

Two Species Open Exclusion Processes

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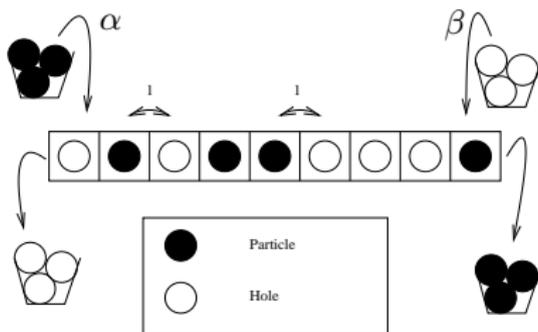
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Colloquium

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Totally Asymmetric Simple Exclusion Processes

- On a one-dimensional lattice of size L .
- Each site is either occupied or empty.
- Particles hop to the right with rate one whenever the site on the right is empty (DDM, DEHP, SD).
- Particles hop onto the first site at rate α from the left reservoir.
- Particles hop out of the last site at rate β into the right one.



Matrix Ansatz

- Satisfies the “matrix ansatz” (DEHP).
- Let \underline{x} be a configuration of the system, an element of $\{0, 1\}^L$.
- The steady state probability of τ is given by

$$P(\underline{x}) = \frac{1}{Z} \langle W | X_{\tau_1} \dots X_{\tau_L} | V \rangle.$$

- Z is the normalization factor

$$Z = \langle W | (X_0 + X_1)^L | V \rangle.$$

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- The matrices and the vectors satisfy the relations

$$X_1 X_0 = X_1 + X_0 \quad X_1 |V\rangle = \frac{1}{\beta} |V\rangle \quad \langle W | X_0 = \frac{1}{\alpha} \langle W |,$$

Example: $L = 2$

$$\begin{aligned}Z_2 P(00) &= \langle W | X_0 X_0 | V \rangle \\ &= \frac{1}{\alpha^2}, \\ Z_2 P(01) &= \langle W | X_0 X_1 | V \rangle \\ &= \frac{1}{\alpha\beta}, \\ Z_2 P(10) &= \langle W | X_1 X_0 | V \rangle = \langle W | (X_1 + X_0) | V \rangle \\ &= \frac{1}{\alpha} + \frac{1}{\beta}, \\ Z_2 P(11) &= \langle W | X_1 X_1 | V \rangle \\ &= \frac{1}{\beta^2}.\end{aligned}$$

$$Z_2 = \frac{\alpha^2 + \alpha\beta + \beta^2 + \alpha\beta(\alpha + \beta)}{\alpha^2\beta^2}.$$

Densities and Currents

- The density at site i is defined to be the probability that site i is occupied by a particle in the steady state, namely

$$\langle \tau_i \rangle = \sum_{\substack{\underline{\tau} \\ \tau_i=1}} P(\underline{\tau})$$

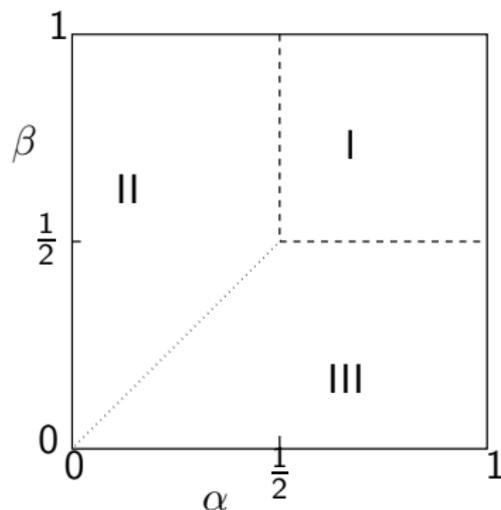
- By the matrix ansatz,

$$\langle \tau_i \rangle = \frac{\langle W | (X_0 + X_1)^{i-1} X_1 (X_0 + X_1)^{L-i} | V \rangle}{\langle W | (X_0 + X_1)^L | V \rangle}$$

- The particle current towards the right is given by

$$J = \langle \tau_i (1 - \tau_{i+1}) \rangle = \sum_{\substack{\underline{\tau} \\ \tau_i=1, \tau_{i+1}=0}} P(\underline{\tau}).$$

Phase Diagram



The phase diagram for the open TASEP. Region I is the maximal current phase. Regions II and III are the low and high density phases respectively. The boundary between II and III represents the shock line.

