ASEP

Asymmetric Simple Exclusion Processes

An introduction on methods

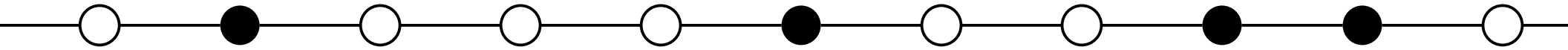Particles moving in one dimension.

Asymmetric: in the direction of motion

Simple: One species

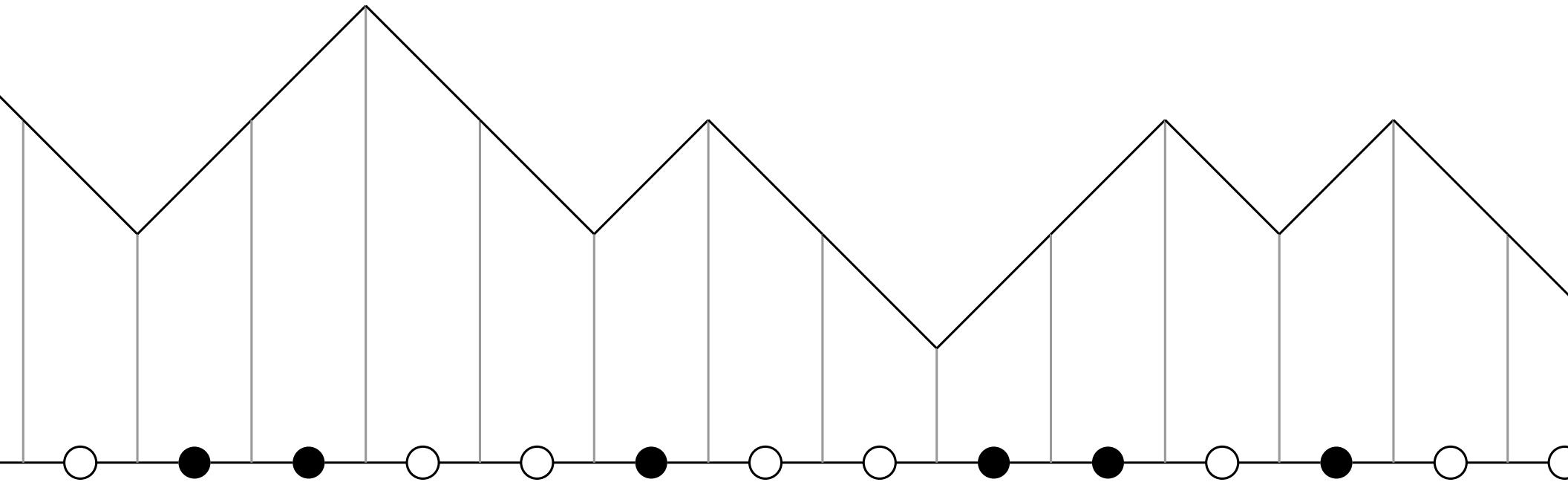Exclusion: particles can not overlap

Special case: TASEP (Totally Asym...): motion only one way
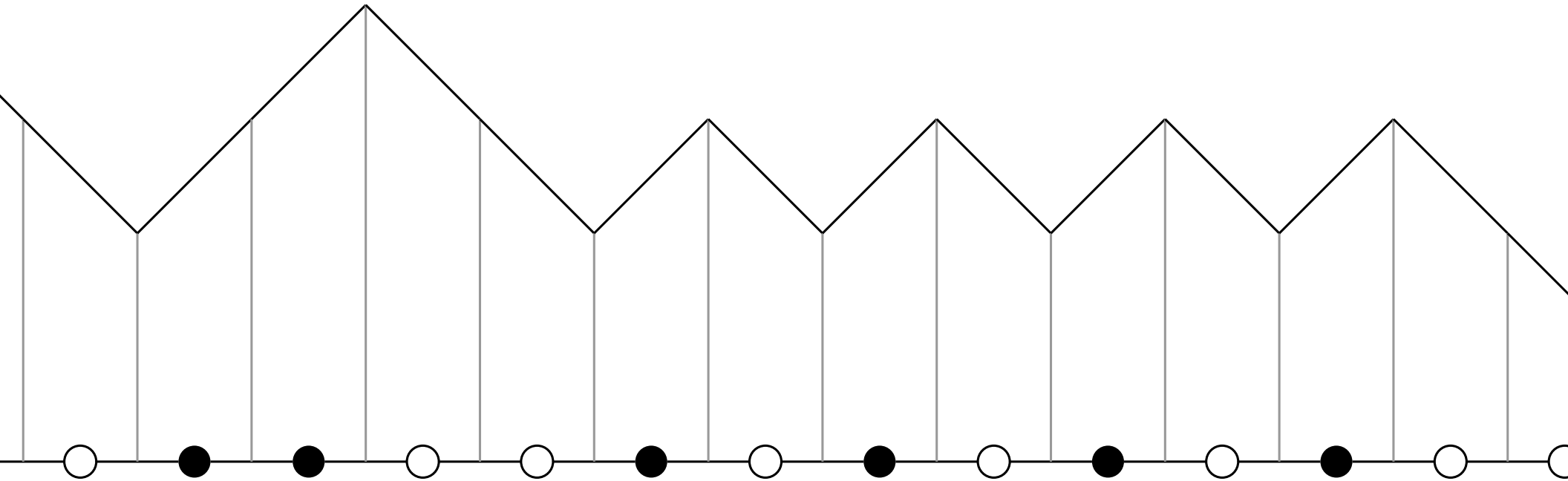
The basic model

- A one-dimensional chain, in continuous time
- the sites can be occupied with at most one particle.
- particles move stochastically
