Grand ensemble results for the Asymmetric Simple Exclusion Process

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Recent accomplishments:

- RG theory of critical phenomena
- Density functional theory
- Monte Carlo methods in computational science

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Used as a tool in many other areas of science, e.g.:

- Condensed matter theory
- Nuclear physics
- Plasma physics
- String theory

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There is no general description for stationary non-equilibrium systems, comparable to the Gibbs-ensembles in equilibrium.

For this reason there is great interest in simple stochastic models of non-equilibrium behavior, for which exact results can be obtained.

An example of this is the Asymmetric Simple Exclusion Process (ASEP) for which many results have been obtained in recent years.

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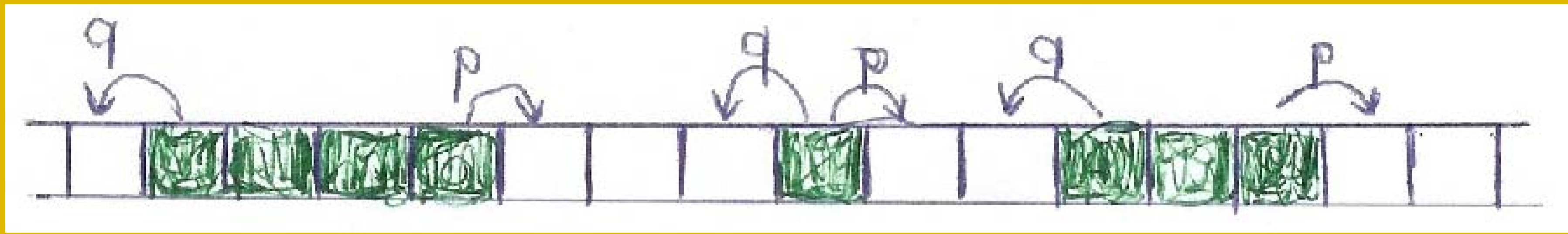

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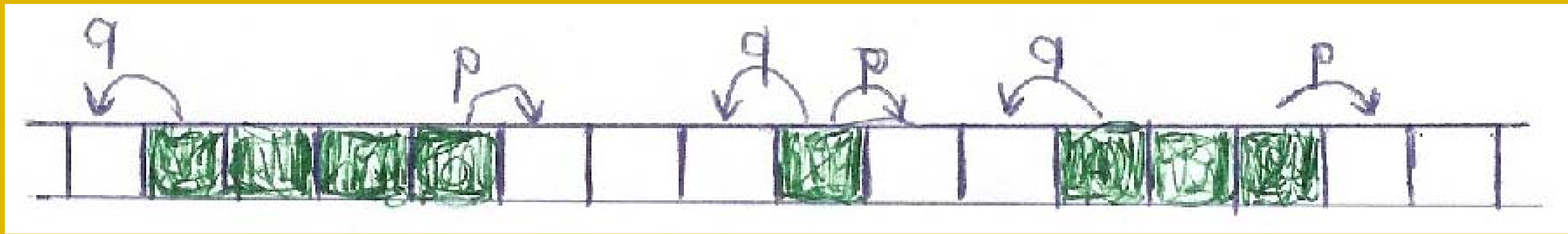

$p=q \rightarrow$ SSEP: Collective dynamics on average identical to those of set of independent random walkers. Tagged particle dynamics are non-trivial (e.g. $< [x(t)- x(0)]^2 \sim t^{1/2}$ for large t) but well understood.