Second Class Particles

- Consider the system on the infinite lattice \mathbb{Z} with starting configuration Bernoulli with density ρ_- to the left of the origin and ρ_+ to the right of the origin and $\rho_- < \rho_+$. Then one notices the occurrence of a shock. The shock front moves with a drift $1 - \rho_- - \rho_+$.
- A second class particle is one which also tries to move to the right with rate one, but the hop succeeds only if the site on the right is empty. The hop for a first class particle succeeds if the site is either empty or is occupied by a second class particle.
- If we inject a single second class particle (ABL) in the system (say at the origin), then the second class particle sits at the location of the shock with high probability. Therefore, a natural definition of the location of the shock is precisely the position of the second class particle.

Factorization

- Suppose one conditions on the presence of second class particles at sites i and $j > i$. Then, in the grand canonical ensemble, one finds that the events which depend only on sites $i + 1, \dots, j - 1$ are completely independent of events which depend only on $j + 1, \dots, L, 1, \dots, i - 1$.
- This is a simple mathematical consequence of a representation of the matrices X_0, X_1, X_2 , but is physically not clear.
- This same factorization occurs if one takes the limit $L \rightarrow \infty$ by conditioning on a second class particle at the origin. Then events on the positive axis are uncorrelated with events on the negative axis.

Particle Hole Symmetry

Under the interchange

$$\begin{aligned}\alpha, \beta &\leftrightarrow \beta, \alpha \\ \tau_i &\leftrightarrow \tau'_{L-i+1} = \begin{cases} \tau_i, & \text{if } \tau_i = 2, \\ 1 - \tau_i, & \text{if } \tau_i = 0, 1, \end{cases}\end{aligned}$$

the system remains invariant. That is

$$P_{\alpha, \beta}(\tau) = P_{\beta, \alpha}(\tau'),$$

and

$$Z_{\alpha, \beta}(L, n) = Z_{\beta, \alpha}(L, n).$$

A matrix ansatz also holds for this model

$$P(\tau) = \frac{1}{Z(L, n)} \langle W_\alpha | X_{\tau_1} \dots X_{\tau_L} | V_\beta \rangle.$$

The matrices themselves satisfy the same relations (1). We work with a representation where the matrices are independent of α and β . This dependence is entirely present in the vectors, with the action by the matrices given by

$$X_1 | V_\beta \rangle = \frac{1}{\beta} | V_\beta \rangle \quad \langle W_\alpha | X_0 = \frac{1}{\alpha} \langle W_\alpha |.$$

Further, the representation has the property

$$\begin{aligned} X_2 &= |V_1\rangle \langle W_1|, \\ \langle W_\alpha | V_1 \rangle &= \langle W_1 | V_\beta \rangle = 1. \end{aligned} \quad \text{for all } \alpha, \beta \tag{2}$$

The Representation

$$X_1 = \begin{pmatrix} 1 & 1 & 0 & 0 & \cdot & \cdot \\ 0 & 1 & 1 & 0 & & \\ 0 & 0 & 1 & 1 & & \\ 0 & 0 & 0 & 1 & \cdot & \\ \cdot & & & & \cdot & \cdot \\ \cdot & & & & & \cdot \end{pmatrix}, \quad X_0 = \begin{pmatrix} 1 & 0 & 0 & 0 & \cdot & \cdot \\ 1 & 1 & 0 & 0 & & \\ 0 & 1 & 1 & 0 & & \\ 0 & 0 & 1 & 1 & & \\ \cdot & & & & \cdot & \cdot \\ \cdot & & & & & \cdot \end{pmatrix}.$$

$$X_2 = X_1 X_0 - X_0 X_1 = [X_1, X_0] = \begin{pmatrix} 1 & 0 & 0 & 0 & \cdot & \cdot \\ 0 & 0 & 0 & 0 & & \\ 0 & 0 & 0 & 0 & & \\ 0 & 0 & 0 & 0 & & \\ \cdot & & & & \cdot & \\ \cdot & & & & & \cdot \end{pmatrix},$$

$$\langle W_\alpha | = \left(1, \left(\frac{1-\alpha}{\alpha} \right), \left(\frac{1-\alpha}{\alpha} \right)^2, \dots \right),$$