- to the right with rate p and to the left with rate q
- only if the targeted sites are available.

Connection to growth

Associating a particle with an up slope of a boundary, and an empty site with a down slope,
translates motion to the left with growth
and motion to the left with shrink

Connection to growth

Associating a particle with an up slope of a boundary, and an empty site with a down slope, translates motion to the left with growth and motion to the left with shrink
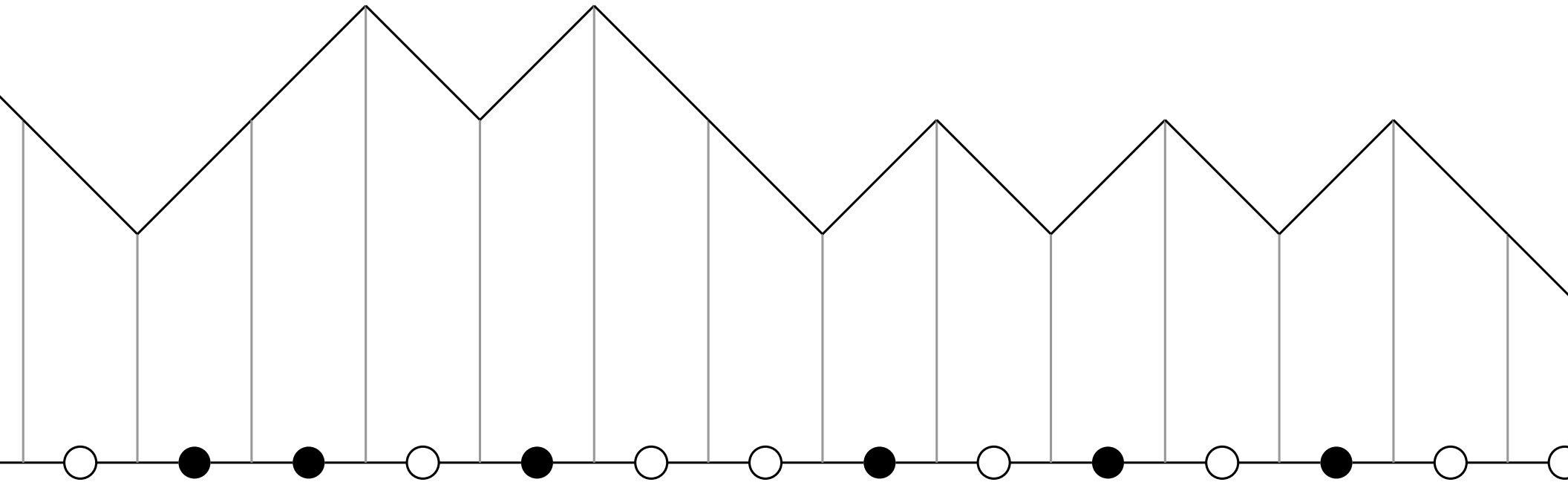
Connection to growth

