

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 [Phys. Rev. Lett. **92**, 180601 (2004)] 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 nonequilibrium [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 nonequilibrium states.

Another macroscopic observable of great physical interest is the current flowing through the system [9–13]. In the present Letter 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 $I_{[0,T]}(j)$. 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 $I_{[0,T]}$. 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], which we call U , may be nonconvex. 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 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 nonequilibrium 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 nonequilibrium 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 $G: \Lambda \rightarrow \mathbb{R}$;

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

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 $N \rightarrow \infty$, to $\rho = \rho(t, u)$ which is the solution of

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

with initial condition ρ_0 . Here D is the diffusion matrix, given by the Green-Kubo formula (see Sec. II.2.2 of [20]), χ is the conductivity, obtained by linear response theory (see Sec. II.2.5 of [20]), and ∇V is the external field. We emphasize that these transport coefficients 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 $S_0'(\rho(u)) = \gamma(u)$ and $u \in \partial \Lambda$; here $\partial \Lambda$ denotes the boundary of Λ and we recall that γ is the chemical potential of the reservoirs. The nonequilibrium 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]

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

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

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

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

$$\partial_t \rho = \mathcal{D}(\rho) - \nabla \cdot [\chi(\rho) \nabla H] \quad (4)$$

with initial condition ρ_0 and the same boundary conditions as the hydrodynamic Eq. (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 $\eta(s)$, $0 \leq s \leq t$, 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 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 J^N , denoted by $J^N(G)$, is given by

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

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 J^N so that it is finite as $N \rightarrow \infty$. Given a density profile ρ let us denote by

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

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 $J^N(t)$ converges, as $N \rightarrow \infty$, to $J(\rho(t))$, the current associated with the solution of the hydrodynamic equation (1). If we let $t \rightarrow \infty$ we have $J(\rho(t)) \rightarrow J(\bar{\rho})$.

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

$$\mathbb{P}_{\eta^N}^N(J^N(t, u) \approx j(t, u)) \sim \exp\{-N^d I_{[0,T]}(j)\}, \quad (6)$$

where the rate functional is

$$I_{[0,T]}(j) = \frac{1}{2} \int_0^T dt \langle [j - J(\rho)], \chi(\rho)^{-1} [j - J(\rho)] \rangle \quad (7)$$

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 $J_{[0,T]}(j) = +\infty$. We present here a heuristic derivation of (6) and (7). Fix a current j ; in order to make j typical, we introduce an external field F . Let ρ be the solution of

$$\partial_t \rho + \nabla \cdot j = 0, \quad \rho(0, u) = \rho_0(u), \quad (8)$$

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

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

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

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

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

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

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

$$\begin{aligned} \mathbb{P}_{\eta^N}^{N,F}(J^N(t, u) \approx j(t, u), (t, u) \in (0, T) \times \Lambda) \\ = \mathbb{P}_{\eta^N}^{N,F}\left(\frac{d\mathbb{P}_{\eta^N}^{N,F}}{d\mathbb{P}_{\eta^N}^{N,F}} \mathbb{1}_{\{J^N \approx j\}}\right) \sim e^{-N^d J_{[0,T]}(j)}. \end{aligned}$$

We emphasize that now we need to allow nongradient 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) and (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

$$\mathbb{P}_{\eta^N}^{N,F}\left(\frac{1}{T} \int_0^T dt J^N(t) \approx J\right) \sim \exp\{-N^d T \Phi(J)\}, \quad (9)$$

where the logarithmic equivalence is understood by sending *first* $N \rightarrow \infty$ and *then* $T \rightarrow \infty$. 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

$$\Phi(J) = \lim_{T \rightarrow \infty} \inf_{j \in \mathcal{A}_{T,J}} \frac{1}{T} J_{[0,T]}(j). \quad (10)$$

By a standard subadditivity 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 $\Phi(J) \leq p\Phi(J_1) + (1-p)\Phi(J_2)$. 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

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

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

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

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

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

$$\Phi(J) \leq U(J). \quad (13)$$

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:

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

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

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

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

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

We next discuss a lower bound for the variational problem (10). We denote by \tilde{U} and \bar{U} the same functionals as in (11) and (12) but now defined on the space of all currents

without the conditions of vanishing divergence. Let also \tilde{U}^{**} be the convex envelope of \tilde{U} .

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

$$\begin{aligned} \frac{1}{T} I_{[0,T]}(j) &= \frac{1}{T} \int_0^T dt \tilde{U}(\rho(t), j(t)) \geq \frac{1}{T} \int_0^T dt \tilde{U}(j(t)) \\ &\geq \frac{1}{T} \int_0^T dt \tilde{U}^{**}(j(t)) \geq \tilde{U}^{**}(J). \end{aligned} \quad (15)$$

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

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 $U^{**} = \tilde{U}^{**}$. 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 $\tilde{U}^{**}(J) < U^{**}(J)$, it is possible that one can further improve the upper bound (14) by exploring currents with nonvanishing 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 Eq. (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 \tilde{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 $\tilde{U}(J)$ is not.

We next discuss an example, with a nonconcave 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 nonconcave 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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