The “Partition Function”

- Call $Z(L, n)$ the partition function with a slight abuse of terminology from equilibrium statistical mechanics.
- The configuration space is

$Y_{L,n} = \{(\tau_1, \dots, \tau_L) \mid \tau_i = 0, 1, 2; \tau_i = 2 \text{ for } n \text{ values of } i\}$,
and thus

$$Z(L, n) = \sum_{\tau \in Y_{L,n}} \langle W_\alpha | X_{\tau_1} \dots X_{\tau_L} | V_\beta \rangle.$$

- The partition function can be written (Arita) in the form

$$Z(L, n) = \sum_{k=0}^{L-n} C_{L-n-k}^{L+n-1} \frac{1/\beta^{k+1} - 1/\alpha^{k+1}}{1/\beta - 1/\alpha}.$$

where the ballot triangle numbers are

$$C_n^m = \frac{m-n+1}{m+1} \binom{m+n}{n} \quad \text{for } n = 0, \dots, m.$$

Factorization again

- Factorization also holds here because of property (2). The probability of all n second class particles being at locations i_1, \dots, i_n is given by

$$\frac{1}{Z(L,n)} \langle W_\alpha | (X_0 + X_1)^{i_1-1} | V_1 \rangle$$

$$\times \left(\prod_{j=1}^{n-1} \langle W_1 | (X_0 + X_1)^{i_{j+1}-i_j-1} | V_1 \rangle \right) \langle W_1 | (X_0 + X_1)^{L-i_n} | V_\beta \rangle$$

- For example, the probability of having a first class particle at site i given that the first second class particle is at site j , $j > i$ is given by

$$\frac{\langle W_\alpha | (X_0 + X_1)^{i-1} X_1 (X_0 + X_1)^{j-i-1} | V_1 \rangle}{\langle W_\alpha | (X_0 + X_1)^{j-1} | V_1 \rangle},$$

independent of the configuration after the j th site.

Density of First Class particles

- It is enough to calculate the density of first class particles to determine all the densities. The density of holes is got by the particle hole symmetry and that of second class particles is got by the fact that the densities sum up to one at each site.
- Let ξ_i be 1 if i is occupied by a first class particle and zero otherwise.

$$\langle \xi_i \rangle = \begin{cases} \frac{1}{Z(L, n)} \sum_{k=n}^{L-1} C_{L-k-1} Z(k, n) & \text{if } i \leq n, \\ \frac{1}{Z(L, n)} \left[\sum_{k=i}^{L-1} C_{L-k-1} Z(k, n) + Z(i-1, n) \sum_{k=0}^{L-i-1} C_k^{L-i-1} \left(\frac{1}{\beta} \right)^{k+1} \right], & n < i < L, \\ \frac{Z(L-1, n)}{\beta Z(L, n)} & i = L. \end{cases}$$

- Here we use the notation

$$C_n = C_n^n = \frac{1}{n+1} \binom{2n}{n},$$

for the Catalan numbers.

- Notice that the density is constant in the first n sites! This in itself is quite counterintuitive. If L and n are fairly large, how can the first class particles at the extreme left “know” that there are exactly n second class particles in the system?

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- But wait, there's more.

Exchangeability

- In a system of L sites and n second class particles, suppose we want to calculate the joint distribution of r first class particles, $r < n$ at site $1 \leq i_1 < i_2 < \dots < i_r \leq n$.
- The steady state probability distribution has a remarkable property of *exchangeability*, by which we mean that this joint distribution is totally independent of i_1, \dots, i_r and only depends on r .
- This gives a strong constraint on the invariant measure by De Finetti's Theorem.

- The proof is by induction on the probability of finding first class particles at sites $i_1, \dots, i_r, i_{r+1}, \dots, i_{r+j-1}$, denoted by $E_r(L, n; i_1, \dots, i_r; j)$.
- Using the matrix algebra, we show that E_r satisfies the recursion

$$E_r(L, n; i_1, \dots, i_r; j) = E_r(L, n; i_1, \dots, i_r; j + 1) + E_r(L - 1, n; i_1, \dots, i_r; j - 1)$$

- We guess an explicit formula for E_r by looking at small systems and show that it satisfies the same recursion and boundary conditions.