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Of interest as very simplified model for traffic flows.
Other applications include:

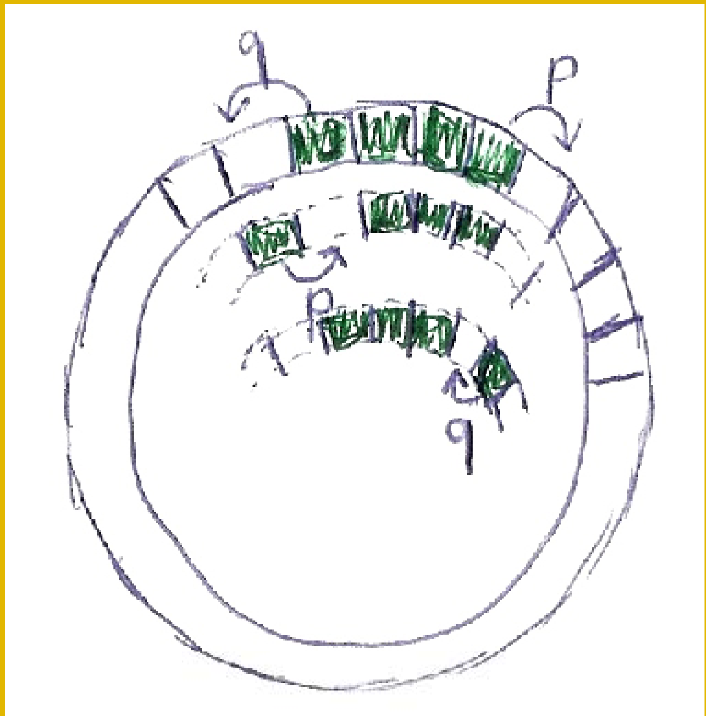
Transport of ions or molecules through pores in membranes.
Dynamics of interfaces in 2d.
Reptation dynamics of polymers in a gel.
Dynamics of motor proteins moving along microtubules.

Good reviews are given in:

B. Derrida, Physics Reports **301** (1998) 65-83
R.A. Blythe and M.R. Evans J. Phys. A **40** (2007) R333-R441

Stationary state on a ring

For n particles on a ring of length N the stationary state gives equal weight to all configurations.



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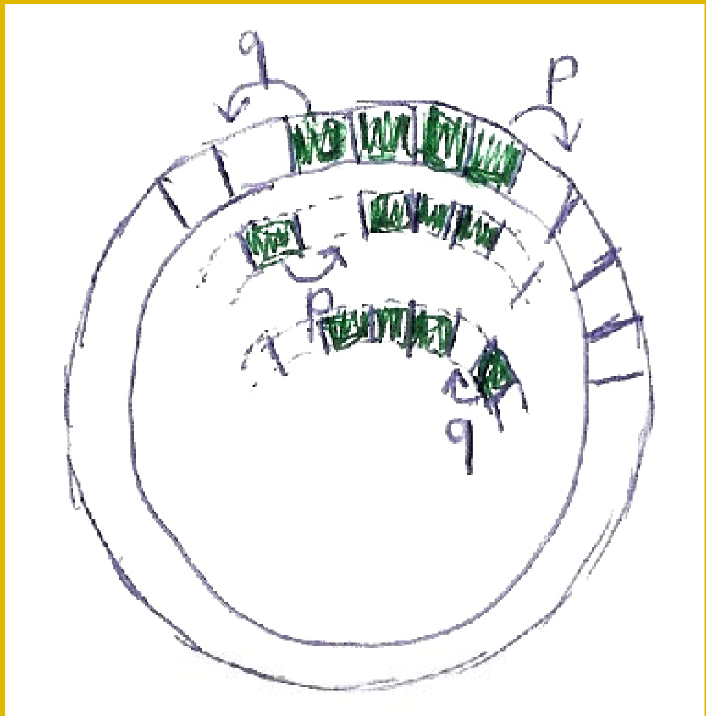

