)), H(T)\rangle - \langle \pi_N(\xi_0), H(0)\rangle - \int_0^T dt\, \langle \pi_N(\xi(t)), \partial_t H(t)\rangle \\ & - N^2 \sum_{x=-N}^{N-1} \int_0^T dt \int_0^1 dp\, \Big\{ e^{[H(t,x/N) - H(t,(x+1)/N)]\,[p\,\xi_{x+1}(t) - (1-p)\xi_x(t)]} - 1 \Big\} \end{aligned}$$

By Taylor expansion we then get

$$
\begin{aligned}
\mathcal{J}^N_{[0,T]}(\xi,H) \approx\ & \langle \pi_N(\xi(T)), H(T)\rangle - \langle \pi_N(\xi_0), H(0)\rangle - \int_0^T dt\ \langle \pi_N(\xi(t)), \partial_t H(t)\rangle \\
& - \int_0^T dt\ \frac{1}{2N} \sum_{x=-N+1}^{N-1} \xi_x(t) \Delta_N H(t, x/N) \\
& - \frac{1}{2}\int_0^T dt\ \xi_{-N}(t)\, N\big[H(t,-1+1/N) - H(t,-1)\big] \\
& + \frac{1}{2}\int_0^T dt\ \xi_N(t)\, N\big[H(t,1) - H(t,1-1/N)\big] \\
& - \int_0^T dt\ \frac{1}{2N} \sum_{x=-N}^{N-1} \frac{-\xi_x(t)\xi_{x+1}(t) + \xi_x^2(t) + \xi_{x+1}^2(t)}{3} \big[\nabla_N H(t,x/N)\big]^2
\end{aligned}
$$

By the same argument given in the derivation of the perturbed hydrodynamic equation (3.9), we can replace $-\xi_x(t)\xi_{x+1}(t) + \xi_x(t)^2 + \xi_{x+1}(t)^2$ by $3[\pi_N(\xi(t))(x/N)]^2$. Recalling that in (3.12) there is the indicator of the event in which $\pi_N(\xi(t))$ is close to $\pi(t)$, we get

$$
\begin{aligned}
\mathcal{J}^N_{[0,T]}(\xi,H) \ \approx\ J_{[0,T]}(\pi) \ =\ & \langle \pi(T), H(T)\rangle - \langle \pi(0), H(0)\rangle - \int_0^T dt\ \langle \pi(t), \partial_t H(t)\rangle \\
& - \frac{1}{2}\int_0^T dt\ \langle \pi(t), \Delta H(t)\rangle - \frac{1}{2}\int_0^T dt\ \langle \pi(t)^2, [\nabla H(t)]^2\rangle \\
& - \frac{1}{2}\int_0^T dt\ \tau_- \nabla H(t,-1) + \frac{1}{2}\int_0^T dt\ \tau_+ \nabla H(t,1)
\end{aligned}
$$

where we used the fact that the value of $\pi$ is fixed at the boundary, $\pi(t,\pm 1) = \tau_\pm$. Recalling that the perturbation $H$ has been chosen as the solution of (3.13), integration by parts shows that

$$
J_{[0,T]}(\pi) = \frac{1}{2}\int_0^T dt\ \langle \nabla H(t), \pi(t)^2 \nabla H(t)\rangle \tag{3.14}
$$

To complete the derivation of the dynamical large deviation functional, we only need to consider the fluctuations of the initial condition. Recalling that we have chosen the initial condition distributed according to the product measure $\nu^N_{\theta_0}$, a straightforward computation on product measures (the one carried out in (2.6)–(2.8)) shows that

$$
\nu^N_{\theta_0}\big(\pi_N(\xi) \sim \pi(0)\big) \asymp \exp\big\{ - N S_0(\pi(0)|\theta_0)\big\}
$$

where $S_0(\pi(0)|\theta_0)$, which represents the contribution to the dynamic large deviation from the initial condition, is given by

$$
S_0(\pi(0)|\theta_0) = \int_{-1}^1 du\ \left[\frac{\pi(0,u)}{\theta_0(u)} - 1 - \log\frac{\pi(0,u)}{\theta_0(u)}\right] \tag{3.15}
$$

By collecting all the computations performed we finally get the dynamical large deviation principle

$$
\mathbb{P}_{\nu^N_{\theta_0}}\Big(\pi_N(\xi(t)) \sim \pi(t), t\in[0,T]\Big) \asymp \exp\big\{ - N\, I_{[0,T]}(\pi|\theta_0)\big\} \tag{3.16}
$$

where

$$
I_{[0,T]}(\pi|\theta_0) = S_0(\pi(0)|\theta_0) + J_{[0,T]}(\pi) \tag{3.17}
$$

We note again that $S_0(\pi(0)|\theta_0)$ represents the cost to create a fluctuation at time zero whereas $J_{[0,T]}(\pi)$ represents the dynamical cost to follow the path $\pi(t)$ in the time interval $[0, T]$. In the case of deterministic initial conditions, as the one discussed in [6] for the SEP, we would have $S_0(\pi(0)|\theta_0) = +\infty$ unless $\pi(0) = \theta_0$.

3.3. **Remarks.** We conclude this section with some remarks on the rigorous derivation of the dynamical large deviation principle (3.16). The probability estimates needed are (not surprisingly) more subtle than discussed here. In fact, while in the proof of the hydrodynamic limit it is enough to show that we can replace $-\xi_x(t)\xi_{x+1}(t) + \xi_x^2(t) + \xi_{x+1}^2(t)$ by $3[\pi_N(\xi(t))(x/N)]^2$ with an error vanishing as $N \to \infty$, in the proof of the large deviations we need such an error to be of $o(e^{-CN})$. This can be proven by the so called super exponential estimate, see [17, 19], which is the key point in the rigorous approach. This estimate has been extended to the non equilibrium SEP in [6]. For the KMP process there is the additional complication of a unbounded single spin space. In [13] the dynamical large deviation principle is proven for the Ginzburg–Landau model; however for the KMP process the situation is more troublesome because the mobility $\pi^2$ is unbounded and the reference measure is only exponentially decaying for large $\pi$. There is also another technical point which requires some care. In the usual proofs of large deviations from hydrodynamic behavior, one first obtains the lower bound for a neighborhood of strictly positive smooth paths $\pi$ and then uses approximations arguments to extend the lower bound to any open set. The approximations arguments used for the SEP, see [17, 19] for the equilibrium case and [6] for nonequilibrium, take full advantage of the fact (special for the SEP) that $J_{[0,T]}(\pi)$ is a convex functional. In order to prove the dynamic large deviation principle for the KMP process a more robust approximation method, possibly analogous to the one in [22], is required.

## 4. The quasi potential and its properties

In this Section we introduce the quasi potential, which measures the minimal cost to produce a fluctuation of the energy profile in the stationary state, and shows that it can be obtained by solving the one–dimensional non linear boundary value problem (2.14). We also characterize the most probable path followed by the KMP process in the spontaneous creation of such a fluctuation. We finally show that the functional $S$ is not convex and derive an *additivity principle* analogous to the one in [11, 12].

Given $T > 0$ and a strictly positive smooth $\theta \in \mathcal{M}$, we introduce the set of energy paths which connect $\bar{\theta}$ to $\theta$ in a time interval $[-T, 0]$, i.e. we define

$$\mathcal{E}_{\theta,T} := \big\{\pi = \pi(t,u) \,:\, \pi(-T,u) = \bar{\theta}(u)\,,\ \pi(0,u) = \theta(u)\big\} \tag{4.1}$$

where we recall that the stationary energy profile $\bar{\theta}$ has been defined in (2.10). Paths $\pi \in \mathcal{E}_{\theta,T}$ must also satisfy the boundary condition $\pi(t, \pm 1) = \tau_\pm$; in fact it can be shown [6] that $J_{[-T,0]}(\pi) = +\infty$ if the path $\pi$ does not satisfy this boundary condition. The *quasi potential* is then defined as

$$V(\theta) := \inf_{T>0} \inf_{\pi \in \mathcal{E}_{\theta,T}} J_{[-T,0]}(\pi) \tag{4.2}$$

where we recall that the functional $J$ is given in (3.14). By the general arguments in [5], see also the rigorous proof in [7] for the SEP, we have that the rate functional $S(\theta)$ for the invariant measure $\mu_{N,\tau_\pm}$, see (2.13), coincides with the quasi potential, i.e. $S(\theta) = V(\theta)$.

