The ABC model on an interval/ring, local measures and beyond

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ABC Model (Evans et al.)

This is a three species system where each lattice site, on an interval with N sites, or on a ring of N sites with cyclic boundary conditions $N+1=1$, is occupied by either an A, B or C type particle. Let $\eta_\alpha(i)=1(0)$ if site i is (is not) occupied by a particle of species $\alpha, \alpha=1,2,3,(A,B,C)$, $i=1,\cdots,N$. A configuration $\underline{\eta}$ of this system then consists of specifying all the $\eta_\alpha(i)$, with $\sum_{\alpha=1}^{3}\eta_\alpha(i)=1$ and $\sum_{i=1}^{N}\eta_\alpha(i)=N_\alpha$.

The dynamics consists of nearest neighbor exchanges between a particle of species α at site i and a particle of species γ at site $i+1, i=1,\cdots,N-1$ on interval (clockwise on ring) with rate $q<1$ if $\alpha<\gamma$ in cyclic order, and with rate 1 otherwise,

$$\mathrm{AB} \underset{q}{\overset{1}{\rightleftharpoons}} \mathrm{BA} \qquad \mathrm{BC} \underset{q}{\overset{1}{\rightleftharpoons}} \mathrm{CB} \qquad \mathrm{CA} \underset{q}{\overset{1}{\rightleftharpoons}} \mathrm{AC}\ .$$

Weakly asymmetric (Clincy et al.)

$$q=\exp[-\beta/N]\sim 1-\frac{\beta}{N}$$

It is "easy" to see that on the **interval**, the dynamics satisfy detailed balance with respect to the canonical Gibbs measure $\nu_\beta(\underline{\eta})$, for all N_A, N_B, N_C,

$$\nu_\beta(\underline{\eta}) = \exp[-\beta E_N(\underline{\eta})]/Z$$

where

$$E_N(\underline{\eta}) = \frac{1}{N} \sum_{i=1}^{N-1} \sum_{j=i+1}^{N} [\eta_C(i)\eta_B(j) + \eta_A(i)\eta_C(j) + \eta_B(i)\eta_A(j)]$$

and Z is the usual canonical partition function with fixed particle numbers, $N_\alpha, \alpha = 1, 2, 3$. The dynamics is ergodic for finite β. Consequently $\nu_\beta(\underline{\eta})$ is the unique stationary measure, for $\beta < \infty$, $N < \infty$.

Note that $E_N(\underline{\eta})$ is of mean field type, with interactions which extend over the whole length of the system. Hence the energy E_N grows like N.

It is easy to check that **if** $N_A = N_B = N_C$ then the energy $E_N(\underline{\eta})$ (given on the previous slide) is also well defined on the ring, i.e. it is independent of the starting site. Thus we can (mentally) connect site N to site 1 clockwise, and "rotate" each configuration on the interval without any cost in energy. The stationary measure is then the same on the interval and on the ring, and is given by $\nu_\beta(\underline{\eta})$.

In fact the observation about the relation between the ABC dynamics and the equilibrium measure with long range interactions was first made for the ring with $N_\alpha = N/3$ (Evans et al.).

When the N_α are different the energy $E_N(\underline{\eta})$ will not be periodic or well defined on the ring. The model on the ring will then generally have a current in the stationary state and will thus not satisfy detailed balance with respect to its stationary measure, which is unknown.

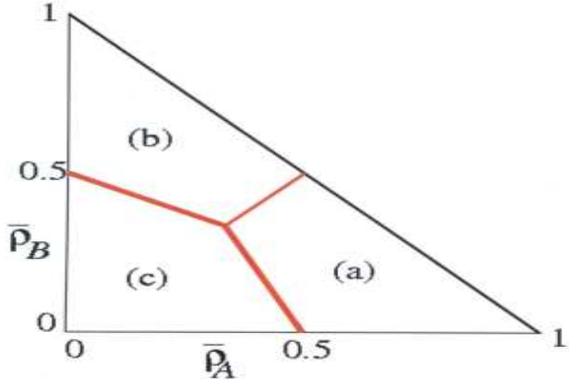
Ground states on the interval

When there is a majority species, e.g. $N_B > \max(N_A, N_C)$, there is a unique ground state consisting of three blocks ABC, with energy per site $e_{\min} = \bar{\rho}_A \bar{\rho}_C$, where $\bar{\rho}_\alpha \equiv N_\alpha / N$.

When $N_A = N_C > N_B$ the ground state will be N_B fold degenerate, with some of the B's at the left side of the interval followed by all the C's then all the A's with the remainder of the B's at the right, i.e. $B_1 C A B_2$.

When $N_A = N_B = N_C$ the ground state is N-fold degenerate, consisting of three blocks ABC with the origin of the A-block at any site i. This corresponds to the "rotational symmetry" on the equivalent ring.

The ground state on the interval is therefore unique everywhere except on the three line segments originating from $\bar{\rho}_A = \bar{\rho}_B = 1/3$ and terminating at the midpoints of the sides of the right triangle. On the edges of the triangle the density of one of the species goes to zero and the system reduces to a two species weakly asymmetric exclusion process with a unique ground state.



Wrong conjecture: the low temperature phase diagram on the interval looks similar.

Properties of the Gibbs measure ν_β

Let $\langle \eta_{\alpha_1}(i_1)\eta_{\alpha_2}(i_2)\cdots\eta_{\alpha_h}(i_h)\rangle_{\nu_\beta}$ be the averages of the occupation variables with respect to the Gibbs measure ν_β with $\alpha_j = A, B, C$. Then it is easy to check that, for any value of the N_α's, $N_\alpha \geq 1$, the following holds

$$\frac{\langle \eta_\alpha(1)\rangle}{\langle \eta_\alpha(N)\rangle} = e^{-\beta[\bar{\rho}_{\alpha+2}-\bar{\rho}_{\alpha+1}]},$$

where α is counted modulo 3. It follows from the above that

$$\prod_{\alpha=1}^{3} \langle \eta_\alpha(1)\rangle = \prod_{\alpha=1}^{3} \langle \eta_\alpha(N)\rangle, \qquad \text{for all } N.$$

One can also show that for fixed j, k with $j \neq k \neq 0$ and $i = [xN]$, $x \in (0, 1)$,

$$\lim_{N\to\infty} \langle \eta_A(i)\eta_B(i+j)\eta_C(i+k)\rangle = K,$$

where K is a constant independent of x, j and k.

Similarly it is "easy" to see that

$$\left\langle \prod_{i=1}^{h} \eta_{\alpha_i}([xN]+j_i) \right\rangle \Big/ \left\langle \prod_{i=1}^{h} \eta_{\alpha_{P(i)}}([xN]+j_{P(i)}) \right\rangle \to 1 \text{ as } N \to \infty$$

where P is any permutation of the $\{j_i\}$, which is kept fixed as $N \to \infty$.