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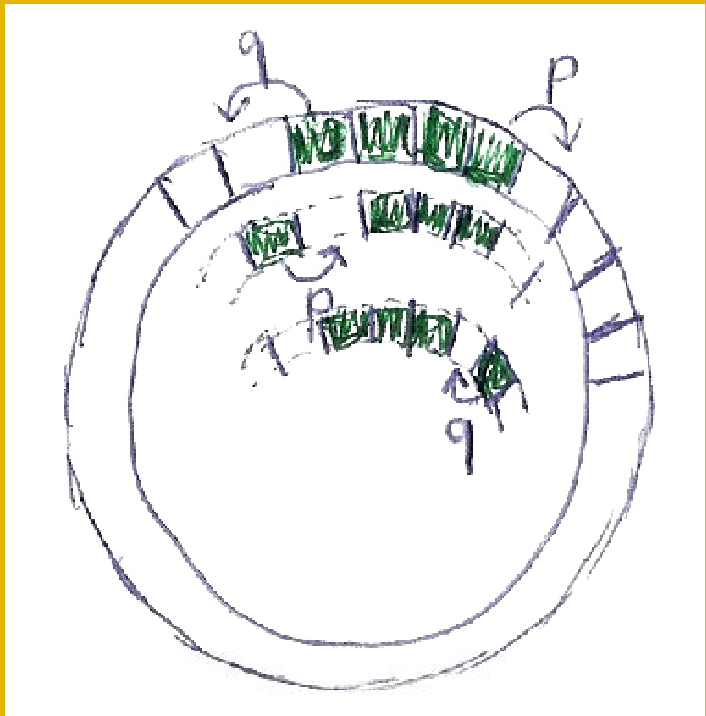
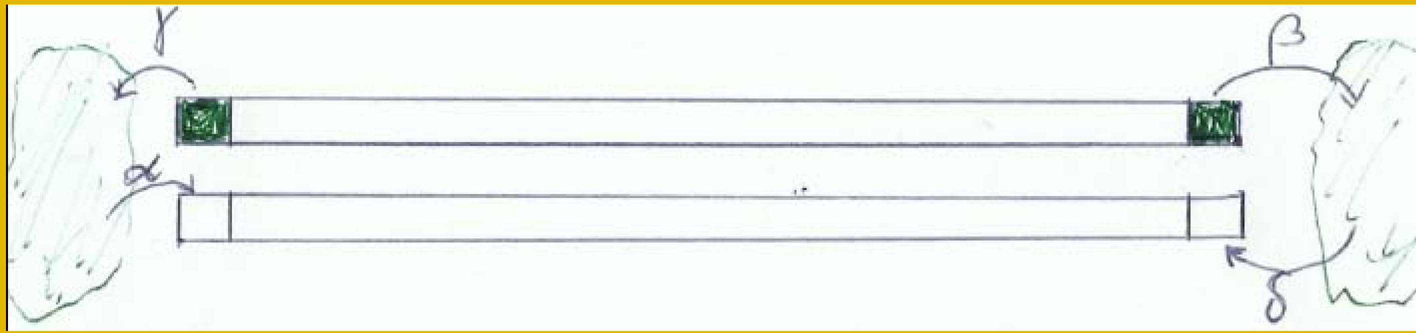


With cluster number n_{cl} both gain and loss rate equal $n_{cl}(p+q)$

As a consequence the occupations of different sites are completely uncorrelated (apart from small finite size effects). In other words: mean-field approximations are exact.

With open boundaries and given rates $\alpha,\beta,\gamma,\delta$ for extracting or inserting particles at the ends the situation becomes much more complicated.



The most elegant and simplest way of attacking this problem is with the Matrix Product Ansatz (MPA) of Derrida and Evans.
They assume one can find matrices D and E, satisfying

$$pDE - qED = D + E$$

$$< W \mid (\alpha E - \gamma D) = < W \mid$$

$$(\beta D - \delta E) \mid V> = \mid V >$$

Then the stationary distribution is given by

$$p_{st}(0,0,1,0 \ldots 1,1,0 \ldots 0,1) = Z^{-1} < W \mid EEDE \ldots DDE \ldots ED \mid V >$$

$$p_{st}(0,0,1,0 \ldots 1,1,0 \ldots 0,1) = Z_N^{-1} < W|\, EEDE \ldots DDE \ldots ED \,|V>$$

with

$$Z_N = < W \mid (E + D)^N \mid V >$$

From the partition function Z_N several quantities can be calculated immediately.