4.1. **Solution of the Hamilton–Jacobi equation.** Recalling that the perturbation $H$ in (3.14) solves (3.13), the variational problem (4.2) consists in minimizing the action that correspond to the Lagrangian

$$\mathcal{L}(\theta, \partial_t\theta) = \frac{1}{2}\Big\langle \nabla^{-1}(\partial_t\theta - \frac{1}{2}\Delta\theta), \frac{1}{\theta^2}\nabla^{-1}(\partial_t\theta - \frac{1}{2}\Delta\theta)\Big\rangle \tag{4.3}$$

The associated Hamiltonian is

$$\mathcal{H}(\theta,H) := \sup_{\zeta}\big\{\langle H,\zeta\rangle - \mathcal{L}(\theta,\zeta)\big\} = \frac{1}{2}\big\langle \nabla H, \theta^2\nabla H\big\rangle + \frac{1}{2}\big\langle H, \Delta\theta\big\rangle \tag{4.4}$$

Noting that $V$ is normalized so that $V(\bar\theta)=0$, we obtain, by a classical result in analytic mechanics, that $V(\theta)$ solves the Hamilton–Jacobi equation $\mathcal{H}(\theta,\frac{\delta V}{\delta\theta})=0$, i.e.

$$\Big\langle \nabla\frac{\delta V}{\delta\theta}, \theta^2\nabla\frac{\delta V}{\delta\theta}\Big\rangle + \Big\langle \frac{\delta V}{\delta\theta}, \Delta\theta\Big\rangle = 0 \tag{4.5}$$

where $\delta V/\delta\theta$ vanishes at the boundary and $\theta(\pm1)=\tau_\pm$. We look for a solution of (4.5) in the form

$$\frac{\delta V}{\delta\theta} = \frac{1}{\tau} - \frac{1}{\theta} \tag{4.6}$$

for some function $\tau=\tau[\theta](u)$ to be determined satisfying the boundary conditions $\tau(\pm1)=\tau_\pm$. By plugging (4.6) into (4.5) and elementary computations, analogous to the ones for the SEP discussed in [5], we get

$$\begin{aligned} 0 &= \Big\langle \nabla\Big(\frac{1}{\tau}-\frac{1}{\theta}\Big), \theta^2\nabla\frac{1}{\tau}\Big\rangle \\ &= -\Big\langle \nabla(\theta-\tau), \frac{\nabla\tau}{\tau^2}\Big\rangle + \Big\langle \frac{(\nabla\tau)^2}{\tau^4}, (\theta^2-\tau^2)\Big\rangle \\ &= \Big\langle \frac{\theta-\tau}{\tau^4},\, \tau^2\Delta\tau + (\theta-\tau)(\nabla\tau)^2\Big\rangle \end{aligned} \tag{4.7}$$

Therefore a solution of (4.7) is obtained when $\tau$ satisfies the non linear boundary value problem (2.14). Let us denote by $\tau[\theta]$ the solution of (2.14); recall the definition (2.11) of the functional $\mathcal{G}(\theta,\tau)$ and that, since (2.14) is the associated Euler–Lagrange equation for fixed $\theta$, we have $[\delta\mathcal{G}/\delta\tau]\,(\theta,\tau[\theta])=0$. By a direct computation we then get

$$\frac{\delta}{\delta\theta}\mathcal{G}(\theta,\tau[\theta]) = \frac{\delta\mathcal{G}}{\delta\theta}(\theta,\tau[\theta]) + \frac{\delta\mathcal{G}}{\delta\tau}(\theta,\tau[\theta])\,\frac{\delta\tau[\theta]}{\delta\theta} = \frac{1}{\tau[\theta]} - \frac{1}{\theta} \tag{4.8}$$

which shows that $V(\theta)=\mathcal{G}(\theta,\tau[\theta])$ is a solution of the Hamilton–Jacobi equation (4.5). To complete the derivation of (2.13) we next show that $V(\theta)$ meets the criterion in [5, §2.6], i.e. it is the "right solution" of the Hamilton–Jacobi equation, and that the infimum in (2.12) is uniquely attained for $\tau=\tau[\theta]$, the solution of (2.14).

4.2. **The exit path.** The characterization of the optimal path for the variational problem (4.2) can be carried out according to the general scheme in [6]. Let $V(\theta)=\mathcal{G}(\theta,\tau[\theta])$ and $\pi(t)$, $t\in[-T,0]$ a strictly positive smooth path such that $\pi(0)=\theta$. By using that $V(\theta)$ solves Hamilton–Jacobi equation (4.5), a simple computation shows that

$$\begin{aligned} J_{[-T,0]}(\pi) = \frac{1}{2}\int_{-T}^{0} dt\, \Big\langle & \nabla^{-1}\Big[\partial_t\pi - \frac{1}{2}\Delta\pi + \nabla\Big(\pi^2\nabla\frac{\delta V}{\delta\theta}(\pi)\Big) - \nabla\Big(\pi^2\nabla\frac{\delta V}{\delta\theta}(\pi)\Big)\Big], \\ & \frac{1}{\pi^2}\nabla^{-1}\Big[\partial_t\pi - \frac{1}{2}\Delta\pi + \nabla\Big(\pi^2\nabla\frac{\delta V}{\delta\theta}(\pi)\Big) - \nabla\Big(\pi^2\nabla\frac{\delta V}{\delta\theta}(\pi)\Big)\Big]\Big\rangle \\ = V(\theta) - V(\pi(-T)) + \frac{1}{2}\int_{-T}^{0} dt\, \Big\langle & \nabla^{-1}\Big[\partial_t\pi - \frac{1}{2}\Delta\pi + \nabla\Big(\pi^2\nabla\frac{\delta V}{\delta\theta}(\pi)\Big)\Big], \\ & \frac{1}{\pi^2}\nabla^{-1}\Big[\partial_t\pi - \frac{1}{2}\Delta\pi + \nabla\Big(\pi^2\nabla\frac{\delta V}{\delta\theta}(\pi)\Big)\Big]\Big\rangle \end{aligned}$$

Since the last term above is positive, the optimal path $\pi^*$ for the variational problem (4.2) solves

$$\partial_t \pi^* = \frac{1}{2}\Delta\pi^* - \nabla\Big((\pi^*)^2\nabla\frac{\delta V}{\delta\theta}(\pi^*)\Big) = -\frac{1}{2}\Delta\pi^* + \nabla\Big(\frac{(\pi^*)^2}{(\tau[\pi^*])^2}\nabla\tau[\pi^*]\Big) \qquad (4.9)$$

where $\tau[\pi^*] = \tau[\pi^*](t,u)$ denotes the solution of (2.14) with $\theta$ replaced by $\pi^*(t)$.

Let us denote by $\theta^*(t) = \pi^*(-t)$, $t \in [0,T]$, the time reversed of the optimal path $\pi^*$. It is then not difficult to show, see [5, Appendix B] for the analogous computation in the case of the SEP, that $\theta^*(t)$ can be constructed by the following procedure. Given $\theta = \pi^*(0) = \theta^*(0)$, first let $\tau_0 = \tau[\theta]$ be the solution of (2.14), then solve the heat equation with initial condition $\tau_0$, i.e. let $\tau(t)$ be the solution of

$$\begin{cases} \partial_t\tau(t) &=& \frac{1}{2}\Delta\tau(t) \\ \tau(t,\pm 1) &=& \tau_\pm \\ \tau(0,u) &=& \tau_0(u) \end{cases}$$

and finally set

$$\theta^*(t) = \tau(t) - \tau(t)^2\frac{\Delta\tau(t)}{[\nabla\tau(t)]^2}$$

Since $\tau(t) \to \bar\theta$ as $t \to \infty$ we get $\pi^*(-T) \to \bar\theta$ as $T \to \infty$, hence $V(\pi^*(-T)) \to V(\bar\theta) = 0$. The identification of the solution of the Hamilton–Jacobi equation with the quasi potential follows from the characterization of the minimizer $\pi^*$ obtained before. In particular $V(\theta)$ satisfies the criterion discussed in [5, §2.6].

4.3. **Solution of equation (2.14).** The existence of a solution for the nonlinear boundary value problem (2.14) can be proven by the same strategy as in [6, 11]. We write (2.14) in the integral–differential form

$$\tau(u) = \tau_- + (\tau_+ - \tau_-)\,\frac{\displaystyle\int_{-1}^{u} dv\ \exp\Big\{\int_{-1}^{v} dw\ \frac{[\tau(w)-\theta(w)]\tau'(w)}{\tau(w)^2}\Big\}}{\displaystyle\int_{-1}^{1} dv\ \exp\Big\{\int_{-1}^{v} dw\frac{[\tau(w)-\theta(w)]\tau'(w)}{\tau(w)^2}\Big\}}$$

Then a solution of (2.14) is a fixed point of the integral–differential operator $\mathcal{K}_\theta[\tau]$ defined as

$$\mathcal{K}_\theta[\tau]\,(u) := \tau_- + (\tau_+ - \tau_-)\,\frac{\displaystyle\int_{-1}^{u} dv\ \exp\Big\{\int_{-1}^{v} dw\ \frac{[\tau(w)-\theta(w)]\tau'(w)}{\tau(w)^2}\Big\}}{\displaystyle\int_{-1}^{1} dv\ \exp\Big\{\int_{-1}^{v} dw\frac{[\tau(w)-\theta(w)]\tau'(w)}{\tau(w)^2}\Big\}}$$

We consider the case in which $\theta$ is bounded, namely we assume that $\|\theta\| := \sup_u|\theta(u)| < +\infty$. Recalling that $\tau$ must be strictly increasing and such that $\tau(\pm 1) = \tau_\pm$, we get

$$-\frac{\|\theta\|\tau'}{\tau_-\tau} \le \frac{(\tau-\theta)\tau'}{\tau^2} \le \frac{\tau'}{\tau}$$

which yields

$$\frac{\tau_+ - \tau_-}{2}\Big(\frac{\tau_-}{\tau_+}\Big)^{1+\frac{\|\theta\|}{\tau_-}} \le \frac{d}{du}\mathcal{K}_\theta[\tau](u) \le \frac{\tau_+ - \tau_-}{2}\Big(\frac{\tau_+}{\tau_-}\Big)^{1+\frac{\|\theta\|}{\tau_-}}$$

It is now easy to show, see [6] for more details, that for each $\theta \in \mathcal{M}$, the operator $\mathcal{K}_\theta[\tau]$ maps a compact convex subset of $\mathcal{T}_{\tau_\pm}$ into itself. Hence, by Schauder's fixed point theorem, we conclude the proof of the existence of solution to (2.14).