The Current

The current of first class particles J_1 is given, as before, by

$$J_1 = \langle \xi_i(1 - \xi_{i+1}) \rangle,$$

and the phase diagram is determined by formulas for the current in the thermodynamic limit

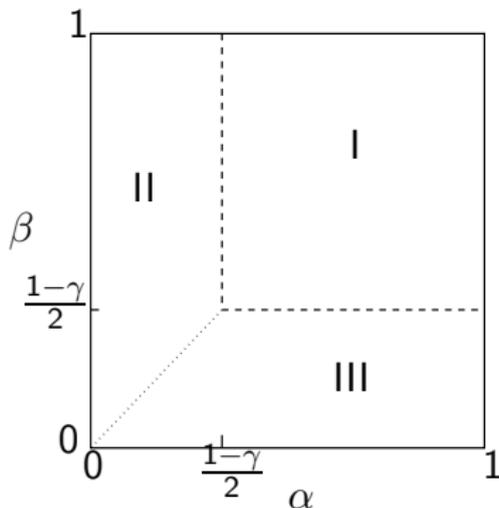
$$J_1 = \begin{cases} \frac{1 - \gamma^2}{4}, & \text{for } \alpha, \beta \geq \alpha_c \text{ (region I),} \\ \alpha(1 - \alpha), & \text{for } \alpha < \alpha_c, \alpha < \beta \text{ (region II),} \\ \beta(1 - \beta), & \text{for } \beta < \alpha_c, \beta < \alpha \text{ (region III),} \end{cases}$$

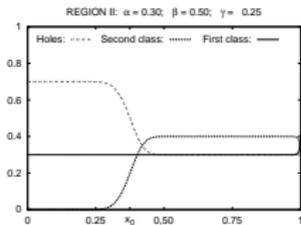
where the critical value α_c of α and β is

$$\alpha_c = \frac{1 - \gamma}{2} \quad \text{and} \quad \gamma = \frac{n}{L}.$$

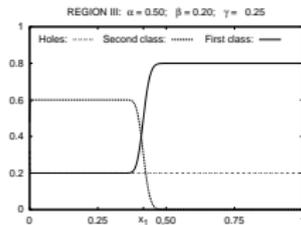
The Phase Diagram

We consider a system of size L and take the number of second class particles to be $n = \lceil \gamma L \rceil$. We then consider the large L limit. The phase diagram thus depends on three parameters — α, β and γ . The cross-section of the phase diagram for fixed γ looks as follows.

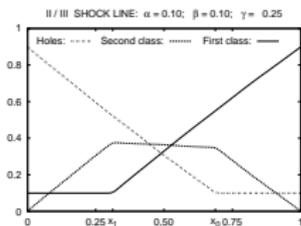




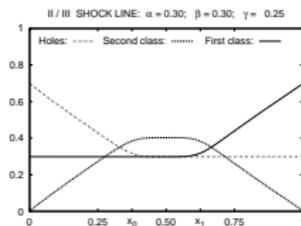
(a)



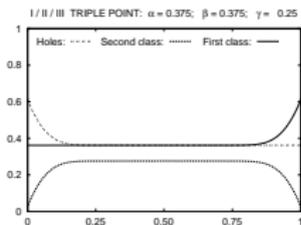
(b)



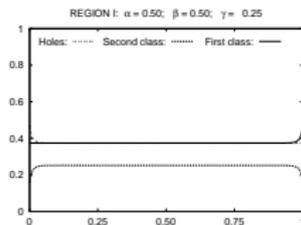
(c)



(d)



(e)



(f)

Macroscopic Density Profiles

- We define the macroscopic density profile $\rho_a(x)$ for $a = 0, 1, 2$ as

$$\rho_a(x) = \lim_{\substack{n/L \rightarrow \gamma \\ i/L \rightarrow x \\ L \rightarrow \infty}} \langle \tau_a(i) \rangle, \quad 0 \leq x \leq 1.$$

- Here $\tau_a(i)$ is one if site i is occupied by particle of type a and zero otherwise. As stated before, knowing $\rho_1(x)$ determines the other two by the particle hole symmetry and $\sum_a \rho_a(x) = 1$.
- For the sake of convenience we will list both $\rho_0(x)$ and $\rho_1(x)$ in all regions. We need to define two variables

$$x_0 = 1 - \frac{\gamma}{1 - 2\alpha}, \quad \text{II and II/III boundary,}$$

$$x_1 = \frac{\gamma}{1 - 2\beta}, \quad \text{III and II/III boundary,}$$

Density profiles in different regions of the phase plane. Note that x_0 is defined only in region II and on its boundaries, and x_1 only in region III and on its boundaries.