The average current is obtained as

$$J = J_{n,n+1} = Z_N^{-1} < W \,|\, (E + D)^{n-1} \, (pDE - qED) \, (E + D)^{N-n-1} \,|\, V >$$
$$= Z_N^{-1} < W \,|\, (E + D)^{N-1} \,|\, V >$$
$$= Z_{N-1}/Z_N$$

Average densities follow from a slight generalization:

$$Z_N\,(\lambda,\mu) = < W \,|\, (\lambda\, E + \mu\, D)^N \,|\, V >$$

as

$$\rho = N^{-1}\, [\partial \log Z_N\,(\lambda,\mu)\, / \partial\, \mu]_{\lambda=\mu=1}$$

Strong simplifications occur for q=0 (TASEP).
Commutation relation reduces to

$$pDE = D + E \quad (\textit{here one may set } p=1)$$

plus one may set $\gamma = \delta = 0$, so $< W \mid \alpha E = < W \mid$; $\beta D \mid V > = \mid V >$

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Most practical is going to a Grand ensemble representation
(*known in the field as generating function method*).

$$p_{st}(N,\tau_1 \ldots \tau_N) = \frac{1}{Z_g(z)} z^N < W \,|\; \Pi_{i=1}^{N}(\tau_i D + (1 - \tau_i)E) \,|\, V >$$

with

$$Z_g(z) = \sum_{N=0}^{\infty} z^N < W \,|\; (D+E)^N \,|\, V >$$

$$= \; < W \,|\; \frac{1}{1 - z(D+E)} \,|\, V >$$

$$Z_g(z) = \; < W | \; \frac{1}{1 - z(D+E)} | V >$$

The average current follows from

$$< j > \; = \; < \frac{Z_{N-1}}{Z_N} > \; = \frac{\sum_{N=0}^{\infty} \frac{Z_{N-1}}{Z_N} z^N Z_N}{Z_g(z)} = z$$

The average length follows as

$$< N > = \frac{\sum_{N=0}^{\infty} N \, z^N Z_N}{Z_g(z)} = z \frac{\partial \log Z_g(z)}{\partial z}$$

Expression for density remains as before.

$$Z_g(z) = \langle W | \frac{1}{1 - z(D+E)} | V \rangle$$

Now use: $(1 - cD)(1 - cE) = 1 - c(D + E) + c^2 DE$

$$= 1 - c(1 - c)(D+E)$$

to rewrite

$$Z_g(z) = \langle W | \frac{1}{1 - \frac{1}{2}(1 - \sqrt{1-4z})E} \; \frac{1}{1 - \frac{1}{2}(1 - \sqrt{1-4z})D} | V \rangle$$

$$= \frac{\alpha}{\alpha - \frac{1}{2}(1 - \sqrt{1-4z})} \; \frac{\beta}{\beta - \frac{1}{2}(1 - \sqrt{1-4z})}$$

$(requiring \; \langle W | V \rangle = 1)$

$$Z_g(z) = \frac{\alpha}{\alpha - \frac{1}{2}(1-\sqrt{1-4z})}\ \frac{\beta}{\beta - \frac{1}{2}(1-\sqrt{1-4z})}$$