Associating a particle with an up slope of a boundary, and an empty site with a down slope,
translates motion to the left with growth
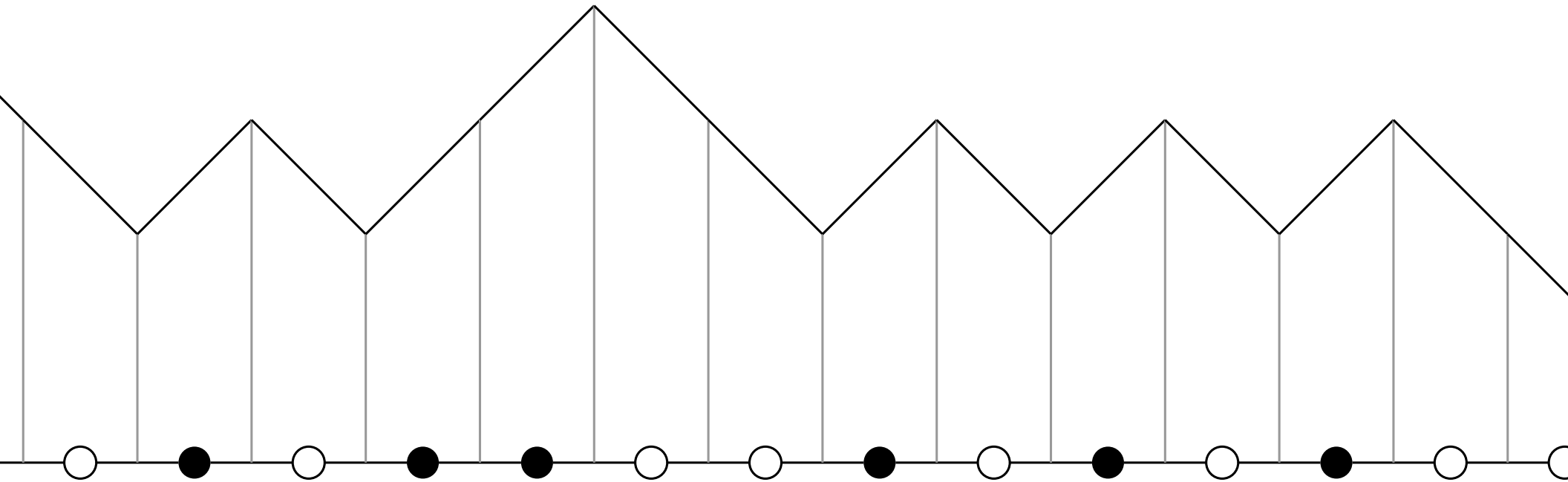and motion to the left with shrink

Connection to growth

Associating a particle with an up slope of a boundary, and an empty site with a down slope, translates motion to the left with growth and motion to the left with shrink

Applications

Molecular motors on a microtubule

Particles flowing through narrow channel

Constrained traffic

Other motivation

Exact solution of many observables is possible
The model is paradigm for non-equilibrium phenomena

Example to try methods

The Master equation

Consider the probability of each configuration

$$P_N(\vec{\tau}; t) \qquad \text{with} \qquad \vec{\tau} = \{\tau_1, \tau_2, \tau_3, \ldots, \tau_N\}$$

How does P_N evolve in time?

