Current fluctuations in stochastic lattice gases

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We study current fluctuations in lattice gases in the macroscopic limit extending the dynamic approach for density fluctuations developed in previous articles. More precisely, we establish a large deviation theory for the space–time fluctuations of the empirical current which include the previous results. We then estimate the probability of a fluctuation of the average current over a large time interval. It turns out that recent results by Bodineau and Derrida in certain cases underestimate this probability due to the occurrence of dynamical phase transitions.

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The Boltzmann–Einstein theory of equilibrium thermodynamic fluctuations, as described for example in [1], states that the probability for a fluctuation from equilibrium in a macroscopic region of volume V is proportional to $\exp\{V\Delta S/k\}$ where ΔS is the variation of entropy density calculated along a reversible transformation creating the fluctuation and k is the Boltzmann constant. This theory is well established and has received a sound mathematical formulation in statistical mechanics via the so called large deviation theory [2]. The study of large deviations has been extended to stochastic dynamics in equilibrium [3] and non–equilibrium [4–6] stationary states. In a dynamical setting one may ask new questions, for example what is the most probable trajectory followed by the density in the spontaneous emergence of a fluctuation or in its relaxation to equilibrium. We showed that: the entropy, as a functional of the local density, satisfies a Hamilton–Jacobi equation, the Onsager–Machlup theory [7] and the minimum dissipation principle [8] extend to stationary non equilibrium states.

Another macroscopic observable of great physical interest is the current flowing through the system [9–13]. In the present article we develop, in the same spirit of [4, 5], a Boltzmann–Einstein formula for the current fluctuations. The asymptotic probability, as the number of degrees of freedom increases, of observing a current fluctuation j on a space–time domain $[0,T]\times\Lambda$ can be described by a rate functional $\mathcal{I}_{[0,T]}(j)$. This functional plays the same role as $-\Delta S$ in the classical Boltzmann–Einstein theory. The present theory for current fluctuations implies the one for the density and leads to a unified approach.

Among the many problems we can discuss within this theory, we consider the behavior of a fluctuation J of the average current over a large time interval. This is the question addressed in [14] in one space dimension by postulating an "additivity principle" which relates the fluctuation of the time averaged current in the whole system to the fluctuations in subsystems. The probability of a fluctuation J can be described by a rate functional $\Phi(J)$ which we characterize, in any dimension, in terms of a variational problem for the functional $\mathcal{I}_{[0,T]}$. The result agrees with [14] only under additional hypotheses. We show by explicit examples that these hypotheses are not always satisfied. More precisely, while the rate functional Φ is always convex for thermodynamic reasons, the functional of [14], that we call U, may be non convex. In such a case $U(J)$ underestimates the probability of the fluctuation J. We interpret the lack of convexity of U as a dynamical phase transition. In a forthcoming more detailed paper [15] we shall study also the behavior of $\mathcal{I}$ and Φ under time reversal and connect it to the well known fluctuation theorem for entropy production of Gallavotti and Cohen [16–18].

The basic microscopic model is given by a stochastic lattice gas with a weak external field and particle reservoirs at the boundary. More precisely, let $\Lambda\subset\mathbb{R}^d$ be a smooth domain and set $\Lambda_N = N\Lambda\cap\mathbb{Z}^d$; we consider a Markov process on the state space X^{Λ_N}, where X is a subset of $\mathbb{N}$, e.g. $X=\{0,1\}$ when an exclusion principle is imposed. The number of particles at the site $x\in\Lambda_N$ is denoted by $\eta_x\in X$ and the whole configuration by $\eta\in X^{\Lambda_N}$. The dynamical evolution is given by a continuous time Markov process on the state space X^{Λ_N}. This is specified by transition rates $c_{x,y}(\eta)$ describing the jump of a particle from a site x to its nearest neighbor y and rates $c_x^{\pm}(\eta)$ describing the appearance or loss of a particle at the boundary site x. The reservoirs are characterized by a chemical potential γ. We assume that the rates satisfy the local detailed balance condition [18] with respect to a Gibbs measure associated to some Hamiltonian $\mathcal{H}$. Typically, for a non equilibrium model, we can consider Λ the cube of side one and the system under a constant force E/N. Moreover we choose the chemical potential

γ so that $\gamma(y/N) = \gamma_0$ if the first coordinate of y is 0, $\gamma(y/N) = \gamma_1$ if the first coordinate of y is N, and impose periodic boundary conditions in the other directions.

