LLN and CLT for IPS: The effect of boundary conditions

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Plan

1. The model: current reservoirs
2. Previous results, key technical issues
3. Fluctuations, challenges

1. The model: current reservoirs

In a region Ω each point (representing a large microscopic system) has reached a local thermal equilibrium.

- Macroscopic states: functions $\rho \in L^1(\Omega)$.
- Postulate: thermodynamics of the system is determined by a free energy functional: $F(\rho) = \int_\Omega f(\rho(r))dr$.
- Dynamics: continuity equation (conservation of mass)

$$\frac{\partial \rho}{\partial t} = -\frac{\partial J}{\partial r}$$

- Constitutive relation for the current (chosen such that free energy decreases)

$$J = -\kappa(\rho)\frac{\partial}{\partial r}\left(\frac{\delta F(\rho)}{\delta \rho(r)}\right)$$

- $\kappa(\rho) > 0$ is a model dependent coefficient called *mobility*.
- Boundary conditions? Periodic, Dirichlet or other?

Density reservoirs: complement the equation with Dirichlet b. c.:

$$\frac{\partial \rho}{\partial t} = -\frac{\partial J}{\partial r}, \qquad J = -\kappa(\rho)\frac{\partial f'(\rho)}{\partial r}, \quad r \in (-1,1)$$

$$\rho(-1,t) = \rho_-, \qquad \rho(1,t) = \rho_+, \quad \rho(r,0) \text{ given}$$

(In some sense, "big" reservoirs maintaining the values of the density at the boundaries.)

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Current reservoirs: play a more active role as they directly force a flux of mass into the system (without freezing the order parameter at the endpoints):

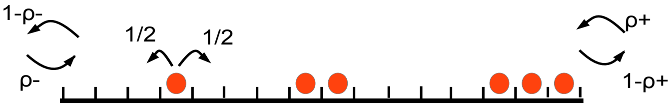
$$J(-1,t) = j\lambda_-\big(\rho(-1,t)\big) \qquad J(1,t) = j\lambda_+\big(\rho(1,t)\big)$$

where $\lambda_-(\cdot), \lambda_+(\cdot)$ are model dependent, mobility parameters. A flux of mass $J(-1,t)$ enters into the system at the point -1 and a flux of mass $J(1,t)$ leaves the system at the point 1 (producing a change of density $\rho(\mp 1,t) \pm J(\mp 1,t)\,dt$).

Density reservoirs: SSEP on $\Lambda_\varepsilon = [-\varepsilon^{-1}, \varepsilon^{-1}] \cap \mathbb{Z} = \{-N, -N+1, ..., N\}$, $N = [\varepsilon^{-1}]$.
Let $\{\eta_t(x) \in \{0,1\}, \, x \in \Lambda_\varepsilon \,, \, t \geq 0\}$ be a process with generator

$$L_0 f(\eta) = \frac{1}{2} \sum_{x \in \Lambda_\varepsilon} \sum_{y:|y-x|=1} \Big(f(\eta^{(x,y)}) - f(\eta) \Big)$$

plus birth/death processes at the boundaries:



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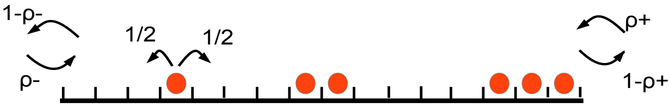


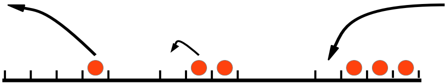
Hydrodynamic limit exists:

$$\frac{\partial \rho}{\partial t} = \frac{1}{2} \frac{\partial^2 \rho}{\partial r^2}, \qquad r \in (-1, 1)$$

with Dirichlet b.c. $\rho(-1, t) = \rho_-$, $\rho(1, t) = \rho_+$.

Current reservoirs: at the boundary ($|I_\pm| = K$, finite!) we impose a (microscopic) current εj with $\varepsilon = 1/N$

$$L_{b,\pm} f(\eta) := \varepsilon \frac{j}{2} \sum_{x \in I_\pm} D_\pm \eta(x) [f(\eta^{(x)}) - f(\eta)],$$



where

$$D_+ \eta(x) = [1 - \eta(x)]\eta(x+1)\eta(x+2)\ldots\eta(N), \quad x \in I_+$$
$$D_- \eta(x) = \eta(x)[1 - \eta(x-1)][1 - \eta(x-2)]\ldots[1 - \eta(-N)], \quad x \in I_-.$$

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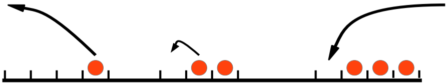