Uniqueness of solution to (2.14) can also be proved with a slight variation of the argument in [11]. Let us consider two different increasing solutions of (2.14) $\tau_1(u)$

and $\tau_2(u)$. If $\tau_1'(-1) = \tau_2'(-1)$ then uniqueness of the Cauchy problem implies $\tau_1 = \tau_2$. On the other hand, if $\tau_1'(-1) > \tau_2'(-1) > 0$ then we denote by $\bar u$ the leftmost point in $(-1,1]$ such that $\tau_1(\bar u) = \tau_2(\bar u)$. The point $\bar u$ exists because $\tau_1(1) = \tau_2(1)$ moreover we have that $\tau_1'(\bar u) \le \tau_2'(\bar u)$. From (2.14) we get

$$\frac{d}{du}\Big(\frac{\tau}{\tau'}\Big) = \frac{\theta}{\tau}$$

which integrated gives

$$\frac{\tau(u)}{\tau'(u)} = \frac{\tau_-}{\tau'(-1)} + \int_{-1}^{u} dv\, \frac{\theta(v)}{\tau(v)}$$

we then deduce

$$\frac{\tau_1(\bar u)}{\tau_1'(\bar u)} - \frac{\tau_2(\bar u)}{\tau_2'(\bar u)} = \frac{\tau_-}{\tau_1'(-1)} - \frac{\tau_-}{\tau_2'(-1)} + \int_{-1}^{\bar u} dv\, \theta(v)\Big[\frac{1}{\tau_1(v)} - \frac{1}{\tau_2(v)}\Big]$$

Since $\tau_1'(-1) > \tau_2'(-1)$ and $\tau_1(v) \ge \tau_2(v)$ for $v \in [-1,\bar u]$, the right hand side above is strictly negative. Recalling that $\tau_1(\bar u) = \tau_2(\bar u)$ we get $\tau_1'(\bar u) > \tau_2'(\bar u)$, the desired contradiction.

In order to prove that the infimum in (2.12) is uniquely attained for $\tau = \tau[\theta]$, the solution of (2.14), we perform the change of variable $\tau = e^{\varphi}$. We then get the functional

$$\widetilde{\mathcal{G}}(\theta,\varphi) := \mathcal{G}(\theta, e^{\varphi}) = \int_{-1}^{1} du\, \Big[\theta(u)\, e^{-\varphi(u)} - 1 - \log\theta(u) - \log\frac{\varphi'(u)}{[\tau_+ - \tau_-]/2}\Big] \tag{4.10}$$

which is strictly convex in $\varphi$; this trivially implies the claim.

4.4. **Non convexity of the quasi potential.** As we mentioned before, in the case of the SEP the quasi potential can be obtained by a variational problem analogous to (2.11) where one maximizes over the auxiliary profile [5,6,10,11]. In such a case, since the functional $\mathcal{G}(\theta,\tau)$ is convex in $\theta$ for fixed $\tau$, the rate functional $S(\theta)$ is trivially convex in $\theta$. In the case of the KMP process we need instead to minimize over the auxiliary profile $\tau$, therefore there is no reason to expect $S(\theta)$ to be convex. We now show, by an explicit computation, that the rate functional is indeed not convex.

We mention that non convexity of the rate functional $S$ has been shown for the asymmetric exclusion process [12]; in that case however the functional is degenerate, in the sense that there are infinitely many profiles for which $S$ vanishes. Therefore the mechanism of the non convexity is somehow different from the one in the KMP process, where $S(\theta)$ vanishes only at $\bar\theta$.

To prove the non convexity of the rate functional $S$ we shall exhibit profiles $\theta$ and $g$ so that, by choosing $\varepsilon$ small enough, we have

$$S(\theta) = S\Big(\frac12[\theta+\varepsilon g] + \frac12[\theta - \varepsilon g]\Big) > \frac12 S(\theta+\varepsilon g) + \frac12 S(\theta - \varepsilon g) \tag{4.11}$$

Let $\tau = \tau[\theta]$ be the strictly increasing solution of the boundary value problem (2.14), then by using (2.12) for $\varepsilon$ small enough and any profile $f$ vanishing at the boundaries, $f(\pm1) = 0$, we have

$$\begin{aligned}
S(\theta+\varepsilon g) &\le \mathcal{G}(\theta+\varepsilon g, \tau+\varepsilon f)\\
&= \mathcal{G}(\theta,\tau) + \varepsilon\int_{-1}^{1} du\,\Big\{\Big(\frac{\theta}{\tau} - 1\Big)\Big(\frac{g}{\theta} - \frac{f}{\tau}\Big) - \frac{f'}{\tau'}\Big\}\\
&\quad + \frac{\varepsilon^2}{2}\int_{-1}^{1} du\,\Big\{\Big(2\frac{\theta}{\tau} - 1\Big)\frac{f^2}{\tau^2} + \frac{g^2}{\theta^2} - 2\frac{gf}{\tau^2} + \frac{(f')^2}{(\tau')^2}\Big\} + o(\varepsilon^2)
\end{aligned}$$

where we brutally Taylor expanded (2.11).

Since $S(\theta) = \mathcal{G}(\theta, \tau)$, the inequality (4.11) will follow if we show that, for an appropriate choice of $f$ (recall that $\tau = \tau[\theta]$ is the solution of (2.14)) we can make the quadratic term in the previous equation strictly negative, i.e.

$$\int_{-1}^{1} du \left\{ \Big(2\frac{\theta}{\tau} - 1\Big)\frac{f^2}{\tau^2} + \frac{g^2}{\theta^2} - 2\frac{gf}{\tau^2} + \frac{(f')^2}{(\tau')^2} \right\} < 0 \tag{4.12}$$

Let us introduce the function

$$h(u) := \begin{cases} \tau_- + \dfrac{64}{81}(\tau_+ - \tau_-)(1-u^6) & \text{if} \quad -1 \le u \le -1/2 \\ \tau_+ + \dfrac{4}{27}(\tau_+ - \tau_-)(u-1) & \text{if} \quad -1/2 < u \le 1 \end{cases}$$

Note that $h \in C^1([-1,1])$, $h(\pm 1) = \tau_\pm$ and $h$ is strictly increasing. We choose the profile $\theta$ as

$$\theta(u) = h(u)\Big[1 - h(u)\frac{h''(u)}{h'(u)^2}\Big] \tag{4.13}$$

Note that $\theta > 0$, i.e. $\theta$ is an allowed profile in $\mathcal{M}$; the corresponding solution of the boundary value problem (2.14) is $\tau[\theta] = h$. We further choose $f(u) = (1-u^2)h'(u)$ (note that $f$ vanishes at the boundaries as required) and $g = f\theta^2/h^2$. With the above choices the left hand side of (4.12) equals

$$\begin{aligned}
&\int_{-1}^{1} du \left\{ \Big(2\frac{\theta}{h} - 1\Big)\frac{f^2}{h^2} - \frac{f^2\theta^2}{h^4} + \frac{(f')^2}{(h')^2} \right\} \\
&\quad = \int_{-1}^{1} du \left\{ -\Big(\frac{\theta}{h} - 1\Big)^2 \frac{f^2}{h^2} + \frac{(f')^2}{(h')^2} \right\} \\
&\quad = \int_{-1}^{1} du \left\{ -\frac{(h'')^2}{(h')^4} f^2 + \frac{(f')^2}{(h')^2} \right\} \\
&\quad = \int_{-1}^{1} du \left\{ -\frac{(h'')^2(1-u^2)^2}{(h')^2} + \frac{1}{(h')^2}\big[-2uh' + (1-u^2)h''\big]^2 \right\} \\
&\quad = 4\int_{-1}^{1} du \left\{ u^2 - u(1-u^2)\frac{h''}{h'} \right\} \\
&\quad = 4\Big\{ \int_{-1}^{1} du\, u^2 - 5\int_{-1}^{-1/2} du\,(1-u^2) \Big\} \;=\; 4\Big\{\frac{2}{3} - \frac{25}{24}\Big\} < 0
\end{aligned}$$

This completes the proof of (4.12) and therefore of the non convexity of the rate functional $S$.