Region	$\rho_1(x)$		$\rho_0(x)$	
I	α_c		α_c	
I/II boundary	α_c		α_c	
I/III boundary	α_c		α_c	
	$x < x_1$	$x > x_1$	$x < x_0$	$x > x_0$
II	α		$1 - \alpha$	α
III	β	$1 - \beta$	β	
II/III boundary (Shock Line)	$\alpha (= \beta)$	linear	linear	$\alpha (= \beta)$

Profiles for the II/III boundary

On the II/III boundary $\alpha = \beta < \alpha_c$, the shock line, the profiles include linear regions:

$$\rho_0(x) = \begin{cases} \frac{x_0 - x}{x_0}(1 - \alpha) + \frac{x}{x_0}\alpha, & 0 \leq x \leq x_0, \\ \alpha, & x_0 \leq x \leq 1 \end{cases}$$

$$\rho_1(x) = \begin{cases} \alpha, & 0 \leq x \leq x_1, \\ \frac{1 - x}{1 - x_1}\alpha + \frac{x - x_1}{1 - x_1}(1 - \alpha), & x_1 \leq x \leq 1. \end{cases}$$

As explained for the single species TASEP, such a linear profile occurs in the presence of shocks. In this model there is a constant region followed by a linear region, which actually occurs because of two separate shocks.

The Intuitive Picture

- Consider a uniform portion of the system where the first class particles, second class particles and holes have densities ρ_1 , ρ_2 and ρ_0 respectively.
- In such a region, the current of first class particles and of holes will be given by $J_1 = \rho_1(1 - \rho_1)$ and $J_0 = -\rho_0(1 - \rho_0)$. The (signed) currents must sum to zero. But we know that there are no second class particles entering or leaving the system. Thus $J_2 = 0$. This implies

$$\rho_1 = \rho_0 = (1 - \rho_2)/2 \quad \text{or} \quad \rho_2 = 0, \quad \rho_1 = 1 - \rho_0.$$

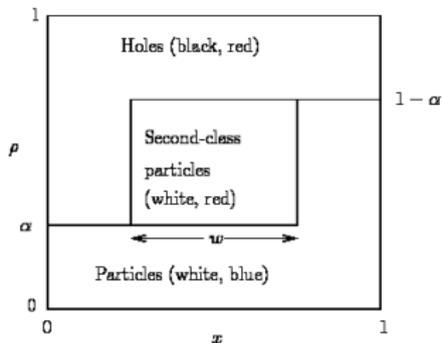
- Therefore in a uniform region either the density of first class particles equals that of holes or there are no second class particles. This is exactly what we see in Regions II and III (Figures (a) and (b)).

The Coloring Idea

- Consider L large and focus on a portion of the system in the bulk.
- Suppose we are colorblind and cannot distinguish between first and second class particles. Color both of these particles white and holes black. Then the dynamics that we see is completely consistent and is in fact the single species TASEP dynamics defined earlier.
- Similarly, if we color second class particles and holes red and first class particles blue, we see yet another single species TASEP dynamics.
- Notice that this identification fails at the boundaries because second class particles are forbidden to enter or leave.

The Fat Shock: Boundary of II/III

We choose $\alpha = \beta < (1 - \gamma)/2$. Then, as shown previously both the white/black and red/blue TASEP will see a shock with a density α on the left and a density $1 - \alpha$ on the right. The velocity of both the shock fronts are therefore $1 - \alpha - (1 - \alpha) = 0$.



The second class particles are completely confined between these two shocks, a region which we call the *fat shock*.