This means that the local measure on microscopic configurations is exchangeable when the system becomes macroscopic.

Consider now the stationary probability distribution of a configuration $\underline{\eta}$, restricted to a finite neighborhood of a site $i = [xN], x \in (0,1)$, e.g. $[i-k, i+k]$. By shifting the origin to $[xN]$ one obtains in the limit $N \to \infty$ a translation invariant measure $\mu_{(x)}$ which, by the exchangeability, is either a product measure, $\widehat{\mu}_{\underline{n}}(\underline{\eta})$, with densities $\underline{n} = (n_1, n_2, n_3)$, or a superposition of such product measures, i.e.,

$$\mu_{(x)}(\underline{\eta}) = \sum_{\underline{n}} \kappa(x; \underline{n}) \widehat{\mu}_{\underline{n}}(\underline{\eta}), \qquad x \in (0,1).$$

The limiting local Bernoulli measures clearly reflect the mean field nature of the interaction giving rise to ν_β without, in principle, any reference to the dynamics.

We note that also on the ring, when the stationary measure is unknown, local probabilities are, in the limit $N \to \infty$, given by a (superposition of) product measures .

This follows dynamically, either on the ring or on the interval, from the observation that when $N \to \infty$, the local generator of the dynamics around $[xN], x \in (0,1)$ is that corresponding to the infinite system, whatever the boundary condition on the finite system. Hence for symmetric or weakly asymmetric exchanges, which become symmetric when $N \to \infty$, the invariant measures are the same as for symmetric exchanges on $\mathbb{Z}$. These are known to be superpositions of extremal Bernoulli measures $\widehat{\mu}_{\underline{n}}(\underline{\eta})$.

This leads, via two independent ways, one dynamic and one equilibrium, to the determination of $\kappa(x;\underline{n})$ in the stationary state on the interval. As we shall see the equilibrium route provides a criteria, minimization of the free energy, for choosing the "right" $\kappa(x;n)$ and leads via some interesting scenic byways, including elliptic functions, to a phase diagram of the ABC system on the interval. By contrast, the local measures on the ring with $\bar{\rho}_\alpha \neq 1/3$, do not come directly from any simple minimization principle, but see Clincy et al. and Bodineau et al, and recent works by Bertini et al.

To determine $\kappa(x;\underline{n})$ we note first that letting $\{\bar{\rho}_\alpha(x)\}$ be the limiting average continuum density profile,

$$\bar{\rho}_\alpha(x) = \lim_{N\to\infty} \langle \eta_\alpha([xN])\rangle,$$

where $\langle\ \rangle$ is taken wrt the stationary measure, known or unknown, then

$$\bar{\rho}_\alpha(x) = \sum_{\underline{n}} \kappa(x;\underline{n}) n_\alpha.$$

But this is clearly not sufficient information for determining $\kappa(x;\underline{n})$. In fact, on the ring we always have $\bar{\rho}_\alpha(x) = \bar{\rho}$ independent of x. The rest of this talk will be devoted to obtaining "typical" density profiles and, using them, to obtain the correct $\mu_{(x)}$. We will do this first from the dynamics and then from ν_β.

Density profiles: derivation from dynamics.

Given any initial state $\mu(\underline{\eta}; s_0)$ we have, for averages with respect to $\mu(\underline{\eta}; s)$, s the microscopic time,

$$\frac{d}{ds}\langle\eta_\alpha(i)\rangle = j_\alpha(i-1,i) - j_\alpha(i,i+1),$$

where the flux of α-particles across the bond $(i, i+1)$ is, for $\alpha = A$,

$$j_A(i,i+1) = \langle\eta_A(i)[q\eta_B(i+1) + \eta_C(i+1)]\rangle - \langle\eta_A(i+1)[\eta_B(i) + q\eta_C(i)]\rangle$$

$$= \langle\eta_A(i)\rangle - \langle\eta_A(i+1)\rangle + (1-q)\langle\eta_A(i)[\eta_C(i-1) - \eta_B(i+1)]\rangle$$

On the interval $j_\alpha(0,1) = j_\alpha(N, N+1) = 0$.

In the stationary state $j_\alpha(i, i+1)$ is independent of i. In the interval it will therefore vanish for all i. On the ring, $\langle\eta_\alpha(i)\rangle = \bar{\rho}_\alpha$ and $j_\alpha(i, i+1) = \bar{j}_\alpha$ independent of i, with $\bar{j}_\alpha \neq 0$ in general, except when $\bar{\rho}_\alpha = 1/3$.

Considering the time evolution of the "typical" density profile in the hydrodynamic (diffusive) scaling limit $i \to [xN], s \to tN^2$, the macroscopic density profiles $\{\rho_\alpha(x,t)\}$ will satisfy the equations,

$$\frac{\partial \rho_\alpha(x,t)}{\partial t} = -\frac{\partial}{\partial x} J_\alpha(x,t), \qquad x \in (0,1),$$

with the **macroscopic** flux J_α given, for $\alpha = A$, by

$$J_A(x,t) = -\frac{\partial}{\partial x}\rho_A(x,t) + \beta \rho_A(x,t)[\rho_C(x,t) - \rho_B(x,t)], \quad \text{etc.},$$

and

$$\sum_\alpha \rho_\alpha(x,t) = 1, \qquad \int_0^1 \rho_\alpha(,t)dx = \bar{\rho}_\alpha, \quad \text{given.}$$

For the **interval**, $J_\alpha(0,t) = J_\alpha(1,t) = 0$, for all t.

In the **stationary** state, $J_\alpha(x) = \bar{J}_\alpha$, with $\bar{J}_\alpha = 0$ on the interval but not necessarily on the ring. This gives the equations determining the "typical" stationary $\rho_\alpha(x)$,

$$\begin{aligned}
\frac{d}{dx}\rho_A(x) &= \beta\rho_A(x)[\rho_C(x) - \rho_B(x)] - \bar{J}_A \\
\frac{d}{dx}\rho_B(x) &= \beta\rho_B(x)[\rho_A(x) - \rho_C(x)] - \bar{J}_B \\
\frac{d}{dx}\rho_C(x) &= \beta\rho_C(x)[\rho_B(x) - \rho_A(x)] - \bar{J}_C.
\end{aligned} \tag{1}$$

Note that the macroscopic flux is related to the microscopic flux by considering (roughly) a limit $J_\alpha(x,t) \sim N j_\alpha([xN],[xN]+1)$. It **cannot** therefore be obtained from $\mu_{(x)}$ in the stationary state.