4.5. **The rate functional on constant profiles.** Here we show that for constant profiles $\theta$ the boundary value problem (2.14) can be integrated; the corresponding value of the rate functional $S(\theta)$ can be expressed in terms of special functions.

We use the variable $\varphi = \log \tau$; we then have $S(\theta) = \widetilde{\mathcal{G}}(\theta, \varphi[\theta])$, where the functional $\widetilde{\mathcal{G}}$ has been defined in (4.10) and $\varphi[\theta]$ is the unique strictly increasing solution of the boundary value problem

$$\begin{cases} e^{\varphi}\dfrac{\varphi''}{(\varphi')^2} + \theta = 0 \\ \varphi(\pm 1) = \log \tau_\pm \end{cases} \tag{4.14}$$

If we restrict to constant profiles $\theta$ this equation can be integrated obtaining

$$\log \varphi'[\theta](u) = \log \varphi'[\theta](-1) + \theta \left\{ e^{-\varphi[\theta](u)} - \frac{1}{\tau_-} \right\} \tag{4.15}$$

and from this

$$S(\theta) = \widetilde{\mathcal{G}}(\theta, \varphi[\theta]) = 2\Big\{ -1 + \frac{\theta}{\tau_-} - \log\theta - \log\varphi'[\theta](-1) + \log\frac{\tau_+ - \tau_-}{2} \Big\}$$

From equation (4.15) we obtain also

$$\varphi'[\theta](-1) = \frac{1}{2} e^{\frac{\theta}{\tau_-}} \int_{\log\tau_-}^{\log\tau_+} d\psi\, e^{-\theta e^{-\psi}}$$

and finally with a change of variables

$$S(\theta) = 2\Big[ -\log\Big(\theta \int_{\frac{1}{\tau_+}}^{\frac{1}{\tau_-}} dy\, \frac{e^{-\theta y}}{y}\Big) - 1 + \log(\tau_+ - \tau_-)\Big] \tag{4.16}$$

In particular for $\theta$ large, from (4.16) we deduce the asymptotic expansion

$$S(\theta) = 2\Big\{ \frac{\theta}{\tau_+} + \Big(\log\frac{\tau_+ - \tau_-}{\tau_+} - 1\Big) + \frac{\tau_+}{\theta} \Big\} + O\Big(\frac{1}{\theta^2}\Big) \tag{4.17}$$

Recall that the equilibrium functional $S_0$ is given in (2.7) and note that for constant and large values of the profile $\theta$ we have $S_0(\theta) \approx 2\theta/\tau$. By comparing this with the expansion (4.17), we see that the leading order is the same but only the warmer thermostat matters, as it is quite reasonable from a physical point of view.

As we showed earlier, the rate functional $S$ is not convex. The restriction of $S$ to constant profiles obtained in (4.16) might however be convex; we do not have an analytic proof of the convexity of (4.16), but rough numerical evidences suggest this is the case.

4.6. **An additivity principle.** In [11] the rate functional $S$ was derived for the SEP by combinatorial techniques. It was then shown that $S$ satisfies a suitable *additivity principle* which allows to construct the rate functional for a system in a macroscopic interval $[a, b]$ from the rate functional of subsystems in the intervals $[a, c]$ and $[c, b]$, here $a < c < b$. More precisely, in [11] is introduced a modified rate functional $\widetilde{S}_{[a,b]}(\tau_a, \tau_b; \theta)$ where $\tau_a$, $\tau_b$ are the density at the endpoints and $\theta = \theta(u)$ is the density profile in $[a, b]$. The additivity principle is then formulated as

$$\widetilde{S}_{[a,b]}(\tau_a, \tau_b; \theta) = \sup_{\tau_c} \big\{ \widetilde{S}_{[a,c]}(\tau_a, \tau_c; \theta\restriction_{[a,c]}) + \widetilde{S}_{[c,b]}(\tau_c, \tau_b; \theta\restriction_{[c,b]}) \big\} \tag{4.18}$$

where $\theta\restriction_{[a,c]}$, respectively $\theta\restriction_{[c,b]}$, denotes the restriction of the profile $\theta$, which is defined on the interval $[a, b]$, to the subinterval $[a, c]$, respectively $[c, b]$. The additivity principle (4.18) plays a crucial role in the derivation of the rate functional for the asymmetric exclusion process. In [12] the expression of the rate functional from this principle is then deduced.

Here we show that the rate functional $S$ for the KMP process satisfies an additivity principle analogous to (4.18). Here, however, we need to minimize on the midpoint value $\tau_c$. This is due to the fact that in (2.12) we need to minimize over the auxiliary profile $\tau$; a direct derivation of the additivity formula, as was done in [12] for the asymmetric exclusion process, would clarify the basic physical difference between the KMP process and the SEP.

Let us consider the KMP process on the macroscopic interval $[a, b]$, here we denote the temperatures of the heat baths at the boundary by $\tau_a$, $\tau_b$. We then let $S_{[a,b]}(\tau_a, \tau_b; \theta)$ be the corresponding rate functional and introduce

$$\widetilde{S}_{[a,b]}(\tau_a, \tau_b; \theta) = S_{[a,b]}(\tau_a, \tau_b; \theta) - (b - a)\log\frac{\tau_b - \tau_a}{b - a} \tag{4.19}$$

by using (2.11) and (2.12) we then get

$$\widetilde{S}_{[a,b]}(\tau_a,\tau_b;\theta) = \inf_{\substack{\tau:\\ \tau(a)=\tau_a,\,\tau(b)=\tau_b}} \int_a^b du\, \Big[\frac{\theta(u)}{\tau(u)} - 1 - \log\frac{\theta(u)}{\tau(u)} - \log\tau'(u)\Big] \tag{4.20}$$

where the infimum is over the strictly monotone auxiliary profiles $\tau(u)$, $u \in [a,b]$. We then get the additivity principle for the KMP process:

$$\widetilde{S}_{[a,b]}(\tau_a,\tau_b;\theta) = \inf_{\tau_c\in[\tau_a,\tau_b]} \big\{\widetilde{S}_{[a,c]}(\tau_a,\tau_c;\theta\restriction_{[a,c]}) + \widetilde{S}_{[c,b]}(\tau_c,\tau_b;\theta\restriction_{[c,b]})\big\} \tag{4.21}$$

It is not difficult to show, see [11], that the expression (2.11)–(2.12) for the rate functional follows from the additivity rule (4.21).

4.7. **Remarks.** We again conclude with a few mathematical remarks. We have discussed existence and uniqueness of (2.14) only for bounded profiles $\theta$; the extension to $\theta \in \mathcal{M}$ should be however straightforward. Let $V(\theta)$ be the quasi potential as defined by the variational problem (4.2). Since the optimal path $\pi^*$ has been explicitly constructed, the rigorous proof of the upper bound $V(\theta) \le \inf_{\tau\in\mathcal{T}_{\tau_\pm}} \mathcal{G}(\theta,\tau)$ should be carried out as in [6]. The proof of the lower bound $V(\theta) \ge \inf_{\tau\in\mathcal{T}_{\tau_\pm}} \mathcal{G}(\theta,\tau)$ is instead more troublesome. The computations presented here essentially prove this bound for strictly positive smooth paths $\pi$, but the argument in [6] to extend it to arbitrary paths in $\mathcal{E}_{\theta,T}$ takes advantages of the convexity (special for the SEP) of the dynamical rate functional $J$. This problem is of course related to the proof of the lower bound for the dynamical large deviation principle for any open set mentioned at the end of Section 3. The identification of the quasi potential $V$ with the rate functional for the invariant measure $S$ has been proven for the SEP in [7]; although the strategy is of wider applicability, the technical points might require some extra effort.

## 5. Higher space dimensions

The KMP process introduced in Section 2 can be easily generalized to the case of space dimensions $d > 1$. Let $\Lambda$ be a smooth domain in $\mathbb{R}^d$ and set $\Lambda_N := \mathbb{Z}^d \cap N\Lambda$. We then define the process on $\Sigma_N := \mathbb{R}_+^{\Lambda_N}$ as follows: every pair of nearest neighbors oscillators exchanges energy according to the rule described in Section 2 and every oscillator at a boundary site $x$ is in contact with a thermostat at temperature $\tilde\tau(x/N)$ for a fixed function $\tilde\tau$.