Equilibrium Distribution of Second Class Particles

- Since the current of second class particles is zero, we can expect the second class particles by themselves to form an equilibrium system.
- The TASEP dynamics gives rise in a natural way to a dynamics on the second class particles with respect to which the dynamics satisfies the detailed balance condition.
- Set

$$\phi_\alpha(d) = -\log(4^{-d} Z_{\alpha,1}(d-1, 0)) = -\log(4^{-d} \langle W_\alpha | (X_0 + X_1)^{d-1} | V_1 \rangle)$$

- Then the probability that the n second class particles are located at sites q_1, \dots, q_n is given by

$$\mu(q_1, \dots, q_n) = \frac{e^{-\phi_\alpha(q_1) - \sum_{i=2}^n \phi(q_i - q_{i-1}) - \phi_\beta(L - q_n)}}{4^{-L} Z_{\alpha,\beta}(L, n)}.$$

where we denote $\phi_1(d)$ by $\phi(d)$.

The rate at which the i th second class particle moves to site $q_i + 1$ is the probability that site $q_i + 1$ is occupied by a hole

$$\frac{\langle W_1 | X_0 (X_0 + X_1)^{q_{i+1} - q_i - 2} | V_1 \rangle}{Z^{1,1}(q_{i+1} - q_i - 1, 0)} = \frac{e^{-\phi(q_{i+1} - q_i - 1)}}{e^{-\phi(q_{i+1} - q_i)}}, \quad \text{if } i < n,$$

$$\frac{\langle W_1 | X_0 (X_0 + X_1)^{L - q_i - 1} | V_\beta \rangle}{Z^{1,\beta}(L - q_i, 0)} = \frac{e^{-\phi_\beta(L - q_i - 1)}}{e^{-\phi_\beta(L - q_i)}}, \quad \text{if } i = n.$$

Similarly, the rate at which the i th second class particle moves to site $q_i - 1$ is the probability that site $q_i - 1$ is occupied by a first class particle

$$\frac{e^{-\phi(q_i - q_{i-1} - 1)}}{e^{-\phi(q_i - q_{i-1})}}, \quad \text{if } i > 1, \quad \frac{e^{-\phi_\alpha(q_1 - 1)}}{e^{-\phi_\alpha(q_1)}}, \quad \text{if } i = 1.$$

One can check that the dynamics satisfies detailed balance with respect to the measure μ . Namely, for any two configurations of second class particles \underline{q} and \underline{q}' ,

$$\mu(\underline{q}) \text{rate}(\underline{q} \rightarrow \underline{q}') = \mu(\underline{q}') \text{rate}(\underline{q}' \rightarrow \underline{q}).$$

Pressure Ensemble

- To obtain the properties of the system described by μ in the thermodynamic limit, $L \rightarrow \infty$, $n/L \rightarrow \gamma$, it is most convenient to consider the *pressure or isobaric ensemble* $\pi_{p,n}^{\alpha,\beta}$.
- Here, instead of keeping the volume L of the system fixed we imagine that the right wall is in contact with a reservoir of pressure p . The value of p is chosen so as to make the average volume equal to L .
- More precisely, we let the position of the right boundary, which we denote q_{n+1} , fluctuate, and add a term involving the pressure p to the measure. This yields the probability distribution in the pressure ensemble:

$$\pi(q_1, \dots, q_n, q_{n+1}) = \frac{e^{-\phi_\alpha(q_1) - \sum_{i=2}^n \phi(q_i - q_{i-1}) - \phi_\beta(q_{n+1} - q_n) - p q_{n+1}}}{\mathcal{Z}^{\alpha,\beta}(p, n)}.$$

The Partition Function

- A nice property of the pressure ensemble is that the partition function $\mathcal{Z}^{\alpha,\beta}(p, n)$ factorizes. In this model, it has a particularly simple expression

$$\mathcal{Z}^{\alpha,\beta}(p, n) = \mathcal{Z}_1(\alpha, p) \mathcal{Z}_2(p)^n \mathcal{Z}_1(\beta, p).$$

- The factors can be written in terms of the variable $z = \sqrt{1 - e^{-p}}$ as

$$\mathcal{Z}_1(\alpha, p) = \frac{\alpha(1-z)}{z+2\alpha-1}, \quad \mathcal{Z}_2(p) = \frac{1-z}{1+z}.$$