Density profiles: equilibrium derivation.

Starting with the equilibrium measure $\nu_\beta(\underline{\eta})$ one can derive an equation for the typical profiles $\{\rho_\alpha(x)\}$ on the **interval** or the ring with $\bar{\rho}_\alpha = 1/3$, when $\bar{J}_\alpha = 0$. These were first derived for the latter case by Clincy et al.

Using the Gibbs canonical distribution ν_β the probability of finding a macroscopic density profile $\rho(x) = \{\rho_\alpha(x)\}$ is given by the Helmholtz free energy (multiplied by β) as a large deviation functional

$$\text{Prob}(\{\rho_\alpha\}) \sim \exp[-N\mathcal{F}(\{\rho_\alpha\})],$$

where

$$\mathcal{F}(\{\rho_\alpha\}) = \beta e(\{\rho_\alpha\}) - s(\{\rho_\alpha\}),$$

with e and s respectively the energy and entropy per site.

For our (mean field) system,

$$\mathcal{F} = \beta \int_0^1 dx \int_0^{1-x} dz \left[\rho_A(x)\rho_C(x+z) + \rho_B(x)\rho_A(x+z) + \rho_C(x)\rho_B(x+z)\right]$$
$$+ \int_0^1 dx \left[\rho_A(x)\ln(\rho_A(x)) + \rho_B(x)\ln(\rho_B(x)) + \rho_C(x)\ln(\rho_C(x))\right],$$

To get the "typical" density profile we have to minimize $\mathcal{F}$ with respect to ρ_A and ρ_B (or ρ_A, ρ_C, or ρ_B, ρ_C) since we can always eliminate one of the densities via $\sum \rho_\alpha(x) = 1$.

The minimizing profile will be a "compromise" between the entropy which wants to keep all the densities uniform and the energy which wants to keep the species segregated, as in the ground state.

Minimization of $\mathcal{F}$ with respect to ρ_A and ρ_B then gives the Euler-Lagrange equations (ELE).

$$\begin{aligned}\frac{\delta\mathcal{F}}{\delta\rho_A(x)} &= \mathcal{F}_A - \mathcal{F}_C = 0,\\ \frac{\delta\mathcal{F}}{\delta\rho_B(x)} &= \mathcal{F}_B - \mathcal{F}_C = 0,\end{aligned}$$

where

$$\begin{aligned}\mathcal{F}_A &= \left(\frac{\delta\mathcal{F}}{\delta\rho_A}\right)_{\rho_B,\rho_C} = \log\rho_A(x) + \beta\int_0^x[\rho_C(y)-\rho_B(y)] + \text{const.}\\ \mathcal{F}_B &= \left(\frac{\delta\mathcal{F}}{\delta\rho_B}\right)_{\rho_C,\rho_A} = \log\rho_B(x) + \beta\int_0^x[\rho_A(y)-\rho_C(y)] + \text{const.}\\ \mathcal{F}_C &= \left(\frac{\delta\mathcal{F}}{\delta\rho_C}\right)_{\rho_A,\rho_B} = \log\rho_C(x) + \beta\int_0^x[\rho_B(y)-\rho_A(y)] + \text{const.}\end{aligned}$$

and we have used the fact that the $\bar{\rho}_\alpha$ are fixed, and $\rho_C(x) = 1 - \rho_A(x) - \rho_B(x)$.

Simple manipulations now show that $\sum \rho_\alpha \frac{\partial \mathcal{F}_\alpha}{\partial x} = 0$, which implies, rather surprisingly, that the solutions of the ELE, will satisfy the equation, $\mathcal{F}_\alpha = \text{const}$, $i.e.$, the functional derivatives of $\mathcal{F}$ can be taken as if the ρ_α were independent.

This gives the ELE,

$$\begin{aligned} \frac{d\rho_A}{dx} &= \beta \rho_A (\rho_C - \rho_B) \\ \frac{d\rho_B}{dx} &= \beta \rho_B (\rho_A - \rho_C) \\ \frac{d\rho_C}{dx} &= \beta \rho_C (\rho_B - \rho_A) , \end{aligned}$$

which are identical to the equations (1) when $\bar{J}_\alpha = 0$. Inspection of these equations show that their solutions satisfy

$$\rho_A(x) + \rho_B(x) + \rho_C(x) = \text{const} = 1.$$

and that

$$\rho_A(x)\rho_B(x)\rho_C(x) = K.$$

The solutions of the ELE correspond to the stationary points of $\mathcal{F}$ which are in the interior of the domain of permissible density profiles, *i.e.*, $\rho_\alpha(x) > 0$ for each α with $x \in [0,1]$ as long as $\bar{\rho}_\alpha \neq 0$.

This will always be the case for the minimizers of $\mathcal{F}$, at nonzero temperature, $\beta < \infty$, due to the form of the entropy terms. For $\beta = \infty$, when only the energy counts, the minimizing densities will be the continuum limit of the ground state configurations described before (slides 5 and 6).