We want $<N> \to \infty$, say $<N> = 1/\varepsilon$. From

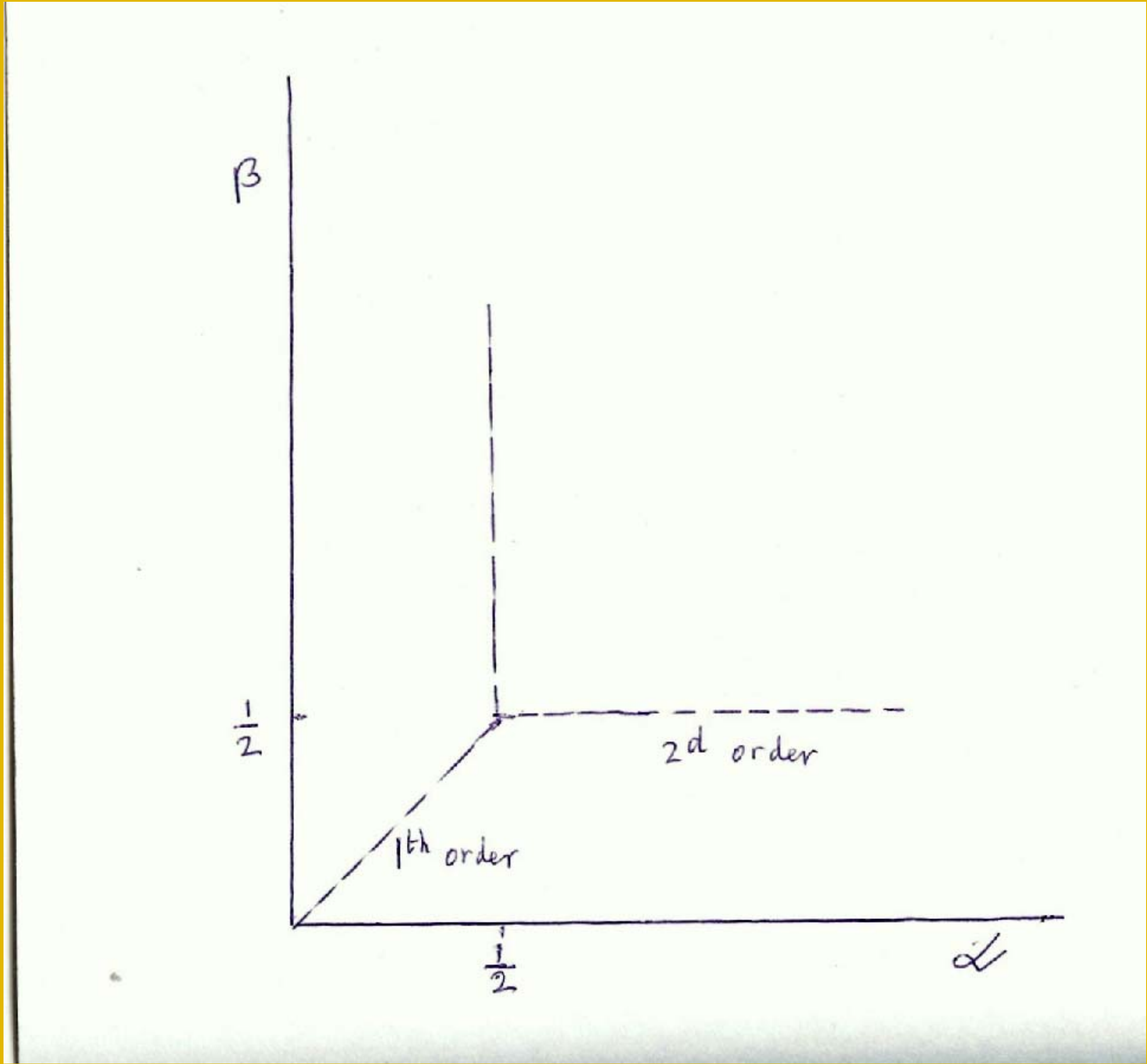
$$<N> = z\frac{\partial \log Z_g(z)}{\partial z}$$

$$= \left[\frac{1}{\alpha - \frac{1}{2}(1-\sqrt{1-4z})} + \frac{1}{\beta - \frac{1}{2}(1-\sqrt{1-4z})}\right]\frac{1}{\sqrt{1-4z}}$$