The parameter z is, for fixed values of α and β , constrained to lie in the range

$$\max\{1 - 2\alpha, 1 - 2\beta\} \leq z \leq 1.$$

The Fat Shock: Equilibrium

The fat shock here is the width between the first and last second class particles — q_1 and q_n . One checks that

$$\begin{aligned}\langle q_1 \rangle_\pi &= -\frac{d}{dp} \log \mathcal{Z}_1(\alpha) = \frac{\alpha(1+z)}{z(z+2\alpha-1)}, \\ \langle q_j - q_{j-1} \rangle_\pi &= -\frac{d}{dp} \log \mathcal{Z}_2 = \frac{1}{z}, \quad j = 2, \dots, n, \\ \langle q_{n+1} - q_n \rangle_\pi &= -\frac{d}{dp} \log \mathcal{Z}_1(\beta) = \frac{\beta(1+z)}{z(z+2\beta-1)}.\end{aligned}$$

To compare with the original system, we set $\langle q_{n+1} \rangle_\pi$ to be the length of the system L which, in the current formulation, is n/γ . We then obtain

$$\frac{\alpha(1+z)}{z(z+2\alpha-1)} + \frac{n}{z} + \frac{\beta(1+z)}{z(z+2\beta-1)} = \frac{n}{\gamma}.$$

Regions of the Phase diagram

We have to choose specific values of the pressure p , or equivalently z , in order to see the same effects that we see in different regions of the phase diagram.

- Region I ($\gamma > 1 - 2\alpha, 1 - 2\beta$): When $z = \gamma + O(1/n)$, the fat shock is of the order of the size of the system and the first and last terms are of order one.
- Region II ($\gamma > 1 - 2\alpha, \alpha < \beta$): When $z = 1 - 2\alpha + O(1/n)$, the first term is of order n and the other two terms are small. This means that the fat shock is forced to the right.
- Region III ($\gamma > 1 - 2\beta, \beta < \alpha$): When $z = 1 - 2\beta + O(1/n)$, the last term is of order n and the other two terms are small. This means that the fat shock is forced to the left.

More General Two-Species Model

	Left		Bulk		Right		
	SP	P			SP	P	
$0 \rightarrow 1$	α	$w(1 - az)$	$10 \rightarrow 01$	1	$1 \rightarrow 0$	β	$v(1 - bz)$
$0 \rightarrow 2$	0	waz	$20 \rightarrow 02$	w	$1 \rightarrow 2$	0	vbz
$2 \rightarrow 1$	0	a	$12 \rightarrow 21$	v	$2 \rightarrow 0$	0	b
$\langle W $	$\langle W_\alpha $	$\langle W_w $			$ V\rangle$	$ V_\beta\rangle$	$ V_v\rangle$

Rates for permeable (P) and semipermeable (SP) boundary conditions.

Matrices and Boundary Vectors

- The matrices now satisfy

$$X_1 X_0 = X_1 + X_0, \quad X_1 X_2 = \frac{1}{v} X_2, \quad X_2 X_0 = \frac{1}{w} X_2,$$

- The boundary vectors depend on whether the boundary is permeable or semipermeable.

- SP:

$$\begin{aligned} \text{Semipermeable left boundary: } \langle W | X_0 &= \frac{1}{\alpha} \langle W |, \\ \text{Semipermeable right boundary: } X_1 | V \rangle &= \frac{1}{\beta} | V \rangle. \end{aligned}$$

- P: Note the absence of a and b .

$$\begin{aligned} \text{Permeable left boundary: } \langle W | X_0 &= \frac{1}{w} \langle W |, \quad \langle W | X_2 = z \langle W |, \\ \text{Permeable right boundary: } X_1 | V \rangle &= \frac{1}{v} | V \rangle, \quad X_2 | V \rangle = z | V \rangle. \end{aligned}$$

Special Case: Triple Shock

- $v = 1$.
- Permeable on the left, semipermeable on the right.
- Let $\alpha = \frac{w}{1+wz}$, and set $\alpha = \beta < 1/2$.
- All density profiles are linear:
 - First class particles: α on the left, $1 - \alpha$ on the right.
 - Second class particles: $\frac{(1-2\alpha)(w-\alpha)}{w(1-\alpha)}$ on the left, 0 on the right.
 - Vacancies: $\frac{\alpha(1-2\alpha+\alpha w)}{w(1-\alpha)}$ on the left, α on the right.