"Explicit" solution of the ELE

Using the above equations we find that each $\rho_\alpha(x)$ is a solution of

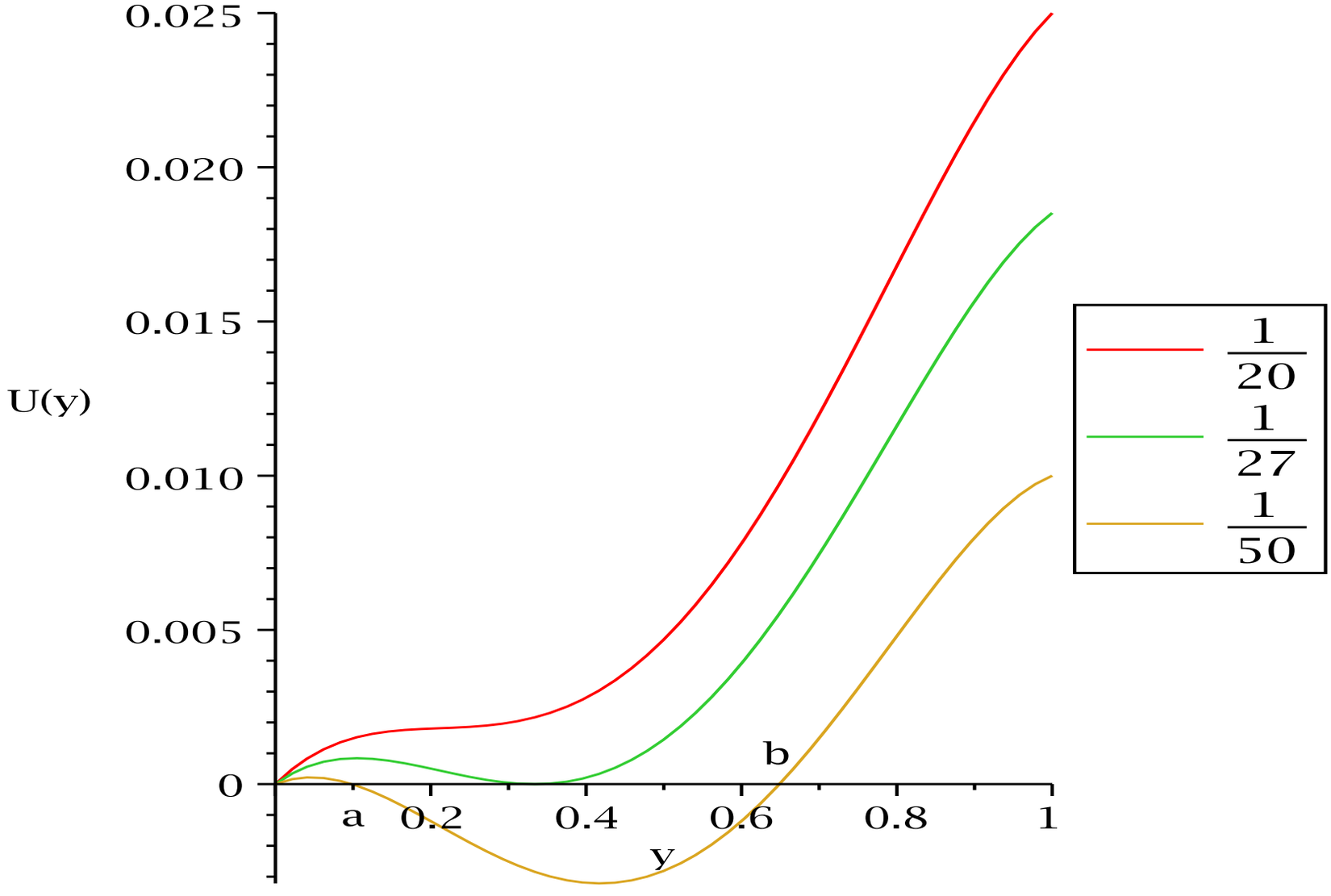
$$\rho'(x)^2 + 8\beta^2 U_K(\rho(x)) = 0; \qquad U_K(\rho) \equiv \frac{1}{2}K\rho - \frac{1}{8}\rho^2(1-\rho)^2.$$

Set $t = 2\beta x$ and let $y(t) = \rho(t/2\beta)$; then y satisfies the equation

$$\frac{1}{2}y'(t)^2 + U_K(y(t)) = 0.$$

This is the equation of the zero energy solution of a mass 1 particle moving in a potential U_K. For $0 < K < 1/27$, U_K has four zeros, with $U_K(y) < 0$ for $a < y < b$. See Figure. Since we are interested in solutions which satisfy $0 < \rho_\alpha(x) < 1$ we consider only the solutions which oscillate between a and b.

These solutions can be expressed in terms of elliptic functions but we do not use the representation in the results described below. In fact our results may even give some new information about some elliptic functions (as far as we know).



Plots of $U_K(y)$ for $K = 1/20$, $1/27$ and $1/50$.

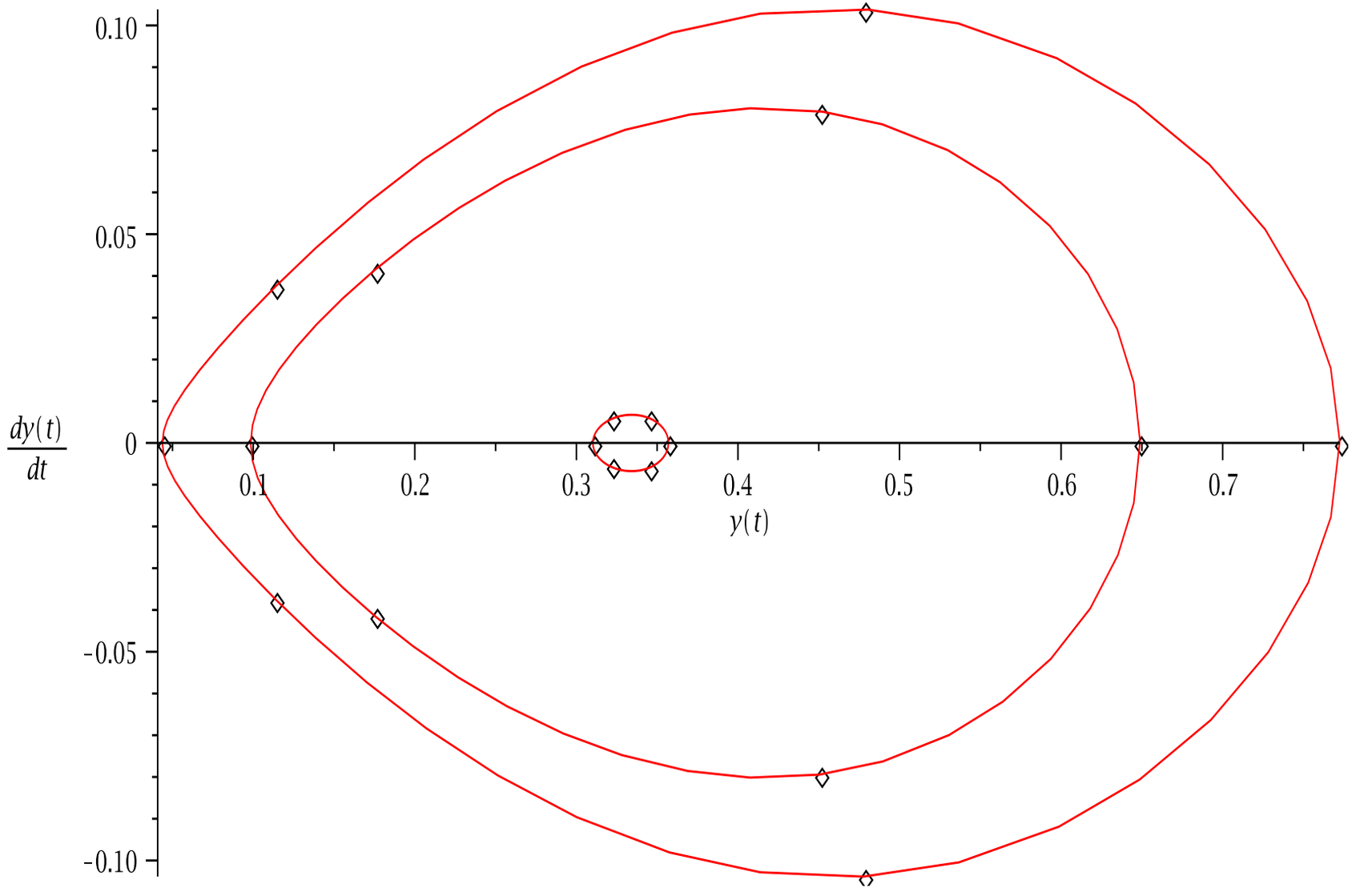
Let y_K denote the solution which satisfies $y_K(0) = a$; $y_K(t)$ then oscillates between a and b with period T_K and can be obtained for all t by extending to an even function of period T_K, where
(a) $\lim_{K \nearrow 1/27} T_K = 4\pi\sqrt{3}$ and $\lim_{K \searrow 0}(T_K/\ln(1/K)) = 6$.
(b) T_K is a strictly monotonic decreasing function of K for $0 < K \leq 1/27$.