Several computations of this paper can be repeated step by step when the model is not one–dimensional. In particular the hydrodynamic equation has still the same form (3.4) with the boundary condition $\theta\restriction_{\partial\Lambda} = \tilde\tau$ and the dynamic large deviation functional $J$ has the same form as (3.14). Formula (4.2) as well as the Hamilton–Jacobi equation (4.5) for the quasi potential holds in any dimension; we can still perform the change of variables (4.6) and reduce (4.5) to (4.7). However the solution of the boundary value (2.14) does not give the quasi potential because, with this choice, the right hand side of (4.6) is a functional derivative only if $d = 1$.

However, by analyzing the variational problem (4.2), we derive an upper bound for quasi potential $V(\theta)$ that holds in any space dimension. We also discuss here the Gaussian fluctuations of the empirical energy when $\xi$ is distributed according to the invariant measure. We shall obtain the covariance of the Gaussian fluctuations by expanding the large deviations functional $S(\theta)$ around the stationary profile $\bar\theta$. We note that in the one–dimensional case the arguments are easier thanks to the more explicit form of $S$.

5.1. **Upper bound for the quasi potential.** Let us denote by $\bar\theta(u)$, $u \in \Lambda$ the stationary solution of (3.4) with boundary condition $\bar\theta(u) = \tilde\tau(u)$, $u \in \partial\Lambda$. Note that, for generic boundary conditions $\tilde\tau$, the profile $\bar\theta$ does not have the simple form (2.10). Of course $\bar\theta$ is still the most likely profile for the empirical energy under the invariant measure. We also introduce the *local equilibrium* large deviation function

$$S_{\rm eq}(\theta) = \int_\Lambda du\ \Big[\frac{\theta(u)}{\bar\theta(u)} - 1 - \log\frac{\theta(u)}{\bar\theta(u)}\Big]\,, \tag{5.1}$$

and note that it coincides with the function defined in (3.15) and it is thus the rate functional for the product measure $\nu^N_{\bar\theta}$.

When $d=1$ we can use (2.11) and easily obtain the upper bound

$$S(\theta) = \inf_{\tau\in\mathcal{M}_{T_{\tau_\pm}}} \mathcal{G}(\theta,\tau) \le \mathcal{G}(\theta,\bar\theta) = S_{\rm eq}(\theta) \tag{5.2}$$

For $d>1$ we use a different strategy. Given a path $\pi = \pi(t,u)$ satisfying the boundary condition $\pi(t,u) = \tilde\tau(u)$, $u \in \partial\Lambda$, a straightforward computation shows that

$$\begin{aligned}
J_{[-T,0]}(\pi) &= \frac12\int_{-T}^0 dt\,\Big\langle \nabla^{-1}\Big[\partial_t\pi - \frac12\Delta\pi\Big], \frac{1}{\pi^2}\nabla^{-1}\Big[\partial_t\pi - \frac12\Delta\pi\Big]\Big\rangle\\
&= \frac12\int_{-T}^0 dt\,\Big\langle \nabla^{-1}\Big[\partial_t\pi + \frac12\Delta\pi + \nabla\Big(\pi^2\nabla\frac{1}{\bar\theta}\Big) - \Delta\pi - \nabla\Big(\pi^2\nabla\frac{1}{\bar\theta}\Big)\Big],\\
&\qquad\qquad \frac{1}{\pi^2}\nabla^{-1}\Big[\partial_t\pi + \frac12\Delta\pi + \nabla\Big(\pi^2\nabla\frac{1}{\bar\theta}\Big) - \Delta\pi - \nabla\Big(\pi^2\nabla\frac{1}{\bar\theta}\Big)\Big]\Big\rangle\\
&= S_{\rm eq}(\pi(0)) - S_{\rm eq}(\pi(-T)) - \frac12\int_{-T}^0 dt\,\Big\langle\frac{(\nabla\bar\theta)^2}{\bar\theta^4}, (\pi-\bar\theta)^2\Big\rangle\\
&\quad + \frac12\int_{-T}^0 dt\,\Big\langle \nabla^{-1}\Big[\partial_t\pi + \frac12\Delta\pi + \nabla\Big(\pi^2\nabla\frac{1}{\bar\theta}\Big)\Big],\\
&\qquad\qquad \frac{1}{\pi^2}\nabla^{-1}\Big[\partial_t\pi + \frac12\Delta\pi + \nabla\Big(\pi^2\nabla\frac{1}{\bar\theta}\Big)\Big]\Big\rangle
\end{aligned}$$

The quasi potential is defined by the variational problem (4.2). Hence, to obtain an upper bound for $V(\theta)$ it is enough to exhibit a path $\pi$ which connects $\bar\theta$ to $\theta$. We choose $\pi(t) = \tilde\theta(-t)$ where $\tilde\theta(t)$ solves

$$\begin{cases}
\partial_t\tilde\theta(t) = \frac12\Delta\tilde\theta(t) + \nabla\Big(\tilde\theta(t)^2\nabla\frac{1}{\bar\theta}\Big)\\
\tilde\theta(t,u) = \tilde\tau(u)\,, \quad u\in\partial\Lambda\\
\tilde\theta(0,u) = \theta(u)
\end{cases}$$

We note that the path $\pi$ connects $\bar\theta$ to $\theta$ since $\tilde\theta(t) \to \bar\theta$ as $t\to\infty$. By using the path $\pi$ in the above expression for $J_{[-T,0]}(\pi)$ and letting $T\to\infty$ we get

$$V(\theta) \le S_{\rm eq}(\theta) - \frac12\int_{-\infty}^0 dt\,\Big\langle\frac{(\nabla\bar\theta)^2}{\bar\theta^4}, [\pi(t)-\bar\theta]^2\Big\rangle \le S_{\rm eq}(\theta)$$

which shows that the upper bound $V(\theta)\le S_{\rm eq}(\theta)$ holds in any space dimension. We also note that the above inequality is strict unless $\theta=\bar\theta$.

5.2. **Gaussian fluctuations.** In the case $d=1$ we can follow step by step the argument given in [11] for the SEP. We consider a small perturbation, $\theta = \bar\theta + \varepsilon\Theta$, of the stationary profile $\bar\theta$, and consequently have $\tau[\theta] = \bar\theta + \varepsilon T$, where, to first order in $\varepsilon$, (2.14) gives

$$\frac{\bar\theta^2}{(\nabla\bar\theta)^2}\Delta T - T = -\Theta \tag{5.3}$$

The functional $S(\theta)$ has a minimum at $\bar\theta$ so that its expansion in $\varepsilon$ is

$$S(\theta) = S(\bar\theta) + \frac{1}{2}\varepsilon^2 \langle \Theta, C^{-1}\Theta\rangle + o\left(\varepsilon^2\right) \tag{5.4}$$

The operator $C$ is the covariance for the Gaussian fluctuations of the empirical energy under the invariant measure $\mu_{N,\tau_\pm}$. Since $S(\theta) = \mathcal{G}(\theta, \tau[\theta])$, we get

$$\begin{aligned}
\langle \Theta, C^{-1}\Theta\rangle &= \int_{-1}^{1} du \left\{ \frac{[T(u)-\Theta(u)]^2}{\bar\theta^2(u)} + \frac{[\nabla T(u)]^2}{[\nabla\bar\theta]^2} \right\} \\
&= \int_{-1}^{1} du \left\{ \frac{\bar\theta(u)^2[\Delta T(u)]^2}{[\nabla\bar\theta]^4} - \frac{T(u)\Delta T(u)}{[\nabla\bar\theta]^2} \right\} = \left\langle \Delta T, \frac{W}{(\nabla\bar\theta)^2}\Delta T \right\rangle
\end{aligned}$$

where we used Taylor expansions, integrations by parts, $T(\pm 1) = 0$, and (5.3). The operator $W$ is defined as

$$W := \frac{\bar\theta^2}{(\nabla\bar\theta)^2}\,\mathbb{1} + (-\Delta)^{-1} \tag{5.5}$$

From equation (5.3) we get $\Theta = -W\Delta T$ and this implies

$$\langle \Theta, C^{-1}\Theta\rangle = \left\langle \Delta T, \frac{W}{(\nabla\bar\theta)^2}\Delta T \right\rangle = \left\langle \Theta, \frac{W^{-1}}{(\nabla\bar\theta)^2}\Theta \right\rangle$$

so that the covariance $C$ is given by

$$C = (\nabla\bar\theta)^2\, W = \bar\theta^2\,\mathbb{1} + (\nabla\bar\theta)^2\,(-\Delta)^{-1} \tag{5.6}$$

The first term above is simply the covariance of the Gaussian fluctuations of the empirical energy for local equilibrium product measure $\nu^N_{\bar\theta}$, while the second term represents the contribution to the covariance due to the long range correlations in the stationary nonequilibrium state. As in the case of the SEP [5, 9–11, 24] this correction is given by $(-\Delta)^{-1}$, the Green function of the Dirichlet Laplacian. Since $(-\Delta)^{-1} > 0$, for the KMP process this correction enhances the Gaussian fluctuations, while in the case of SEP it decreases them. We also note that, by exploiting the duality of the KMP process with the process we shall introduce in Section 6, the expression (5.6) for the covariance could be rigorously deduced as in the case of the SEP [9, 24].