The sequence $\ldots,1,0,\ldots$ turns into $\ldots,0,1,\ldots$ with rate p, while the reverse move occurs with rate q.

We can formally write the differential equation

$$\frac{\partial}{\partial t} P(\vec{\tau}; t) = \sum_{\vec{\sigma}} W(\vec{\sigma} \to \vec{\tau}) \, P(\vec{\sigma}; t) - \sum_{\vec{\sigma}} W(\vec{\tau} \to \vec{\sigma}) \, P(\vec{\tau}; t)$$

where $W(\vec{\sigma} \to \vec{\tau})$ is the rate with which $\vec{\sigma}$ turns into $\vec{\tau}$.

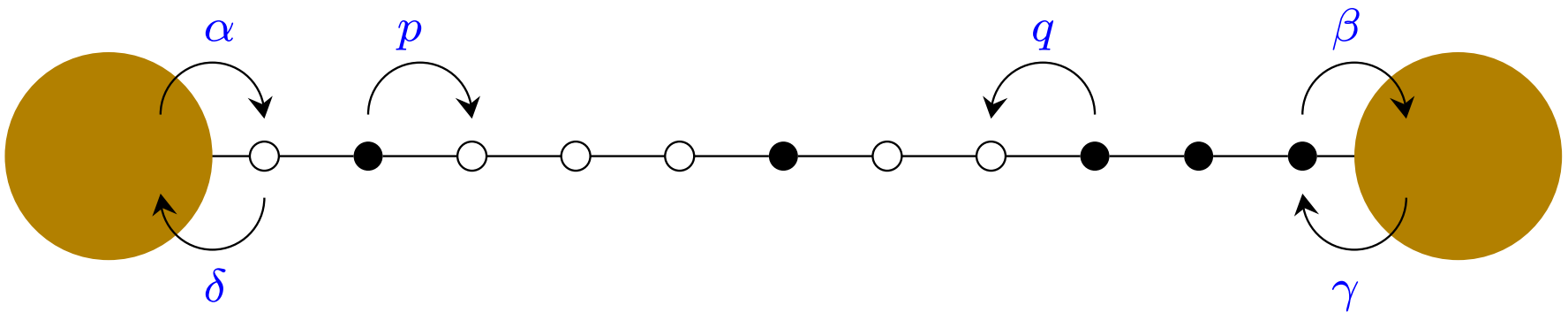This is the **Master Equation**, with its characteristic gain and loss term.

One of the interests is to obtain the stationary state, satifying

$$\sum_{\vec{\sigma}} W(\vec{\sigma} \rightarrow \vec{\tau}) P(\vec{\sigma}; t) = \sum_{\vec{\sigma}} W(\vec{\tau} \rightarrow \vec{\sigma}) P(\vec{\tau}; t)$$

NB: no symmetry between LHS and RHS.

Consider a chain with open ends:

Phenomenology, continuum approach

If the density varies only slowly in space and there are only weak correlations, we can justify a continuum space approach, and assume that the current J is determined by the density ρ. For ASEP this would be $J \propto \rho(1 - \rho)$.

Conservation of particles:

$$\frac{\partial \rho}{\partial t} + \frac{\partial J}{\partial x} = 0$$

then turns into

$$\frac{\partial \rho}{\partial t} + \frac{\mathrm{d}J}{\mathrm{d}\rho}\frac{\partial \rho}{\partial x} = 0$$

We call $\frac{\mathrm{d}J}{\mathrm{d}\rho} = v(\rho)$, the profile velocity. Because of the implicit solution

$$\rho(x,t) = f\left(x - v(\rho)t\right)$$

The density profile moves but with a velocity that depends on the density itself.

Note that the profile velocity $\frac{\mathrm{d}J}{\mathrm{d}\rho} = v(\rho)$ is not the mean velocity of the particles which is J/ρ.

Unlike diffusion, a density profile does not spread, but it tilts: the high density part of the profile may move to the right faster than the low density part.

One slope sharpens up, while the opposite softens.