For $\alpha = A, B, C$ there must be a phase shift t_α such that

$$\rho_\alpha(x) = y_K(2\beta(x - 1/2) + t_\alpha), \qquad 0 \leq x \leq 1,$$

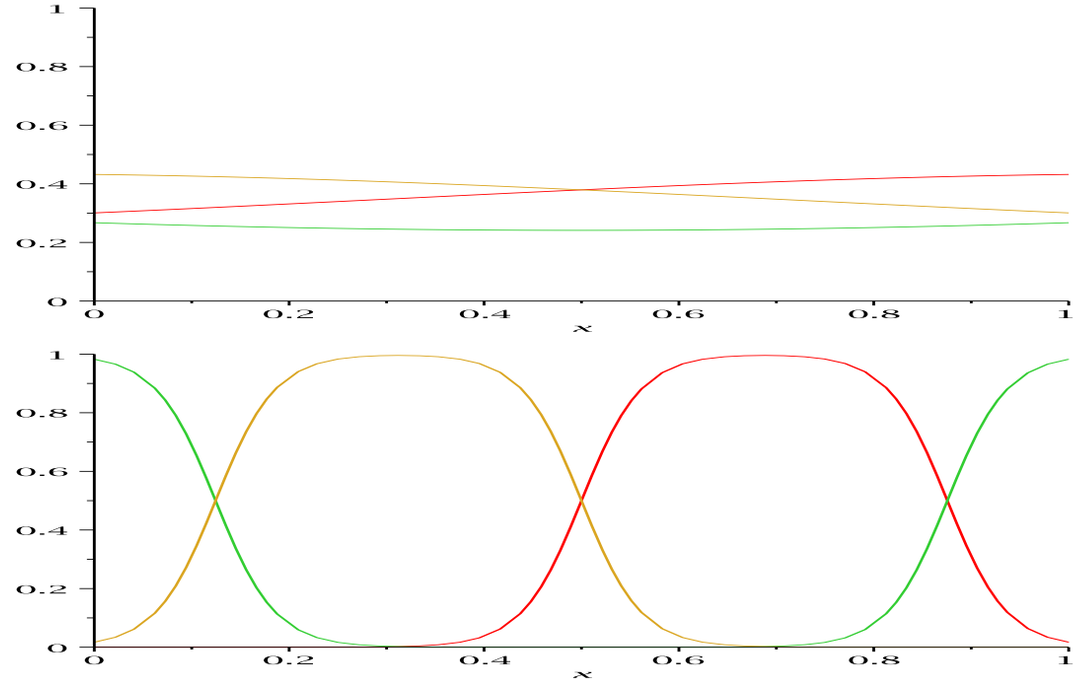
that is, each $\rho_\alpha(x)$ is obtained by looking at the solution $y_K(x)$ within a window of length 2β centered at some value t_α, and rescaling from t to x.

It can be shown that if $\rho_A(x)$, $\rho_B(x)$, and $\rho_C(x)$ satisfy the ELE then $t_A = t_B + T_K/3$ and $t_C = t_B - T_K/3$.



Phase plane orbit of $y_K(t)$ for $K = 1/100, 1/50, 1/27.1$. The time intervals between the six marked points are all equal to $T_K/6$.

The figure below shows the curves $\rho_\alpha(x)$ obtained from $y_K(t)$ and $y_K(t \pm T_K/3)$ for two values of β, with the same $\bar{\rho}_\alpha$'s.



Plots of ρ_A (red), ρ_B (green), ρ_C (yellow) when

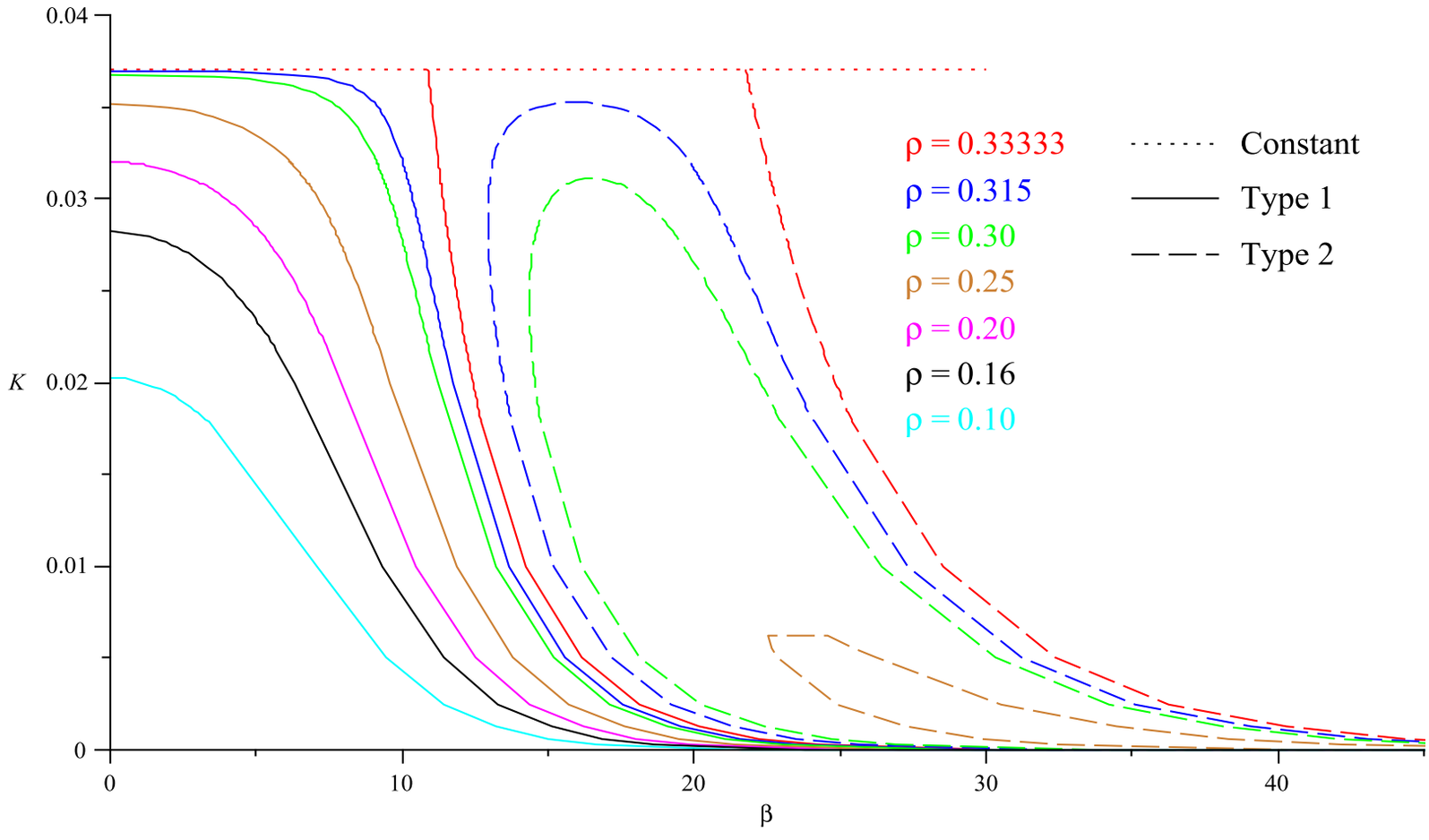
$\bar{\rho}_B = 0.25, \bar{\rho}_A = \bar{\rho}_C = 0.375.$