To obtain the covariance of Gaussian fluctuations in the case $d > 1$ we instead argue as in [5]. Let us introduce the "pressure" as the Legendre transform of the rate functional $S(\theta)$, i.e.

$$G(h) := \sup_\theta \left\{ \langle \theta, h\rangle - S(\theta) \right\} \tag{5.7}$$

We then get that $G(h)$ satisfies the Hamilton–Jacobi equation dual to (4.5), i.e.

$$\left\langle \nabla h, \left(\frac{\delta G}{\delta h}\right)^2 \nabla h \right\rangle = \left\langle \nabla h, \nabla \frac{\delta G}{\delta h} \right\rangle \tag{5.8}$$

where $h(u)$ satisfies the boundary conditions $h(u)|_{\partial\Lambda} = 0$.

Let us denote by $G_{\rm eq}$ the pressure associated via (5.7) to the local equilibrium functional $S_{\rm eq}$; we look for a solution of (5.8) in the form

$$G(h) = G_{\rm eq}(h) + \langle g, h\rangle + \frac{1}{2}\langle h, B\, h\rangle + o(h^2) \tag{5.9}$$

for some function $g = g(u)$ and some linear operator $B$. From (5.4) we get

$$G(h) = \langle \bar\theta, h\rangle + \frac{1}{2}\,\langle h, C\, h\rangle + o(h^2) \tag{5.10}$$

hence the second derivative of $G$ at $h = 0$ is the covariance of the density fluctuations. By comparing (5.9) to (5.10) we find

$$C = \frac{\delta^2 G_{\mathrm{eq}}}{\delta h^2}\Big|_{h=0} + B = \bar{\theta}^2\, \mathbb{1} + B \tag{5.11}$$

By plugging (5.9) into (5.8) and expanding up to second order in $h$, it is not difficult to show, see [5] for the case of the SEP, that $g = 0$ and

$$\langle h, \Delta B\, h\rangle = -\big\langle h, |\nabla\bar{\theta}|^2 h\big\rangle \tag{5.12}$$

The operator $B$ therefore satisfies

$$\frac{1}{2}[\Delta B + B\Delta] = -|\nabla\bar{\theta}|^2 \tag{5.13}$$

See [24] for another derivation of this equation based on fluctuating hydrodynamic instead of large deviations.

From (5.13) we see that if $\nabla\bar{\theta}$ is constant (this condition can be realized by a suitable choice of the thermostat $\tilde{\tau}$), the operator $B$ has the kernel

$$B(u, v) = |\nabla\bar{\theta}|^2(-\Delta)^{-1}(u, v) \tag{5.14}$$

where $(-\Delta)^{-1}(u, v)$ is the Green function of the Dirichlet Laplacian in $\Lambda$. The interpretation of (5.11) and (5.14) is as in the one dimensional case (5.6); we note the fact that $B$ is a positive operator can also be obtained as a consequence of the bound $S(\theta) \le S_{\mathrm{eq}}(\theta)$.

## 6. The dual process

The analysis in [18] is based on a duality relationship between the KMP process and another process we discuss next in the one–dimensional case. The state space is $\Sigma_N := \mathbb{N}^{\Lambda_N}$ where $\mathbb{N} := \{0, 1, \dots\}$ is the set of natural numbers. If $\xi = \{\xi_x\,,\ x \in \Lambda_N\} \in \Sigma_N$, the value $\xi_x$ at the site $x$ can therefore be interpreted as the number of particles at $x$. As for the KMP process, at each bond $\{x, x+1\}$ there is an exponential clock of rate one; when it rings the total number of particles $\xi_x + \xi_{x+1}$ is redistributed uniformly across the bond $\{x, x+1\}$. Moreover the boundary sites $\pm N$ evolve according to a heat bath dynamics with respect to a geometric distribution with parameter $p_\pm$. More formally, the infinitesimal generator has still the form (2.1) but now the bulk dynamics is defined by

$$L_{x,x+1} f\,(\xi) := \frac{1}{\xi_x + \xi_{x+1} + 1} \sum_{k=0}^{\xi_x+\xi_{x+1}} \big[f(\xi^{(x,x+1),k}) - f(\xi)\big] \tag{6.1}$$

where the configuration $\xi^{(x,x+1),k}$ is defined as

$$\big(\xi^{(x,x+1),k}\big)_y := \begin{cases} \xi_y & \text{if } \ y \neq x, x+1 \\ k & \text{if } \ y = x \\ \xi_x + \xi_{x+1} - k & \text{if } \ y = x+1 \end{cases}$$

The boundary part of the generator is defined as follows

$$L_\pm f\,(\xi) := \sum_{k=0}^{\infty} p_\pm (1 - p_\pm)^k \big[f(\xi^{\pm N,k}) - f(\xi)\big] \tag{6.2}$$

where $p_\pm \in (0, 1)$ are the parameters of the reservoirs and the configuration $\xi^{x,k}$ is defined as

$$\big(\xi^{x,k}\big)_y := \begin{cases} \xi_y & \text{if } \ y \neq x \\ k & \text{if } \ y = x \end{cases} \tag{6.3}$$

If $p_+ = p_- = p$ the dynamics is reversible with respect to the product of geometric distributions of parameter $p$, i.e. the invariant measure is

$$\mu_{N,p}(\xi) = \prod_{x\in\Lambda_N} \left[p\,(1-p)^{\xi_x}\right] \tag{6.4}$$

By a computation analogous to (2.6)–(2.8), it is easy to show that when $\xi$ is distributed according to $\mu_{N,p}$ then the empirical density $\pi_N(\xi)$, which is defined as in (2.3), satisfies a large deviation principle with the rate functional

$$S_0(\theta) = \int_{-1}^{1} du \left\{\theta(u)\log\frac{\theta(u)}{\bar\theta} + [1+\theta(u)]\log\frac{1+\bar\theta}{1+\theta(u)}\right\} \tag{6.5}$$

where the parameter $\bar\theta$ is related to $p$ by the relation $\bar\theta = \sum_{k=0}^{\infty} k\,p(1-p)^k = (1-p)/p$.

When $p_+ \neq p_-$ the model is no longer reversible and the invariant measure $\mu_{N,p_\pm}$ is not explicitly known. In the sequel we shall assume $p_- > p_+$. We can repeat the computations done for the KMP process and get the hydrodynamic equation. This is still the linear heat equation with the appropriate boundary conditions, i.e.

$$\begin{cases} \partial_t\theta(t) &= \frac{1}{2}\Delta\theta(t) \\ \theta(t,\pm1) &= \theta_\pm = \dfrac{1-p_\pm}{p_\pm} \\ \theta(0,u) &= \theta_0(u) \end{cases} \tag{6.6}$$

As before the most likely density profile $\bar\theta$ is the stationary solution of (6.6).

To obtain the dynamic large deviation principle we introduce a smooth function $H = H(t,u)$ vanishing at the boundary and consider the following time dependent perturbation of the generator $L_{x,x+1}$ in (6.1)

$$\begin{aligned} L^H_{x,x+1}f\,(\xi) \quad := \quad & \frac{1}{\xi_x+\xi_{x+1}+1}\sum_{k=0}^{\xi_x+\xi_{x+1}} e^{(\xi_x-k)[H(t,(x+1)/N)-H(t,x/N)]} \\ & \qquad\qquad \times\ \left[f(\xi^{(x,x+1),k}) - f(\xi)\right] \end{aligned}$$

The hydrodynamic equation associated to this perturbed dynamics is given by

$$\partial_t\theta(t) = \frac{1}{2}\Delta\theta(t) - \nabla\Big(\theta(t)[1+\theta(t)]\nabla H(t)\Big) \tag{6.7}$$

with the same boundary conditions as (6.6). By the same computations as in Section 3, we get that the dynamical large deviation functional is

$$J_{[0,T]}(\pi) = \frac{1}{2}\int_0^T dt\,\big\langle\nabla H(t), \pi(t)[1+\pi(t)]\nabla H(t)\big\rangle \tag{6.8}$$

where $H$ has to be obtained from the path $\pi$ by using equation (6.7) with $\theta(t)$ replaced by $\pi(t)$.

This leads to the following Hamilton–Jacobi equation for the quasi potential

$$\Big\langle\nabla\frac{\delta V}{\delta\theta}, \theta(1+\theta)\nabla\frac{\delta V}{\delta\theta}\Big\rangle + \Big\langle\frac{\delta V}{\delta\theta}, \Delta\theta\Big\rangle = 0 \tag{6.9}$$

where $\delta V/\delta\theta$ vanishes at the boundary and $\theta(\pm1) = \theta_\pm$.