The macroscopic fluctuation theory of stochastic lattice gases, as discussed below, is expected to apply to a wider class of non equilibrium systems with conservation laws, e.g. the Hamiltonian anharmonic chain of [19] and fluids driven by thermal gradients. We introduce the empirical density π^N associated to a microscopic configuration $\eta \in X^{\Lambda_N}$ by requiring for each smooth function $G : \Lambda \to \mathbb{R}$,

$$\langle \pi^N, G \rangle = \int_\Lambda du\, \pi^N(u)\, G(u) = \frac{1}{N^d} \sum_{x \in \Lambda_N} G(x/N) \eta_x$$

so that $\pi^N(u)$ is the local density at the macroscopic point $u = x/N$ in Λ. Consider a sequence of initial configurations η^N such that $\pi^N(\eta^N)$ converges to some density profile ρ_0. Under diffusive scaling the empirical density at time t converges, as $N \to \infty$, to $\rho = \rho(t,u)$ which is the solution of

$$\partial_t \rho = \nabla \cdot \Big[\frac{1}{2} D(\rho) \nabla \rho - \chi(\rho) \nabla V \Big] = \mathcal{D}(\rho) \tag{1}$$

with initial condition ρ_0. Here D is the diffusion matrix, given by the Green–Kubo formula, see [20, II.2.2], χ is the conductivity, obtained by linear response theory, see [20, II.2.5], and ∇V the external field. We emphasize that these transport coefficient are defined in terms of the equilibrium Gibbs measure. In particular if we denote by $S_0(\rho)$ the entropy associated to $\mathcal{H}$, the usual Einstein relation $D(\rho) = R^{-1}(\rho)\chi(\rho)$ holds, here $R(\rho) = S_0''(\rho)^{-1}$ is the compressibility. The interaction with the reservoirs appears as a boundary condition to be imposed on solutions of (1). More precisely, we require that $S_0'(\rho(u)) = \gamma(u)$, $u \in \partial\Lambda$, here $\partial\Lambda$ denotes the boundary of Λ and we recall that γ is the chemical potential of the reservoirs. The non equilibrium stationary profile $\bar\rho$ is the unique stationary solution of (1).

The probability to observe a density trajectory different from the hydrodynamic behavior (1) is exponentially small in N^d and given by [4, 5]

$$\mathbb{P}^N_{\eta^N}\big(\pi^N \approx \rho,\ t \in [0,T]\big) \sim \exp\big\{ -N^d I_{[0,T]}(\rho) \big\} \tag{2}$$

where $\approx$ denotes closeness in some metric, $\sim$ logarithmic equivalence as $N \to \infty$, and $\mathbb{P}_{\eta^N}$ stands for the distribution of the process starting from η^N. The rate functional $I_{[0,T]}(\rho)$ is given by

$$I_{[0,T]}(\rho) \;=\; \frac{1}{2} \int_0^T dt\, \langle \nabla H, \chi(\rho) \nabla H \rangle \tag{3}$$

where the external potential H has to be chosen so that ρ solves

$$\partial_t \rho = \mathcal{D}(\rho) - \nabla \cdot \big(\chi(\rho) \nabla H \big) \tag{4}$$

with initial condition ρ_0 and the same boundary conditions as the hydrodynamic equation (1). Equations (2)–(4) are the analog of the Boltzmann–Einstein formula for dynamical fluctuations.

We give now a parallel discussion for the current. Denote by $\mathcal{N}_t^{x,y}$ the number of particles that jumped from x to y in the macroscopic time interval $[0,t]$. Here we adopt the convention that $\mathcal{N}_t^{x,y}$ represents the number of particles created at y due to the reservoir at x if $x \notin \Lambda_N$, $y \in \Lambda_N$ and that $\mathcal{N}_t^{x,y}$ represents the number of particles that left the system at x by jumping to y if $x \in \Lambda_N$, $y \notin \Lambda_N$. The difference $J_t^{x,y} = \mathcal{N}_t^{x,y} - \mathcal{N}_t^{y,x}$ is the net number of particles flown across the bond $\{x,y\}$ in the time interval $[0,t]$. In other words, given a path $\eta(s)$, $0 \le s \le t$, the instantaneous current $dJ_t^{x,y}/dt$ is a sum of δ–functions localized at the jump times across the bond $\{x,y\}$ with weight $+1$, respectively -1, if a particle jumps from x to y, respectively from y to x.