(1) $\beta = 2.898, K = 5/144$, (2) $\beta = 32.5683, K = 1/204800.$

To obtain solutions ρ_α for some K one views the curves $y_K(t)$ in a window of length 2β.

We label the solutions of the ELE by an integer which is one more than the number of full periods that fit into the window.

A solution $\rho(x)$ of the ELE with $K < 1/27$ is of *type* n, for $n = 1, 2, \ldots$, if $(n-1)T_K < 2\beta \leq nT_K$.



Plot of K versus β for different solutions for $\bar{\rho}_B = \rho \leq 1/3, \bar{\rho}_A = \bar{\rho}_C = (1 - \bar{\rho}_B)/2$. The solid lines are the type 1 solutions, the dashed lines are the type 2 solutions and the dotted line is the constant solution.

As can be seen from the figure there will in general be many solutions for the ELE for a given β and $\{\bar{\rho}_\alpha\}$. We know that at least one of these solutions will be the minimizer of $\mathcal{F}$.

Question: (i) Is the minimizing profile $\tilde{\rho}(x) = \{\tilde{\rho}_\alpha(x)\}$ unique?
(ii) If not unique, identify the minimizing profiles.

Answer: For $\bar{\rho} = (1/3, 1/3, 1/3)$ and $\beta \leq 2\pi\sqrt{3}$ there is a unique solution of the ELE and therefore ipso facto a unique minimizer. It is (as expected from Clincy et al.) $\tilde{\rho}_\alpha(x) = \bar{\rho}_\alpha = 1/3$ corresponding to $K = 1/27$.

For $\bar{\rho} = (1/3, 1/3, 1/3)$ and $\beta > 2\pi\sqrt{3}$ all type 1 solutions with $2\beta = T_K$ and t_B any point in $[0, T_K]$ are minimizing profiles. The constant solution as well as the $n > 1$ type solutions, which will exist for $\beta > 2\pi n\sqrt{3}$ are not minimizers.

We can also prove for all β and $\bar{\rho}_\alpha$'s, that the minimizing solution has to be of type 1.

We have strong evidence that for $\bar{\rho} \neq (1/3, 1/3, 1/3)$ there is a unique minimizer for all $\beta < \infty$. This is actually proven for $\beta < 2\pi/\sqrt{3}$, all $\bar{\rho}_\alpha$, and for $\bar{\rho}_B < \bar{\rho}_A = \bar{\rho}_C$, all β.

Local measures for ABC from equilibrium

- $\bar{\rho} = (1/3, 1/3, 1/3)$, $\beta \leq 2\pi\sqrt{3}$, and for all $\bar{\rho}_\alpha$ with $\beta < 2\pi/\sqrt{3}$ as well as for $\bar{\rho}_B < \bar{\rho}_A = \bar{\rho}_C$ and $\beta < \infty$,

$$\kappa(x, \underline{n}) = \delta(\tilde{\rho}(x) - \underline{n}), \qquad \mu_{(x)}(\underline{\eta}) = \hat{\mu}_{\tilde{\rho}(x)}$$

  (As noted before, we believe, but have not proven, that this uniqueness holds for all $\beta < \infty$ when not all the $\bar{\rho}_\alpha$ are equal.)

- For $\bar{\rho} = (1/3, 1/3, 1/3)$, $\beta > 2\pi\sqrt{3}$

$$\mu_{(x)}(\underline{\eta}) = \int_0^1 \widehat{\mu}_{\tilde{\rho}(x+z)}(\underline{\eta})dz$$

where, remembering that $y_K(t)$ is periodic with period $T_K = 2\beta$, we have

$$\begin{aligned}
\tilde{\rho}_A(x) &= y_K(2\beta(x - 1/2)) \\
\tilde{\rho}_B(x) &= y_K(2\beta(x - 1/6)) \\
\tilde{\rho}_A(x) &= y_K(2\beta(x + 1/6))
\end{aligned}$$

(I will not write this out in terms of $\kappa(x, \underline{n})$.)

Local measures: general

The ABC model illustrates the general problem of finding the local microscopic structure of macroscopic systems. This structure can be uniform across the system (away from the boundaries) or it can vary with x; $x \in \Lambda$ being a point in a macroscopic domain $\Lambda \in \mathbb{R}^d$, say a unit cube. The macroscopic system in Λ is obtained as the $N \to \infty$ limit of a microscopic system in a stationary state with specified bulk and boundary dynamics.

The finite microscopic system is assumed to have a unique stationary measure. This can be either an equilibrium measure, defined (for the present) to be one in which there is detailed balance for the dynamics, or not.

As a simple example of the equilibrium case consider the Ising model in the cube $[-N, N]^d \subset \mathbb{Z}^d$, evolving according to Glauber dynamics satisfying detailed balance with respect to the Gibbs measure $\sim \exp(\beta \sum_{<i,j>} \sigma_i \sigma_j +$ boundary terms). The boundary terms come from boundary conditions which I will take to be either all $+$ or of the Dobrushin type, $\pm$ bc, ie $+(-)$ for $i_2 \geq 0$ ($i_2 < 0$).