We look for a solution of the form

$$\frac{\delta V}{\delta\theta} = \log\frac{\theta}{1+\theta} - \log\frac{F}{1+F} \tag{6.10}$$

By the same computations as in Section 4, we reduce the Hamilton–Jacobi equation (6.9) to

$$\Big\langle \frac{\theta - F}{F^2(1+F)^2}\, ,\, F(1+F)\Delta F + (\theta - F)(\nabla F)^2 \Big\rangle = 0 \tag{6.11}$$

We thus obtain a solution of (6.9) considering the functional

$$V(\theta) = \int_{-1}^{1} du\, \Big\{ \theta(u) \log \frac{\theta(u)}{F(u)} + [1+\theta(u)] \log \frac{1+F(u)}{1+\theta(u)} - \log \frac{F'(u)}{[\theta_+ - \theta_-]/2} \Big\} \tag{6.12}$$

where $F(u)$ has to be computed from $\theta(u)$ as the unique strictly increasing solution of the boundary value problem

$$\begin{cases} F(1+F)\dfrac{F''}{\big(F'\big)^2} + \theta - F = 0 \\ F(\pm 1) = \theta_\pm \end{cases} \tag{6.13}$$

As for the KMP process it is possible to check that this is the right solution of the Hamilton–Jacobi equation (6.9).

By the change of variable $F = e^{\varphi}$, it is easy to verify that the right hand side of (6.12) is strictly convex in $\varphi$. We therefore have, analogously to the KMP process,

$$V(\theta) = \inf_F \int_{-1}^{1} du\, \Big\{ \theta(u) \log \frac{\theta(u)}{F(u)} + [1+\theta(u)] \log \frac{1+F(u)}{1+\theta(u)} - \log \frac{F'(u)}{[\theta_+ - \theta_-]/2} \Big\}$$

where the infimum is carried out over all strictly increasing functions $F$ satisfying the boundary condition $F(\pm 1) = \theta_\pm$.

## 7. Conclusions: few comments on generic models

For the SEP, the derivation of the rate function for the stationary non equilibrium state obtained in [10,11] depends heavily on the details of the microscopic process. On the other hand, the variational approach in [5] depends only on the macroscopic transport coefficients, bulk diffusion $D$ and mobility $\sigma$ of the system. These are not independent functions, they are related by the Einstein relation $D(\rho) = \sigma(\rho)\chi(\rho)^{-1}$ where $\chi(\rho)$ is the *compressibility*. It is defined as $\chi(\rho)^{-1} = \lambda'(\rho) = f_0''(\rho)$ where $f_0$ is the (equilibrium) Helmholtz free energy of the system and $\lambda$ is the chemical potential. This means in particular that while the derivation in [10,11] is only valid for nearest neighbor jumps, the result holds for the general SEP. In this paper we have discussed a model, the KMP process (in fact two models if we consider also its dual process), in which the rate functional has an expression very similar to the one for the SEP. Here we discuss what are the essential features of the functional form of these coefficients in the derivation of the rate functional $S$. In this discussion we shall consider $D$ and $\sigma$ as given and discuss the large deviations properties of the nonequilibrium state.

We discuss only one–dimensional (symmetric) diffusive system with a single conservation law and particle reservoirs at the boundary. Here it will be convenient to think of the conserved quantity as the density of particles. For general models, the hydrodynamic equation is expected (proven for equilibrium models in [26] and in [14,15] for nonequilibrium under the so called *gradient condition*), to be given by a nonlinear diffusion equation with Dirichlet data at boundary, i.e.

$$\begin{cases} \partial_t \rho(t,u) &=& \dfrac{1}{2}\nabla\Big(D\big(\rho(t,u)\big)\nabla\rho(t,u)\Big) \\ \rho(t,\pm 1) &=& \rho_\pm \\ \rho(0,u) &=& \rho_0(u) \end{cases} \tag{7.1}$$

where the bulk diffusion $D(\rho) = \sigma(\rho)\chi(\rho)^{-1}$ is given by a Green–Kubo formula, see e.g. [25, II.2.2]. For the KMP process, as well as for the SEP, we simply have $D = 1$, i.e. $\sigma = \chi$.

The probability of a large deviations from the hydrodynamic behavior are expected (to our knowledge for open systems this has been proven only for the SEP in [6], see however [25, II.3.7] for an heuristic derivation for equilibrium lattice gas models) to have the form (3.16)–(3.17) where the dynamical cost $J_{[0,T]}$ should be of the form

$$J_{[0,T]}(\pi) = \frac{1}{2}\int_0^T dt\, \langle \nabla H(t), \sigma(\pi(t))\nabla H(t)\rangle \tag{7.2}$$

in which the perturbation $H$ has to be chosen so that the fluctuation $\pi$ solves the perturbed hydrodynamic

$$\begin{cases} \partial_t \pi(t) &= \frac{1}{2}\nabla\Big(D\big(\pi(t)\big)\nabla\pi(t)\Big) - \nabla\Big(\sigma\big(\pi(t)\big)\nabla H(t)\Big) \\ \pi(t,\pm 1) &= \rho_\pm \\ \pi(0,u) &= \rho_0(u) \end{cases} \tag{7.3}$$

and $\sigma(\pi)$ is the *mobility* of the system. For the SEP process we have $\sigma(\pi) = \pi(1-\pi)$ (note that in this case we have $0 \le \pi \le 1$) while for the KMP process, respectively its dual, we have $\sigma(\pi) = \pi^2$, respectively $\sigma(\pi) = \pi(1+\pi)$.

We first mention the few examples in which it is possible to obtain the rate function $S$ in a closed form. The following models are however even simpler than the SEP or the KMP process since they do not exhibit the non–locality of $S$, which reflects, at the large deviation level, the long range correlations of the system which are expected [1, 24] to be a generic feature of nonequilibrium models.

The easiest example is provided by independent particles. In this case we have $D$ constant and $\sigma$ linear. The nonequilibrium state is a product measure and it is easy to verify that $S(\rho) = \int_{-1}^1 du\, f\big(\rho(u), \bar\rho(u)\big)$, where

$$f(\rho,\tau) = f_0(\rho) - f_0(\tau) + (\rho-\tau)f_0'(\tau) = \rho\log(\rho/\tau) - (\rho-\tau) \tag{7.4}$$

and $\bar\rho$ is the stationary solution of (7.1). Another example is the so called zero range process, see e.g. [25, II.7.1]. In this case $D(\rho) = \Phi'(\rho)$ and $\sigma(\rho) = \Phi(\rho)$ where the (increasing) function $\Phi$ depends on the microscopic rates. As shown in [8] the nonequilibrium state is again a product measure and, as discussed in [4, 5], its rate function is $S(\rho) = \int_{-1}^1 du\, f\big(\rho(u), \bar\rho(u)\big)$ for $f$ again given by (7.4) with the appropriate $f_0$. . These examples (the first being a special case of the second) are characterized by the fact that $\sigma(\rho) = C\exp\{\lambda(\rho)\}$ where $C > 0$ is a constant and $\lambda$ is the chemical potential. The Einstein formula then gives $D(\rho) = \sigma'(\rho)$. The last example is the Ginzburg–Landau model, see e.g. [25, II.7.3], where $\sigma$ is a constant while $D$ is determined by the Einstein relation. In this case the nonequilibrium state is still a product measure and its rate function has the same expression as in the zero range process.

We note that for the SEP, as well as for the KMP process and its dual, we have $D(\rho)$ constant and $\sigma(\rho)$ a second order polynomial in $\rho$. We next show that an expression of the rate function $S$ of the nonequilibrium state can be derived under a general hypothesis. More precisely, we shall assume that the diffusion coefficient $D(\rho)$ and the mobility $\sigma(\rho)$ satisfy the following condition. There exists a constant $a \in \mathbb{R}$ such that for any $\rho \neq \tau$

$$\frac{\sigma(\rho)-\sigma(\tau)}{\int_\tau^\rho dr\, D(r)} = \frac{\sigma'(\tau)}{D(\tau)} + a\,(\rho-\tau) \tag{7.5}$$

This condition, of course, identifies a rather tiny class of models that in fact coincides with the class of all the examples discussed. We should not expect to be able to obtain $S$ in almost a closed form for *any* model. As we shall see, the locality of the functional $S$ corresponds to the special case (in this class) $a = 0$.

Let us first discuss which functions $D$ and $\sigma$ satisfy condition (7.5). We rewrite it with $\rho$ and $\tau$ exchanged

$$\frac{\sigma(\tau) - \sigma(\rho)}{\int_\rho^\tau dr\ D(r)} = \frac{\sigma'(\rho)}{D(\rho)} + a(\tau - \rho)$$

This equation together with (7.5) imply

$$\frac{\sigma'(\tau)}{D(\tau)} - \frac{\sigma'(\rho)}{D(\rho)} = 2a(\tau - \rho)$$

It is easy to see that this is equivalent to

$$\frac{\sigma'(r)}{D(r)} = 2ar + c \tag{7.6}$$

with $c$ an arbitrary constant. Condition (7.6) is a necessary condition for the validity of (7.5). We rewrite (7.6) in the integrated form

$$\sigma(\rho) - \sigma(\tau) = 2a \int_\tau^\rho dr\ rD(r) + c \int_\tau^\rho dr\ D(r)$$

and substitute it inside (7.5). We thus obtain

$$\frac{2a \int_\tau^\rho dr\ rD(r)}{\int_\tau^\rho dr\ D(r)} = a(\rho + \tau) \tag{7.7}$$

A pair $(\sigma, D)$ is a solution of (7.5) if and only if is a solution of (7.6) and (7.7).