Fix a macroscopic time T and denote by $\mathcal{J}^N$ the empirical measure on $[0,T] \times \Lambda$ associated to the current. For smooth vector fields $G = (G_1, \dots, G_d)$, the integral of G with respect to $\mathcal{J}^N$, denoted by $\mathcal{J}^N(G)$, is given by

$$\begin{aligned} \mathcal{J}^N(G) \;&=\; \int_0^T dt \int_\Lambda du\, G(t,u) \cdot \mathcal{J}^N(t,u) \\ &=\; \frac{1}{N^{d+1}} \sum_{i=1}^d \sum_x \int_0^T dt\, G_i(t, x/N)\, \frac{dJ_t}{dt}^{x,x+e_i} \end{aligned}$$

where $\cdot$ is the inner product in $\mathbb{R}^d$, e_i is the canonical basis, and we sum over all x such that either $x \in \Lambda_N$ or $x + e_i \in \Lambda_N$. We normalized $\mathcal{J}^N$ so that it is finite as $N \to \infty$. Given a density profile ρ let us denote by

$$J(\rho) = -\frac{1}{2} D(\rho) \nabla \rho + \chi(\rho) \nabla V \tag{5}$$

the current associated to ρ. The hydrodynamic equation (1) can then be written as $\partial_t \rho + \nabla \cdot J(\rho) = 0$. Recall that the initial configuration η^N is such that the empirical density $\pi^N(\eta^N)$ converges to the density profile ρ_0 and denote by $\rho(t)$ the solution of (1). Then the empirical current $\mathcal{J}^N(t)$ converges, as $N \to \infty$, to $J(\rho(t))$, the current associated to the solution of the hydrodynamic equation (1). If we let $t \to \infty$ we have $J(\rho(t)) \to J(\bar\rho)$.

We next discuss the large deviation properties of the empirical current. Fix a smooth vector field $j : [0,T] \times \Lambda \to \mathbb{R}^d$. The large deviation principle for the current states that

$$\mathbb{P}^N_{\eta^N}\big(\mathcal{J}^N(t,u) \approx j(t,u)\big) \sim \exp\big\{ -N^d \mathcal{I}_{[0,T]}(j) \big\} \tag{6}$$

where the rate functional is

$$\mathcal{I}_{[0,T]}(j) \;=\; \frac{1}{2} \int_0^T dt\, \big\langle [j - J(\rho)], \chi(\rho)^{-1} [j - J(\rho)] \big\rangle \tag{7}$$

in which $J(\rho)$ is given by (5) and $\rho = \rho(t,u)$ is obtained by solving the continuity equation $\partial_t \rho + \nabla \cdot j = 0$ with initial condition $\rho(0) = \rho_0$. Of course there are compatibility conditions to be satisfied, for instance if we have chosen a j such that $\rho(t)$ becomes negative for some $t \in [0,T]$ then $\mathcal{I}_{[0,T]}(j) = +\infty$. We present here a heuristic derivation of (6)–(7). Fix a current j; in order to make j typical, we introduce an external field F. Let ρ be the solution of

$$\begin{cases} \partial_t \rho + \nabla \cdot j = 0 \\ \rho(0,u) = \rho_0(u) \end{cases} \tag{8}$$

and $F : [0,T] \times \Lambda \to \mathbb{R}^d$ be the vector field such that

$$\begin{aligned} j &= J(\rho) + \chi(\rho) F \\ &= -\frac{1}{2} D(\rho) \nabla \rho + \chi(\rho)\{\nabla V + F\} \end{aligned}$$

We introduce a perturbed measure $\mathbb{P}^{N,F}_{\eta^N}$ which is obtained by modifying the rates as follows

$$c^F_{x,y}(\eta) \; = \; c_{x,y}(\eta)\, e^{N^{-1} F(t,x/N)\cdot(y-x)}$$

Following a similar argument as the one for the large deviation principle of the empirical density [5], one can show that

$$\begin{aligned} \frac{d\mathbb{P}^N_{\eta^N}}{d\mathbb{P}^{N,F}_{\eta^N}} &\sim \exp\Big\{ - N^d \frac{1}{2} \int_0^T dt\, \langle F, \chi(\rho) F \rangle \Big\} \\ &= \exp\big\{ - N^d \mathcal{I}_{[0,T]}(j) \big\} \end{aligned}$$