When $\beta < \beta_c(d)$ there is only one extremal measure, $\mu(\underline{\sigma}; \beta)$ for the infinite system on $\mathbb{Z}^d$ and so $\mu_{(x)}(\underline{\sigma}) = \mu(\underline{\sigma}; \beta)$ for all x. When $\beta > \beta_c(d)$, in $d \geq 2$, there are two extremal translation invariant states, $\mu_{(+)}(\underline{\sigma}, \beta)$ and $\mu_{(-)}(\underline{\sigma}, \beta)$, with $\mu_{(+)}(\underline{\sigma}, \beta)$ and $\mu_{(-)}(\underline{\sigma}, \beta)$ corresponding to the measures obtained from the all $+$ or all $-$ boundary conditions.

It is known that for Dobrushin boundaries $\mu_{(x)}, x \in \Lambda$, will for $x_2 > 0$ be $\mu_{(+)}(\underline{\sigma}, \beta)$ while for $x_2 < 0$ it will be $\mu_{(-)}(\underline{\sigma}, \beta)$. When $x_2 = 0$ we will get something which depends on the way the limit is taken and on the dimension.

In the simplest case consider the microscopic site $\underline{i} = (i_1, 0, i_3) = [xN]$. Then in $d = 2$, $\mu_{(x)} = (\mu_{(+)}(\underline{\sigma}, \beta) + \mu_{(-)}(\underline{\sigma}, \beta))/2$ for all $\beta > \beta_c(2)$. In $d = 3$, we will instead get for $\beta > \beta_{\text{rough}} \geq \beta_c(3)$, a $\mu_{(x)}$ which is non translation invariant, in the x_2 direction corresponding to a "rigid" Dobrushin interface.

Taking the limit at $\underline{i}$ such that $i_2 = \lambda\sqrt{N}$ will give a superposition $\mu_{(x)} = c(\lambda)\mu_{(+)}(\underline{\sigma}, \beta) + (1 - c(\lambda))\mu_{(-)}(\underline{\sigma}, \beta)$ in $d = 2$ with $c(\lambda)$ an error function for $\beta > \beta_c(2)$. In $d = 3$, with $\beta > \beta_{\text{rough}}$ one will get $c(\lambda) = 1$ for $\lambda > 0$ and $c(\lambda) = 0$ for $\lambda < 0$. It is not clear what one gets for $\beta \in (\beta_{\text{rough}}, \beta_c(3))$.

Going now to a nonequilibrium example consider the case of the open simple exclusion process.

Open Systems

SSEP $\rho_a = \frac{\alpha}{\alpha+\gamma}$, $\rho_b = \frac{\delta}{\beta+\delta}$.

TASEP $\gamma = \delta = 0$, $\rho_a = \alpha$, $\rho_b = 1 - \beta$

Consider the stationary measure $\mu(\underline{\eta})$ for the open system corresponding to the SSEP or TASEP centered on $j = [xN]$ then, in the limit $N \to \infty$, $\mu_{(x)}$ is given by

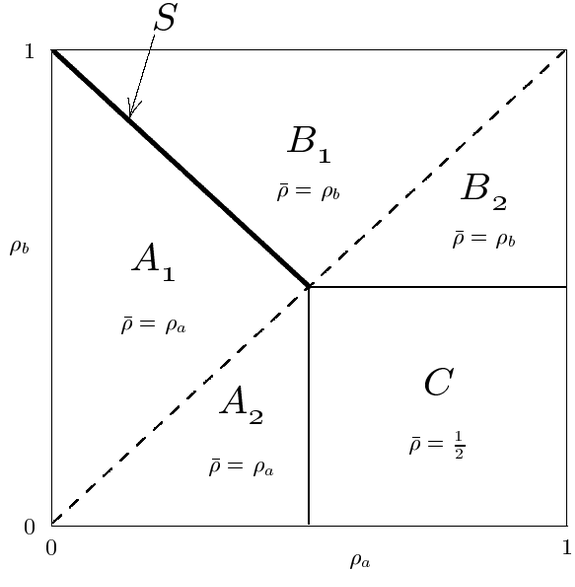
$$\mu_{(x)} = \int \kappa(x;\lambda)\nu_\lambda d\lambda$$

where $\{\nu_\lambda\}$ are the infinite volume extremal stationary measures for the SSEP or TASEP on $\mathbb{Z}$.

For the SSEP there are only the Bernoulli measures, and it follows from the work of Eyink, Spohn, L. that $\kappa(x;\lambda) = \delta(\lambda - \tilde{\rho}(x))$, $\tilde{\rho}(x) = \rho_a + x(\rho_b - \rho_a)$.

For the TASEP the infinite volume stationary measures are either of the blocking type, with all sites empty to the left and all sites occupied to the right of some fixed site, or are translation invariant Bernoulli measures at density $\bar{\rho}$. Liggett proves that the blocking measures do not enter in the decomposition of $\mu_{(x)}$. When one is not on the "shock line" S, $\tilde{\rho}(x) = \bar{\rho}$, constant, and Liggett proves that $\kappa(x;\lambda) = \delta(\lambda - \bar{\rho})$. On the shock line S

$$\kappa(x;\lambda) = x\delta(\lambda - \rho_a) + (1-x)\delta(\lambda - \rho_b).$$



The phase diagram can be understood in terms of solutions of the Burgers equation

$$\frac{\partial \rho(x,t)}{\partial t} = -\frac{\partial}{\partial x}\left(\rho(x)(1-\rho(x))\right), \qquad x \in \mathbb{R},$$

which have shocks of the form

$$\rho(x,t) = \begin{cases} \rho_-, & x \le X(t), \\ \rho_+, & x > X(t), \end{cases} \qquad \rho_- < \rho_+;$$

this shock moves with velocity $dX(t)/dt = v = 1 - \rho_- - \rho_+$.

In A_1 the shock sticks to right,
in B_1 the shock sticks to left,
in S, the shock has no net drift, $v = 0$.
In A_2, B_2 and C we are in the "fan" region,
C is the maximal current phase.

The proof given by Liggett is rather special — making use of some inequalities to prove that the extremal states entering into the superposition all have the same current,

$$j = \rho_a(1 - \rho_a) = \rho_b(1 - \rho_b).$$

We (Ayyer, L, Speer) have used a different argument which also works (with modifications) for the case with a fixed density of second class particles where we also find that all infinite volume extremal stationary states appearing in the superposition giving any local measures have the same current.

There ought to be a general argument for this!