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$$D_- \eta(x) = \eta(x) [1 - \eta(x-1)] [1 - \eta(x-2)] \dots [1 - \eta(-N)], \quad x \in I_-.$$

More general dynamics:

$$D_\pm \eta(x) = \frac{1}{N^\theta} F(\eta|_{I_\pm}), \quad \text{for some} \quad \theta > 0$$

2. Previous results

$$\begin{aligned}\frac{d}{dt}\mathbb{E}_\varepsilon[\eta(x,t)] &= \mathbb{E}_\varepsilon[L_0(\eta)+L_b(\eta)] \\ &= \frac{1}{2}\Delta_\varepsilon \mathbb{E}_\varepsilon[\eta(x,t)] + \mathbb{E}_\varepsilon \frac{j}{2}\sum_{x\in I_\pm} D_\pm \eta(x)[f(\eta^{(x)})-f(\eta)]\end{aligned}$$

Can we close it with respect to $\rho_\varepsilon(x,t) := \mathbb{E}_\varepsilon[\eta(x,t)]$?

2. Previous results

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Can we close it with respect to $\rho_\varepsilon(x,t) := \mathbb{E}_\varepsilon[\eta(x,t)]$?

- Propagation of chaos. Considering the correlation functions:

$$v^\varepsilon(\underline{x},t|\mu^\varepsilon) := \mathbb{E}_\varepsilon\Big[\prod_{i=1}^n\{\eta(x_i,t)-\rho_\varepsilon(x_i,t)\}\Big], \quad \underline{x}\in\Lambda_N^{n,\neq},\ n\geq 1$$

Theorem (De Masi, Presutti, T., Vares)

$\exists\tau>0, c^*>0$, s.t. $\forall\beta^*>0, n\in\mathbb{Z}_+$, $\exists c_n$ s.t. $\forall\varepsilon>0$

$$\sup_{\underline{x}\in\Lambda_N^{n,\neq}}|v^\varepsilon(\underline{x},t|\mu^\varepsilon)| \leq \begin{cases} c_n(\varepsilon^{-2}t)^{-c^*n}, & t\leq\varepsilon^{\beta^*} \\ c_n\varepsilon^{(2-\beta^*)c^*n} & \varepsilon^{\beta^*}\leq t\leq\tau\log\varepsilon^{-1}\end{cases}$$

- In the limit $\varepsilon \to 0$: heat equation with special boundary conditions:

$$\frac{\partial}{\partial t}\rho(r,t) = \frac{1}{2}\frac{\partial^2}{\partial r^2}\rho(r,t), \qquad r \in (-1,1),$$

$$\frac{\partial \rho(r,t)}{\partial r}|_{r=1} = j(1-\rho(1,t)^K), \quad \frac{\partial \rho(r,t)}{\partial r}|_{r=-1} = j(1-(1-\rho(-1,t))^K)$$

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- Validity of Fourier law: the expected current through $x+\frac{1}{2}$ is

$$j^{(\varepsilon)}(x,t) = \frac{\varepsilon^{-2}}{2}\,\mathbb{E}_\varepsilon\big[\varepsilon\{\eta(x,t)-\eta(x+1,t)\}\big] = -\frac{1}{2}\mathbb{E}_\varepsilon\big[\frac{\eta(x+1,t)-\eta(x,t)}{\varepsilon}\big].$$

and we prove that for $r \in (-1,1)$

$$\lim_{\varepsilon\to 0} j^{(\varepsilon)}([\varepsilon^{-1}r],t) = -\frac{1}{2}\,\frac{\partial \rho(r,t)}{\partial r}.$$

3. Fluctuations

(joint work with P. Birmpa and P. Gonçalves, in progress)

Look at

$$Y(\phi) := \frac{1}{\sqrt{N}} \sum_{x=-N}^{N} \phi(x)(\eta(x) - \rho(x))$$

Goal: The limit exists, it is unique and Gaussian (generalized Ornstein-Uhlenbeck process).

1. the process is a Gaussian being the limit of a martingale. Then it suffices to compute $\mathbb{E}(Y(\phi)^2)$.
2. find the full distribution $\mathbb{E}(f(Y(\phi)))$ and use Holley-Stroock theory
3. need: tightness, uniqueness

Let

$$
\begin{aligned}
M_t(\phi) &:= Y_t(\phi) - Y_0(f) - \int_0^t \Lambda(\phi)\,ds \\
N_t(\phi) &:= (M_t(\phi))^2 - \int_0^t \Gamma(\phi)\,ds
\end{aligned}
$$

where

$$
\begin{aligned}
&\Lambda(\phi) := (\partial_t + L)Y(\phi) \\
&\Gamma(\phi) := L(Y(\phi))^2 - 2Y(\phi)LY(\phi).
\end{aligned}
$$

For a general test function f we have:

$$
f(Y(\phi)) = f'(Y(\phi))\Lambda(\phi) + \frac{1}{2}f''(Y(\phi))\Gamma(\phi) + \dots
$$

(check the case $f(r) = r^2$). How shall we proceed?