Moreover, under $\mathbb{P}^{N,F}_{\eta^N}$, as $N \to \infty$, $\mathcal{J}^N$ converges to j. Therefore,

$$\begin{aligned} &\mathbb{P}^N_{\eta^N} \Big(\mathcal{J}^N(t,u) \approx j(t,u), \;\; (t,u) \in [0,T] \times \Lambda \Big) \\ &= \mathbb{P}^{N,F}_{\eta^N} \Big(\frac{d\mathbb{P}^N_{\eta^N}}{d\mathbb{P}^{N,F}_{\eta^N}} \, \mathbb{1}_{\{\mathcal{J}^N \approx j\}} \Big) \sim e^{-N^d \mathcal{I}_{[0,T]}(j)} \end{aligned}$$

We emphasize that now we need to allow non–gradient external fields F, while in the large deviation principle for the empirical density (2) it is sufficient to consider gradient external fields [3, 21]. The latter is therefore a special case and can be recovered from (6)–(7).

We want to study the fluctuations of the time average of the empirical current over a large time interval $[0,T]$; the corresponding probability can be obtained from the space–time large deviation principle (6). Fix some divergence free vector field $J = J(u)$ constant in time and denote by $\mathcal{A}_{T,J}$ the set of all currents j such that $T^{-1} \int_0^T dt\, j(t,u) = J(u)$. The condition of vanishing divergence on J is required by the local conservation of the number of particles. By the large deviations principle (6), for T large we have

$$\mathbb{P}^N_{\eta^N} \Big(\frac{1}{T} \int_0^T dt\; \mathcal{J}^N(t) \approx J \Big) \sim \exp\big\{ - N^d T \Phi(J) \big\} \tag{9}$$

where the logarithmic equivalence is understood by sending *first* $N \to \infty$ and *then* $T \to \infty$. In [15] we show that for the so–called zero range process the limits can be taken in the opposite order; we expect this to be true in general. The functional Φ is given by

$$\Phi(J) = \lim_{T \to \infty} \inf_{j \in \mathcal{A}_{T,J}} \frac{1}{T}\, \mathcal{I}_{[0,T]}(j) \tag{10}$$

By a standard sub–additivity argument it is indeed easy to show that the limit exists. We now prove that Φ is a convex functional. Let $J = pJ_1 + (1-p)J_2$: we want to show that $\Phi(J) \le p\Phi(J_1) + (1-p)\Phi(J_2)$. Let us call $(j_1(t), \rho_1(t))$, $t \in [0, pT]$ (respectively $(j_2(t), \rho_2(t))$, $t \in [0, (1-p)T]$) the optimal path of current and density which implements the minimum in (10) at J_1 (respectively J_2). We then consider a path $(j(t), \rho(t))$ which spends a time interval pT following (j_1, ρ_1) and a time interval $(1-p)T$ following (j_2, ρ_2) (and a finite time to go continuously from (j_1, ρ_1) to (j_2, ρ_2)). With such a path we get

$$\begin{aligned} \Phi(J) &\le \frac{1}{T} \mathcal{I}_{[0,pT]}(j_1) + \frac{1}{T} \mathcal{I}_{[0,(1-p)T]}(j_2) + O(1/T) \\ &\le p\Phi(J_1) + (1-p)\Phi(J_2) + O(1/T) \end{aligned}$$

where we used the existence of the limit (10).

We next study the variational problem on the right hand side of (10). We begin by deriving an upper bound. Given $\rho = \rho(u)$ and $J = J(u)$, $\nabla \cdot J = 0$, let us introduce the functionals

$$\mathcal{U}(\rho, J) \; = \; \frac{1}{2} \langle J - J(\rho), \chi(\rho)^{-1} [J - J(\rho)] \rangle \tag{11}$$

$$U(J) \; = \; \inf_{\rho} \, \mathcal{U}(\rho, J) \tag{12}$$

where the minimum in (12) is carried over all profiles ρ satisfying the boundary conditions and $J(\rho)$ is given by (5). When J is constant, that is in the one–dimensional case, the functional U is the one introduced in [14].