This results in shock waves, that eventually violate the approximation that J depends on ρ only: $J(\rho)$.
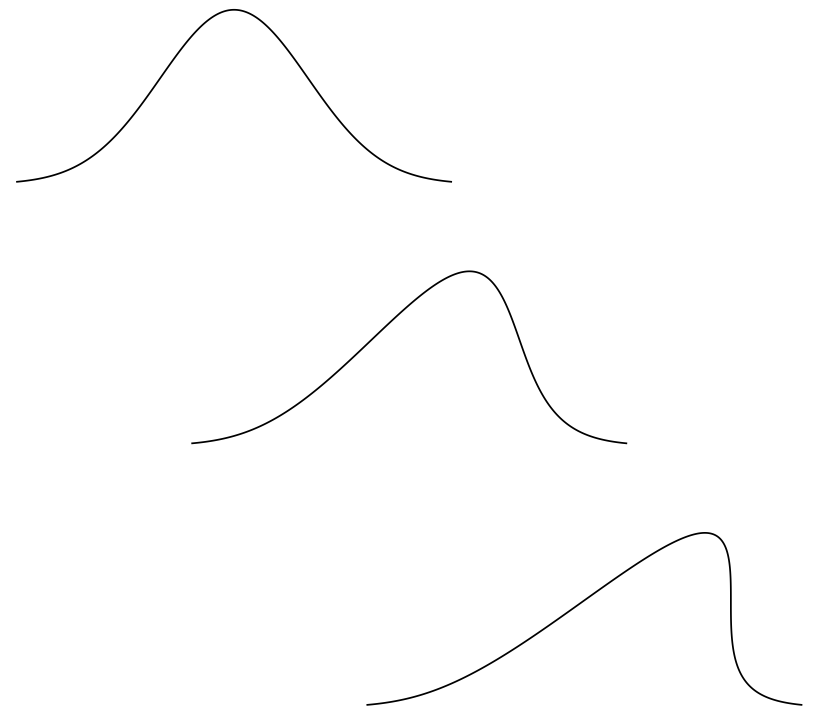
Mean Field approximation

Mean field is an easy method that can be applied on almost any many body system.

Central approximation: neglect correlations.
In this case its starting point is the independence of the τ_i variables.

As an example, we keep here only the forward motion: $q = \gamma = \delta = 0$, and we scale time by setting $p = 1$.
The remaining control parameters are α and β.

The relevant quantities are the density $\rho_i = \langle \tau_i \rangle$ and the current $J_i = \langle \tau_i (1 - \tau_{i+1}) \rangle$.
In Mean Field: $J_i = \rho_i (1 - \rho_{i+1})$.

In the steady state the current J_i does not depend on i.

The equation $J = \rho_i(1 - \rho_{i+1})$ gives us a recursion that controls the density profile:

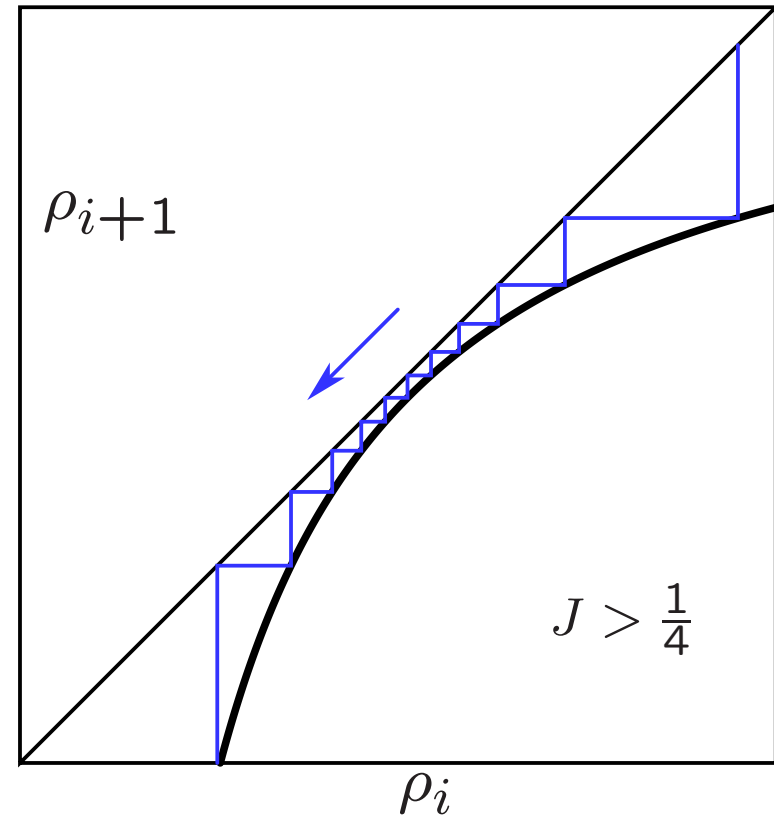$$\rho_{i+1} = 1 - \frac{J}{\rho_i}$$

But, while J is fixed, it is not given.

The inflow corresponds to a virtual site 0 with $\rho_0 = \alpha$,
and the outflow with a virtual site with density $\rho_{N+1} = 1 - \beta$.

So, what happens is that the system 'finds' a J such that the recursion corresponds to $\rho_0 = \alpha$ and $\rho_{N+1} = 1 - \beta$.

To see what happens we have to study the recursion:
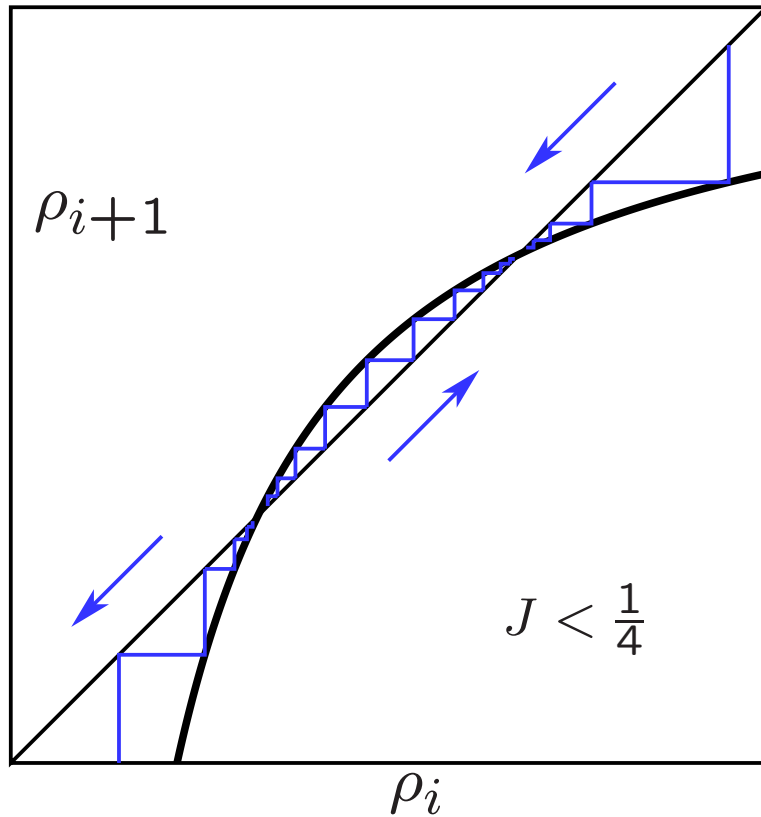
for $J = 1/4$ the curve $\rho_{i+1} = 1 - J/\rho_i$ would just touch the line $\rho_{i+1} = \rho_i$.

The recursion $\rho_{i+1} = 1 - \frac{J}{\rho_i}$ follows one of the blue staircases, initiating at $\rho_0 = \alpha$ and terminating on $\rho_{N+1} = 1 - \beta$. In the steady state the system must find a J that accomodates these.