When $a = 0$, equation (7.7) is always satisfied and (7.6) becomes $\sigma'(r) = cD(r)$. If $c \neq 0$ we have the solutions corresponding to zero range dynamics (with an extra multiplicative factor $c$); if $c = 0$ we have the solutions corresponding to Ginzburg–Landau models.

When $a \neq 0$, equation (7.7) becomes

$$2 \int_\tau^\rho dr\ rD(r) = (\rho + \tau) \int_\tau^\rho dr\ D(r) \tag{7.8}$$

We differenciate with respect to $\rho$ and obtain

$$(\rho - \tau)D(\rho) = \int_\tau^\rho dr\ D(r)$$

that is satisfied if and only if $D$ is constant. Now condition (7.6) imposes that $\sigma(\rho)$ is a second order polynomial in $\rho$. In this class of solutions fall the simple exclusion model, the KMP model and its dual.

To write the rate functional $S$ we need to introduce a little more notation. We let $d(\rho) = \int_0^\rho dr\ D(r)$, since $D > 0$ the function $d$ is strictly increasing; we denote its inverse by $b$. We finally set $A(\varphi) := \sigma\big(b(\varphi)\big)$. We next denote partial derivatives by a subscript. Let us introduce a function of two variables $f = f(\rho, \tau)$ such that $f_{\rho\rho}(\rho, \tau) = D(\rho)\sigma(\rho)^{-1} = \chi^{-1}(\rho)$ and normalize $f$ so that $f(\cdot, \tau)$ has a minimum at $\tau$ and $f(\tau, \tau) = 0$. Therefore

$$f(\rho, \tau) = \int_\tau^\rho dr \int_\tau^r dr'\ \frac{1}{\chi(r')}$$

It is easy to verify that in the equilibrium case, $\rho_+ = \rho_- = \bar\rho_0$, the rate function $S_0$ is simply given by $S_0(\rho) = \int_{-1}^1 du\, f\big(\rho(u), \bar\rho_0\big)$. To obtain the rate function $S$ in the nonequilibrium case $\rho_+ \neq \rho_-$ we introduce the functional of two variables

$$\mathcal{G}(\rho,\varphi) := \int_{-1}^{1} du \, \Big\{ f\big(\rho(u), b(\varphi(u))\big) - \frac{1}{a} \log \frac{\nabla\varphi(u)}{\nabla d(\bar\rho(u))} \Big\} \tag{7.9}$$

where $\bar\rho$ is the equilibrium profile. Note that $\nabla d(\bar\rho(u)) = D(\bar\rho(u))\nabla u$ is a constant since its divergence must vanish in the stationary state.

We claim that, under condition (7.5), the rate function $S$ can be expressed as $S(\rho) = \mathcal{G}(\rho, \varphi[\rho])$ where, given $\rho$, the auxiliary function $\varphi = \varphi[\rho]$ is the solution of the Euler–Lagrange equation $\delta\mathcal{G}(\rho,\varphi)/\delta\varphi = 0$, that is

$$\begin{cases} \dfrac{1}{a}\dfrac{\Delta\varphi}{\big(\nabla\varphi\big)^2} + \dfrac{\rho - b(\varphi)}{A(\varphi)} = 0 \\ d(\varphi(\pm 1)) = d(\rho_\pm) \end{cases} \tag{7.10}$$

where we used $f_\tau(\rho,\tau) = -D(\tau)(\rho-\tau)/\sigma(\tau)$, $b'(\varphi) = D(b(\varphi))^{-1}$ and the definition of $A$.

The definition of the functional $\mathcal{G}$ and the above equation are not really meaningful if $a = 0$, as it is the case for the simple models in which $S$ is local discussed above. However, in such a case we understand (7.10) as $\Delta\varphi = 0$ whose solution is $\varphi(u) = d(\bar\rho(u))$. Plugging it into the functional $\mathcal{G}$ we get, by understanding $(\log 1)/0 = 0$, the correct local functional $S(\rho)$. On the other hand, as soon as $a \neq 0$, the functional $S$ is nonlocal.

To establish the claim, we next show that the functional $S$ solves the Hamilton–Jacobi equation

$$\Big\langle \nabla\frac{\delta S}{\delta\rho}, \sigma(\rho)\nabla\frac{\delta S}{\delta\rho}\Big\rangle + \Big\langle \frac{\delta S}{\delta\rho}, \nabla\Big(D(\rho)\nabla\rho\Big)\Big\rangle = 0 \tag{7.11}$$

The argument to conclude the identification of $S$ with the quasi potential, as defined in (4.2), is indeed essentially the one carried out in section 4.2 and it is therefore omitted.

By the definition of $S$, we get $\delta S(\rho)/\delta\rho = \delta\mathcal{G}(\rho,\varphi)/\delta\rho = f_\rho(\rho, b(\varphi))$ so that the left hand side of (7.11), after an integration by parts, reduces to

$$\begin{aligned} &\Big\langle f_{\rho\rho}(\rho,b(\varphi))\nabla\rho + \frac{f_{\rho\tau}(\rho,b(\varphi))}{D(b(\varphi))}\nabla\varphi, \\ &\qquad\qquad \sigma(\rho) f_{\rho\rho}(\rho,b(\varphi))\nabla\rho + \sigma(\rho)\frac{f_{\rho\tau}(\rho,b(\varphi))}{D(b(\varphi))}\nabla\varphi - D(\rho)\nabla\rho \Big\rangle \\ &= \Big\langle f_{\rho\rho}(\rho,b(\varphi))\nabla\rho + \frac{f_{\rho\tau}(\rho,b(\varphi))}{D(b(\varphi))}\nabla\varphi, \sigma(\rho)\frac{f_{\rho\tau}(\rho,b(\varphi))}{D(b(\varphi))}\nabla\varphi \Big\rangle \\ &= \Big\langle \nabla d(\rho), \frac{-\nabla\varphi}{A(\varphi)} \Big\rangle + \Big\langle \nabla\varphi, \frac{\sigma(\rho)}{A(\varphi)^2}\nabla\varphi \Big\rangle \end{aligned}$$

where we used the Einstein relation $\sigma(\rho) f_{\rho\rho}(\rho, b(\varphi)) = D(\rho)$ in the first step and $f_{\rho\tau}\big(\rho, b(\varphi)\big) = -D(b(\varphi))/A(\varphi)$ in the second one.

We next write $\nabla d(\rho) = \nabla[d(\rho) - \varphi] + \nabla\varphi$ and integrate by parts the first term in the last expression above (recall that $d(\rho)$ and $\varphi$ satisfy the same boundary conditions). We finally get that the left hand side of (7.11) equals

$$\Big\langle d(\rho) - \varphi, \nabla\Big(\frac{\nabla\varphi}{A(\varphi)}\Big) + \frac{\sigma(\rho) - A(\varphi)}{d(\rho) - \varphi}\frac{1}{A(\varphi)^2}\big(\nabla\varphi\big)^2 \Big\rangle$$

We therefore find that the functional $S$ solves the Hamilton–Jacobi equation (7.11) provided $\varphi$ satisfies the equation

$$A(\varphi)\Delta\varphi + \Big[ -A'(\varphi) + \frac{\sigma(\rho) - A(\varphi)}{d(\rho) - \varphi} \Big] \big(\nabla\varphi\big)^2 = 0 \tag{7.12}$$

In general, we have no reason to expect to be able to express the solution of the functional derivative equation (7.11) by a boundary value problem analogous to (7.12), it simply works under our special assumption.

Up to this point we did not yet really use condition (7.5) but, to complete the argument, we need to show that (7.12) is equivalent to the Euler–Lagrange equation (7.10). By writing (7.5) with $\tau = b(\varphi)$ we get

$$\frac{\sigma(\rho) - A(\varphi)}{d(\rho) - \varphi} = A'(\varphi) + a\big[\rho - b(\varphi)\big]$$

and, by comparing (7.10) with (7.12), we see that they are indeed equivalent under the above condition.

As we emphasized, the rate function for SEP is obtained by taking the supremum over $\varphi$ of $\mathcal{G}(\rho, \varphi)$, while for the the KMP process we need to take the infimum. We can now realize that this depends on the sign of $a$. Indeed for $a > 0$ (as in the KMP process) the functional $\mathcal{G}(\rho, \varphi)$ is concave in $\nabla\varphi$ while it is convex for $a < 0$ (as in the SEP).

It is quite tempting to extend the previous derivation to a broader class of models, possibly by a different definition of the trial functional $\mathcal{G}$, however our attempts in this direction were not successful.

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