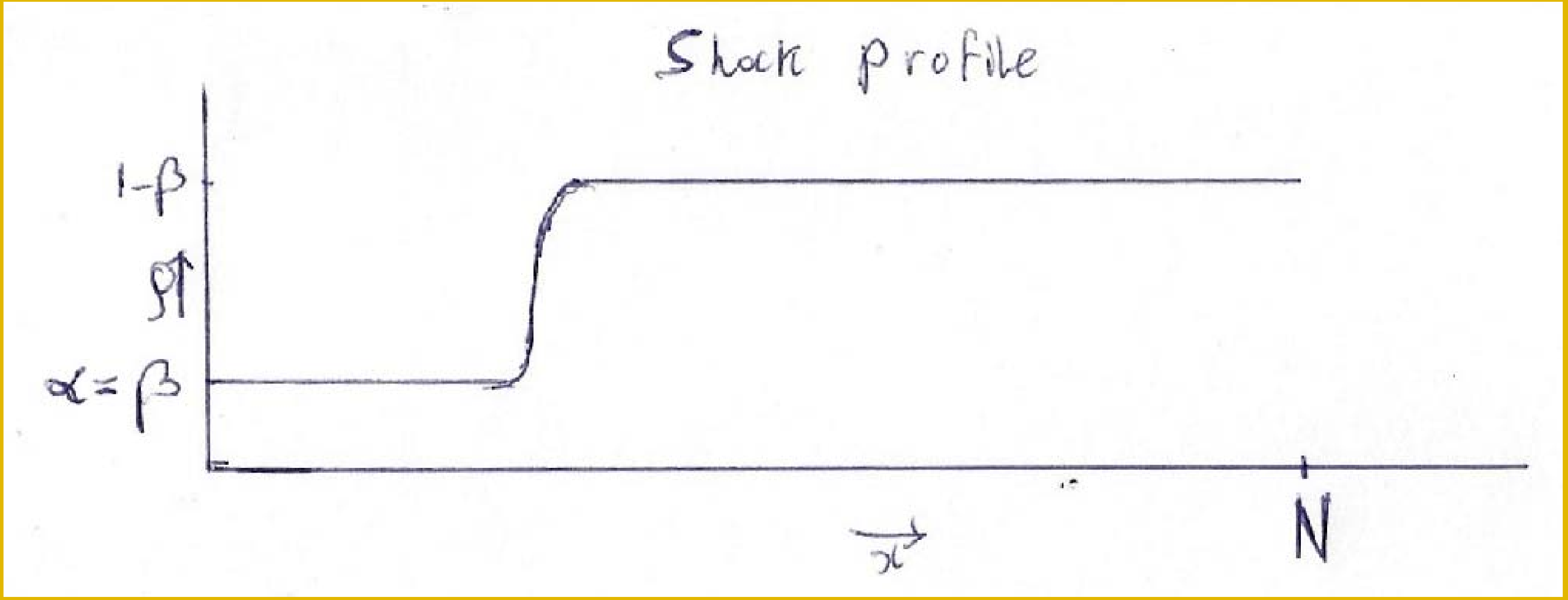
we see there are three ways this can be obtained:

1) z = $\alpha(1-\alpha)$ (*with* $\alpha < \beta$ *and* $\alpha < 1/2$) Low density phase
2) z = $\beta(1-\beta)$ (*with* $\beta < \alpha$ *and* $\beta < 1/2$) High density phase
3) z = $1/4$ Maximal current phase

Leads to phase diagram below:



Special case for $\alpha = \beta < ½$. In this case low-density and high-density phase compete and one obtains solutions showing a shock profile. Interpretable as solutions with coexisting phases.



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Multispecies models

References: V. Karimipour, PRE **59** (1999) 205-212
V. Karimipour, Europhys. Lett. 47 (1999) 304-310
M. Khorrami and V. Karimipour, J. Stat. Phys. 100 (2000) 999-1030

n species represented by matrices D_i. Exchange rates p_{ij} between neighboring particles with $p_{ij} \neq 0$ only if $i < j$.

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n species represented by matrices D_i. Exchange rates p_{ij} between neighboring particles with $p_{ij} \neq 0$ only if $i < j$.