E.g. when

$\alpha = \rho_0 > \rho_{N+1} = (1 - \beta)$,
the J will find the value
just above 1/4 such that
precisely $N + 1$ steps are
needed to get from $\rho_0 = \alpha$
to $\rho_{N+1} = 1 - \beta$.
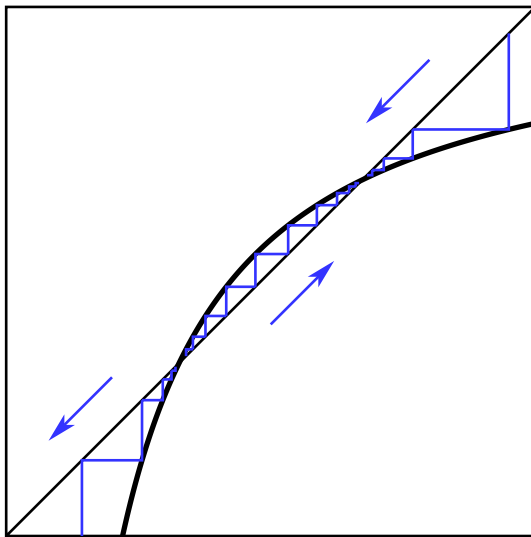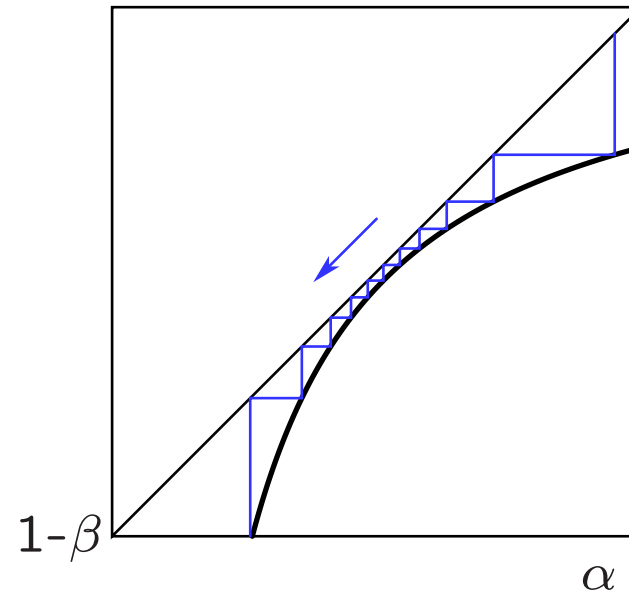
corresponding to the four staircases.