Boundary terms

$$\begin{aligned}\Gamma(\phi) &= \epsilon \sum_{x=-N}^{N} (\nabla_\epsilon^+ \phi(\epsilon x))^2 (\eta_t(x) - \eta_t(x+1))^2 + \\ &+ \frac{j}{2} \sum_{x \in I_+} (\phi(\epsilon x))^2 D_+ \eta_t(x) + \frac{j}{2} \sum_{x \in I_-} (\phi(\epsilon x))^2 D_- \eta_t(x)\end{aligned}$$

and

$$\begin{aligned}\Lambda(\phi) &= Y_t^\epsilon(\partial_t \phi) + \sqrt{\epsilon} \sum_{x=-N+1}^{N-1} \frac{1}{2} \Delta_\epsilon \phi(\epsilon x) \bar{\eta}_t(x) - \frac{1}{2\sqrt{\epsilon}} \nabla_\epsilon^- \phi(1) \bar{\eta}_t(N) \\ &+ \frac{1}{2\sqrt{\epsilon}} j \sum_{x=N-K+1}^{N-1} \phi(\epsilon x) \left(D_+ \eta_t(x) - D_+ \rho_t(x)]\right) - \frac{1}{2\sqrt{\epsilon}} j \phi(1) \bar{\eta}_t(N) \\ &+ \text{ similarly at } I_-\end{aligned}$$

Linearization:

$$\frac{\partial}{\partial r}(\rho+\epsilon\xi)|_{r=1} = j(1-(\rho+\epsilon\xi)(1)^{K}) \Rightarrow \frac{\partial}{\partial r}\xi|_{r=1} = -jK\rho(1)^{K-1}\xi$$

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From equation $\frac{\partial}{\partial t}\xi = \xi''$, integrating by parts, we obtain:

$$\begin{aligned} -\xi\frac{\partial}{\partial t}\phi = \phi\frac{\partial}{\partial t}\xi = \phi\xi'' &= \phi''\xi + (\phi\xi')|_{-1}^{1} - (\phi'\xi)|_{-1}^{1} \\ &= \phi''\xi + [-jK\rho(1)^{K-1}\phi(1) - \phi'(1)]\xi(1) + \dots \end{aligned}$$

Similarly, computing $\mathbb{E}(Y(\phi)^2)$ in order to obtain the limit $\varepsilon \to 0$ we need to make the same choice of the space of ϕ.

$K = 2$:

$$(1-\eta(N-1))\eta(N) - (1-\rho(N-1))\rho(N)$$
$$= \bar{\eta}(N) - [\bar{\eta}(N-1) + \rho(N-1)][\bar{\eta}(N) + \rho(N)] + \rho(N-1)\rho(N)$$
$$= \bar{\eta}(N) - 2\bar{\eta}(N)\rho(N)$$
$$+ \text{ terms of the type } ...(\bar{\eta}(N-1) - \bar{\eta}(N)), \bar{\eta}(N-1)\bar{\eta}(N)$$

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&= \bar{\eta}(N) - [\bar{\eta}(N-1) + \rho(N-1)][\bar{\eta}(N) + \rho(N)] + \rho(N-1)\rho(N) \\
&= \bar{\eta}(N) - 2\bar{\eta}(N)\rho(N) \\
&+ \text{terms of the type } ...(\bar{\eta}(N-1) - \bar{\eta}(N)), \bar{\eta}(N-1)\bar{\eta}(N)
\end{aligned}
$$

At the limit, we need to control the extra terms:

$$
\mathbb{E}\left[\left(\int_0^t \varepsilon^{-\frac{1}{2}} \bar{\eta}_s(x)\, ds\right)^2\right] = 2\varepsilon^{-1} \int_0^t ds \int_0^s dr\, \mathbb{E}_{\mathcal{F}_r}\left[\mathbb{E}[\bar{\eta}_s(x) | \mathcal{F}_r] \bar{\eta}_r(x)\right]
$$

Conclusions

1. General boundary dynamics
2. Choice of test functions
3. v-estimates at different times
4. large deviations?