By choosing a suitable path $j(t,u) \in \mathcal{A}_{T,J}$ we first show that

$$\Phi(J) \le U(J) \tag{13}$$

The strategy is quite simple, see also [14]. Let $\hat\rho = \hat\rho(J)$ be the density profile which minimizes the variational problem (12). Given the initial density profile ρ_0, we construct a path $j = j(t,u)$, $(t,u) \in [0,T] \times \Lambda$ as follows

$$j(t) = \begin{cases} \hat{\jmath} & \text{if } \; 0 \le t < \tau \\ \frac{T}{T - 2\tau} J & \text{if } \; \tau \le t < T - \tau \\ -\hat{\jmath} & \text{if } \; T - \tau \le t \le T \end{cases}$$

where $\hat{\jmath}$ is a vector field such that $\tau \nabla \cdot \hat{\jmath} = \rho_0 - \hat\rho$ and $\tau > 0$ is some fixed time. It is now straightforward to verify that $j \in \mathcal{A}_{T,J}$, as well as $\lim_{T \to \infty} \frac{1}{T}\, \mathcal{I}_{[0,T]}(j) = U(J)$.

From (13) and the convexity of $\Phi(J)$ it immediately follows that

$$\Phi(J) \leq U^{**}(J) \tag{14}$$

where U^{**} denotes the convex envelope of U.

We next discuss a lower bound for the variational problem (10). We denote by $\widetilde{\mathcal{U}}$ and $\widetilde{U}$ the same functionals as in (11)–(12), but now defined on the space of all currents without the conditions of vanishing divergence. Let also $\widetilde{U}^{**}$ be the convex envelope of $\widetilde{U}$.

Let $j \in \mathcal{A}_{T,J}$. By the convexity of $\widetilde{U}^{**}$ in the set of all currents, we get

$$\begin{aligned} \frac{1}{T}\mathcal{I}_{[0,T]}(j) &= \frac{1}{T}\int_0^T dt\, \widetilde{\mathcal{U}}(\rho(t), j(t)) \geq \frac{1}{T}\int_0^T dt\, \widetilde{U}(j(t)) \\ &\geq \frac{1}{T}\int_0^T dt\, \widetilde{U}^{**}(j(t)) \geq \widetilde{U}^{**}(J) \end{aligned} \tag{15}$$

The upper and lower bounds (14) and (15) are, in general, different. For a divergence free J we have $\widetilde{U}(J) = U(J)$ but since the convex envelopes are considered in different spaces, we only have $\widetilde{U}^{**}(J) \leq U^{**}(J)$.

To understand the physical meaning of the convex envelope in (14), suppose $J = pJ_1 + (1-p)J_2$ and $U(J) > U^{**}(J) = pU(J_1) + (1-p)U(J_2)$ for some p, J_1, J_2. The values p, J_1, J_2 are determined by J and U. In addition we assume that $U^{**} = \widetilde{U}^{**}$. If we condition on observing an average current J, the corresponding density profile is not determined, but rather we observe with probability p the profile $\hat{\rho}(J_1)$ and with probability $1-p$ the profile $\hat{\rho}(J_2)$. When U is not convex we have thus a situation in which the time averaged current J is realized with the coexistence of two dynamical regimes: we have a dynamical phase transition.

The derivation of the upper bound shows that, if U is not convex, our result differs from the one in [14]. On the other hand if $\widetilde{U}^{**}(J) < U^{**}(J)$ it is possible that one can further improve the upper bound (14) by exploring currents with non vanishing divergence. In such a situation it is not clear to us if Φ can be directly related to U.

We can consider the large time behavior of the empirical current as in equation (9) with the additional constraint that the associated density is asymptotically time independent. In such a case it is not difficult to show that (9) holds with $\Phi = U$. With this extra constraint we are in fact forbidding the system from oscillating.

In the models where the diffusion coefficient $D(\rho)$ is constant and the mobility $\chi(\rho)$ is concave, for example in the symmetric simple exclusion where $\chi = \rho(1-\rho)$, it is not difficult to see that $\widetilde{U}$ is convex. Therefore in these cases $\Phi = U$. In [15] we shall show that in the Kipnis-Marchioro-Presutti model [22, 23] at equilibrium $U(J)$ is convex while $\widetilde{U}(J)$ is not.

We next discuss an example, with a non–concave χ, where the functional U is not convex. We fix equilibrium boundary conditions $\rho_0 = \rho_1 = \bar{\rho}$. We take $D(\rho) = 1$ and $\chi(\rho)$ a smooth function with $\chi(0) = \chi(1) = 0$ which has a non concave part $\chi(\rho) = Ke^{-C\rho}$, for ρ in a given interval, where C is a positive parameter. An explicit calculation gives that $U(J) = \frac{1}{C^2}e^{C\bar{\rho}}F(CJ)$ where $F(z) = z\frac{e^z-1}{e^z+1}$, if J is in an appropriate interval. Since the second derivative of $F(z)$ can be negative, $U(J)$ is not convex.

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