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Large deviations of the current in stochastic systems

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(joint work with A. De Sole, D. Gabrielli, G. Jona-Lasinio, C. Landim)

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 $\mathbb{N}$. 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 dynamics of the particles is described by a continuous time Markov process on the state space X^{Λ_N} with transition rates $c_{x,y}(\eta)$ from a configuration η to the configuration obtained from η by moving a particle from x to a neighbor site y. Similar rates $c_x^{\pm}$ describe the appearance or loss of a particle at the boundary site x. We assume the rates satisfy the *local detailed balance*, see [4, II.2.6]. The reservoirs are characterized by a chemical potential γ.

We introduce the empirical measure π^N corresponding to the density as follows. For each microscopic configuration $\eta \in X^{\Lambda_N}$ and each smooth function $G : \Lambda \to \mathbb{R}$, we set $\pi^N(G) = N^{-d} \sum_{x\in\Lambda_N} G(x/N)\eta_x$ Consider a sequence of initial configurations η^N such that $\pi^N(\eta^N)$ converges weakly to some density profile ρ_0. Under diffusive scaling, the empirical density at time t converges weakly, as $N \to \infty$, to $\rho = \rho(t, u)$ which is the solution of the hydrodynamic equation [3, 4]

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

with initial condition ρ_0 and boundary condition fixed by the reservoirs. Here D is the diffusion matrix, given by the Green–Kubo formula, see [4, II.2.2], χ is the conductivity, obtained by linear response theory, see [4, II.2.5], and ∇V the external field.

We now introduce the empirical current as follows. 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 $J_t^{x,y} = \mathcal{N}_t^{x,y} - \mathcal{N}_t^{y,x}$ represents the total current across the bond $\{x, y\}$ in the time interval $[0, t]$. 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 $\mathcal{J}^N$ is given by $\mathcal{J}^N(G) = N^{-(d+1)} \sum_{i=1}^d \sum_x \int_0^T G_i(t, x/N)\, dJ_t^{x,x+e_i}$, where 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 $J(\rho) = -\frac{1}{2}D(\rho)\nabla\rho + \chi(\rho)\nabla V$ the current associated to ρ. If we consider an initial configuration η^N such that the empirical density $\pi^N(\eta^N)$ converges to some density profile ρ_0, 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.

We next discuss the large deviation properties of the empirical current. Fix a smooth vector field $j : [0,T] \times \Lambda \to \mathbb{R}^d$ and a sequence of configurations η^N whose empirical density converges to some profile ρ_0. Then, by the methods in [3, Ch. 10], it is possible to show that

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

where the rate function is given by

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

in which $\rho = \rho(t,u)$ is obtained by solving the continuity equation $\partial_t \rho + \nabla \cdot j = 0$ with initial condition $\rho(0) = \rho_0$ and $\langle \cdot, \rangle$ is the inner product in $L_2(\Lambda, du)$. 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 next discuss how, from the time dependent large deviation principle stated above, we obtain an extension of the results of [2] for the time average of the empirical current. Given time independent profiles $\rho = \rho(u)$ and $J = J(u)$, let us introduce the functionals

$$\begin{aligned} \mathcal{U}(\rho, J) &= \frac{1}{2}\langle J - J(\rho), \chi(\rho)^{-1}[J - J(\rho)]\rangle \\ U(J) &= \inf_{\rho} \mathcal{U}(\rho, J) \end{aligned}$$

where the infimum is carried over all profiles ρ satisfying the boundary conditions and $J(\rho)$ has been defined above. When J is constant, the functional U is the one introduced in [2].

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. From the large deviations principle for the current we get

$$\mathbb{P}^N_{\eta^N}\Big(\frac{1}{T}\int_0^T dt\; \mathcal{J}^N(t,u) \approx J(u)\Big) \sim \exp\big\{ - N^d \inf_{j \in \mathcal{A}_{T,J}} \mathcal{I}_{[0,T]}(j)\big\}$$

Let U^{**} be the convex envelope of U, in [1] it is shown that

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

we therefore have

$$\mathbb{P}^N_{\eta^N}\Big(\frac{1}{T}\int_0^T dt\,\mathcal{J}^N(t,u)\approx J(u)\Big)\sim\exp\big\{-N^d\,T\,U^{**}(J)\big\}$$

where the logarithmic equivalence is understood by sending *first* $N\to\infty$ and *then* $T\to\infty$. This result extends [2] to $d\geq 1$, allows divergence free J, and shows that, in general, U has to replaced by its convex envelope U^{**}. An example where U is not convex is discussed in [1].

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Simulations of Diffusion Induced Segregation

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Diffusion Induced Segregation (DIS) processes represent a particular class of segregation phenomena where the formation of (two) phases only starts after the concentration of a particular diffusor exceeds a certain threshold. The objective of the present work is to develop suitable models for the so-called chalcopyrite disease within sphalerite which is one example of DIS, compute at least approximately the actual physical free energies and make simulations closer to reality.

Model A: For $t\geq 0$ find $c=(c_1,c_2,c_3,c_4),\chi$ such that in $\Omega\subset\mathbb{R}^D$ for $t>0$

$$0 = \mathrm{div}\Big(\sum_{j=1}^4 L_{1j}\nabla\mu_j\Big)+k^{1/b_\chi}(c_2^2-(\kappa)^{1/b_\chi}c_1c_3), \tag{1}$$

$$\partial_t c_i = \mathrm{div}\Big(\sum_{j=1}^4 L_{ij}\nabla\mu_j\Big)+r_i(c,\chi),\ i=2,3,4, \tag{2}$$

$$\mu_i = \frac{\partial f}{\partial c_i}(c,\chi),\ 1\leq i\leq 4, \tag{3}$$

$$\tau\partial_t\chi = \gamma\triangle\chi-\omega(c,\chi) \tag{4}$$

together with initial values for c and χ and Dirichlet boundary conditions for c, μ and χ. Here, c is a concentration vector, χ measures the volume fraction of the chalcopyrite phase, μ is the chemical potential. Reaction terms: $r=(r_1,\dots,r_4)$ with $r_1=r_3=-\frac{1}{2}r_2=k^{1/b_\chi}\Big(c_2^2-\kappa^{1/b_\chi}c_1c_3\Big)$, $r_4=0$. Let $\Omega_T:=\Omega\times(0,T_0)$.