Our argument goes as follows: For the one component TASEP **not** on the shock line one has from the exact solution of the finite system (Derrida et al.) that

$$\begin{aligned} \tilde{\rho}(x) &= \int \lambda \kappa(x;\lambda) d\lambda = \bar{\rho}, \text{ constant} \\ \bar{j}(x) &= \int \lambda(1-\lambda)\kappa(x;\lambda) d\lambda = \bar{\rho}(1-\bar{\rho}). \end{aligned}$$

This implies that

$$\langle \lambda^2 \rangle_\kappa = \langle \lambda \rangle_\kappa^2$$

and hence that

$$\kappa(x;\lambda) = \delta(x - \bar{\rho}).$$

On the shock line one can use a "second class" particle which tracks the shock microscopically and is uniformly distributed in $[0,1]$.

This suggests a way of looking at what is happening globally in a macroscopic system (S. Goldstein). Think of a general $\kappa(x;\lambda)$ as arising from a random field $\psi(x)$ which gives the (random) value of "λ" at position x. For the cases considered, $\psi(x)$ would either be a deterministic field or, in the case of the TASEP on S,

$$\psi(x) = \theta(x - Y)\rho_b + (1 - \theta(x - Y))\rho_a,$$

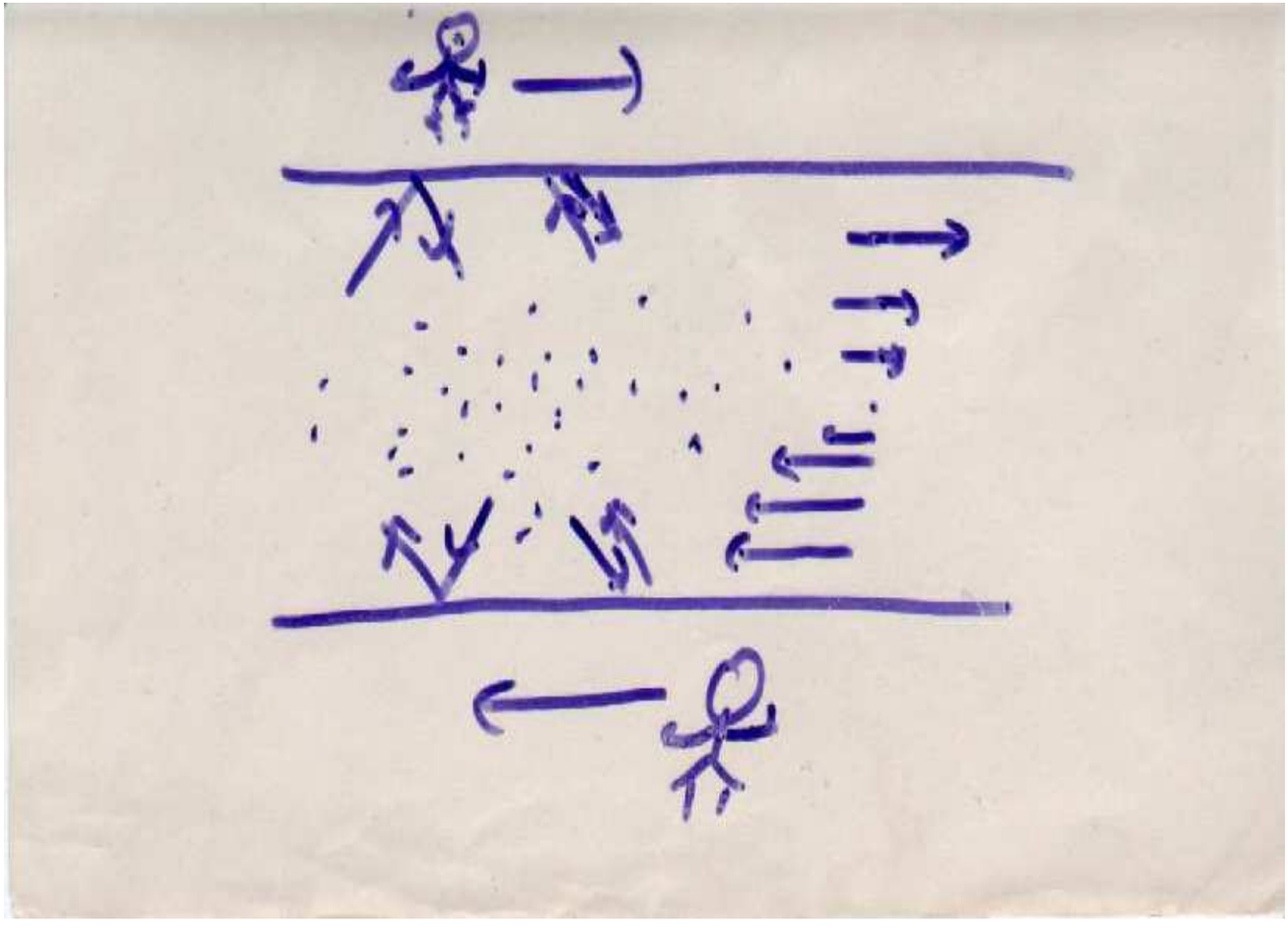
with Y uniformly distributed on the interval. Similarly for the ABC model with $\bar{\rho} = (1/3, 1/3, 1/3)$, $\beta > 2\pi\sqrt{3}$, the phase shift t_B is uniformly distributed in $[0, 1]$.

In the general case one would hopefully get a global space-time picture of what is happening in a nonequilibrium stationary state of a macroscopic system which would go beyond the "local" measures $\mu_{(x)}, x \in \Lambda$. For example for the TASEP on S one would expect the shock position to undergo a diffusion on a longer time scale.

This is a challenging task, related to recent work by Bertini et al. We know that even in the simplest case of the SSEP the large deviation function for finding density profiles $\rho(x) \neq \tilde{\rho}(x)$ is not given by the local equilibrium formulas. These reflect the $O(1/N)$ corrections to local equilibrium.

Is there a universal way of capturing this global behavior? Does the global structure always depend only on the locally conserved quantities described by hydrodynamic equations like the Navier-Stokes equations?

Example: Stationary shear flow (Chernov, L).



References for ABC on ring

1. M.R. Evans, Y. Kafri, H.M. Koduvely, and D. Mukamel,
   Phys. Rev. Lett. **80**, 425 (1998);
   Phys. Rev. E. **58**, 2764 (1998)

2. M. Clincy, B. Derrida, and M.R. Evans,
   Phys. Rev. E. **67**, 066115 (2003)

3. T. Bodineau, B. Derrida, V. Lecomte and F. van Wijland,
   arXiv: 0809.2394 (2008)

4. G. Fayolle and C. Furtlehner,
   J. Stat. Phys. **114**, 229 (2004);
   arXiv:cond-mat/0603243 (2006)