Require that these matrices satisfy the relations

$$p_{ij} D_i D_j = c_i D_j - c_j D_i$$

They have to obey the associative property $D_i [D_j D_k] = [D_i D_j] D_k$
This imposes the conditions

$$p_{ij} = \mathrm{v}_i - \mathrm{v}_j, \text{ so } \mathrm{v}_1 > \mathrm{v}_2 > \ldots > \mathrm{v}_n$$

Passing rates are proportional to velocity differences.

Choose one of the species, say m+1 as the empties and set $v_{m+1} = 0$.

Then species 1…m are right movers. Can be inserted on left with rates $f_1 \ldots f_m$ if first site is occupied by an empty; and extracted (= exchanged for an empty) with rates $g_1 \ldots g_m$ if they occupy the last site. Species m+2, … n are left movers, with similar input and exit rates.

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Introduce again vectors < W | and | V > and require:
1. | V > is right eigenvector of $D_1 ... D_{m+1}$, with all eigenvalues 1.
2. < W | is left eigenvector of $D_{m+1} ... D_n$, also with eigenvalues 1.

The relations $(v_i - v_j) D_i D_j = c_i D_j - c_j D_i$ then impose severe conditions on the allowed values of the c_i, namely

$$c_i = v_i - v_0$$

The stationarity condition fixes the entrance and exit rates:

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If we require that the stationary distribution is of the form

$$p_{st}(i_1 \ldots i_N) = \frac{< W \mid z_{i_1} D_{i_1} \ldots z_{i_N} D_{i_N} \mid V >}{Z_g(z_1 \ldots z_n)}$$

the entrance and exit frequencies must be chosen as

$$f_j = \frac{z_j}{z_e} \mid \mathrm{v}_j - \mathrm{v}_0 \mid \qquad j \neq m+1 \qquad (with\ z_e \equiv z_{m+1})$$

$$g_j = \mid \mathrm{v}_j - \mathrm{v}_0 \mid$$

In addition z_e depends on the other z_j. So the fugacities are fixed by the entrance rates plus v_0, up to a multiplicative constant that determines the average length $< N >$.

Grand partition function:

$$Z_g = \langle W | \frac{1}{1-\sum_{j=1}^{n} z_j D_j} | V \rangle$$

$$= \langle W | \frac{1}{1-b_n D_n} \cdots \frac{1}{1-b_1 D_1} | V \rangle$$

Simple to express z_i in terms of b_j. The inverse problem requires solving polynomial equations of order n.
In terms of b's the partition function simply satisfies

$$\log Z_g = -\sum_{i=1}^{n} \log(1-b_i) \qquad (with \quad \langle W | V \rangle = 1)$$

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The large-system limit again can be obtained either by having $b_i \to 1$ (i-dominated phase) or Det $(\partial z_i / \partial b_j) = 0$ (maximal current phase). Phase transitions happen whenever as function of external parameters one jumps from one condition to another.

By and large one finds the same phenomena as in the single species case. Some remarks can be made, however:

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2. If one has at least two kinds of right (left) movers plus at least one kind of left (right) mover, the matrices can be reduced to constants and solutions basically reduce to product measures. All densities become uniform, with values $\rho_i = z_i / \sum_j z_j$. This can be cured by considering models with only right and left movers and no empties.

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3. Except in shock states, where both a right and a left mover have a $b_i \approx 1$ the occupations in the bulk are uncorrelated in the large-system limit.

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4. It is nice having a model that can describe multi-speed and two-lane traffic. However, it is a pity that solvability conditions restrict the passing rates to single values.

Remark: There are several other solution methods, which can be used e.g. to treat the Partially Asymmetric Simple Exclusion Process (PASEP). See e.g. Blythe and Evans.

Open problems:

1. Systems with disorder. Both by having different hopping rates of particles and by having hopping rates that vary between sites. Especially the latter problem is hard.

2. PASEP with two types of empty sites with interchanged p's and q's. This models DNA electrophoresis.

3. Higher dimensional systems.