$\rho_{N+1} < 1/2 < \rho_0 \quad$ and $\quad J \approx 1/4$

$1/2 < \rho_{N+1} < \rho_0 \quad$ and $\quad J = \beta(1 - \beta)$

$\rho_{N+1} > \rho_0 \quad$ and

$$J = \min\left[\alpha(1 - \alpha), \beta(1 - \beta)\right]$$

$\rho_{N+1} < \rho_0 < 1/2 \quad$ and $\quad J = \alpha(1 - \alpha)$

$J = \frac{1}{4}$

$J = \beta(1 - \beta)$

$\alpha =$

ρ_0

$J = \alpha(1 - \alpha)$

$\rho_{N+1} = 1 - \beta$
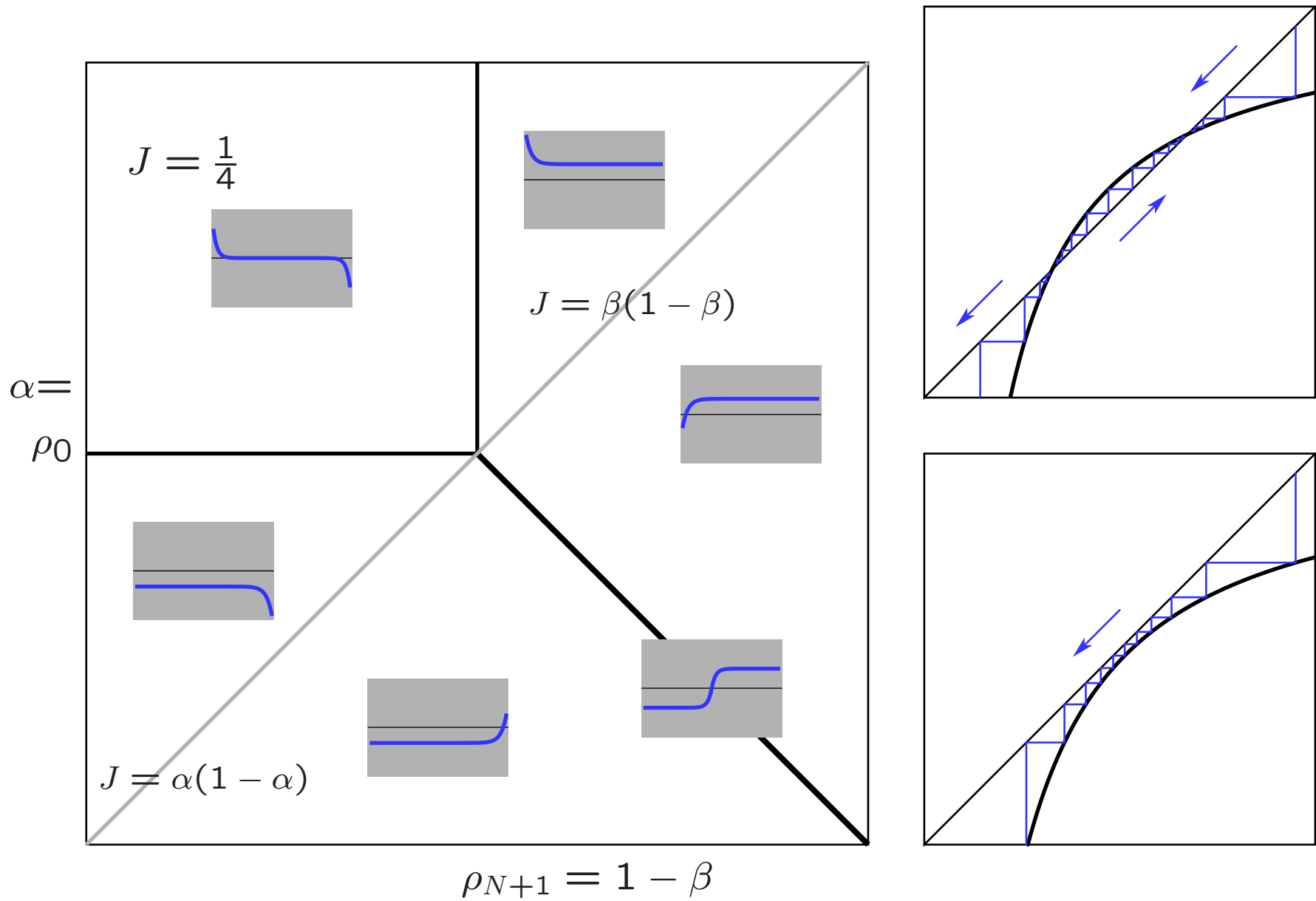
This gives rise to a rich phase diagram.

Clearly we see a (stationary) shock wave solution in the case $\alpha = \beta < 1/2$. In all other cases the shock is driven to the boundaries.

If we identify a phase transition as a singularity in $J(\alpha, \beta)$, the black lines are phase transitions, but the gray one is not.

The choice to set $q = \gamma = \delta = 0$ is not essential, but made here only to keep the presentation simple.

Clearly the mean field approach yields a very rich behavior.
The resulting phase diagram is correct, but the density profile is only qualitative, and correlations are neglected altogether.

The Mean Field approximation is good at finding a qualitative phase diagram, (here even quantitative).
It can be generalized to incorporate restricted correlations.

We now look into other approaches without approximation.

Exact approaches

The master equation for the steady state:

$$\sum_{\vec{\sigma}} W(\vec{\sigma} \to \vec{\tau}) P_N(\vec{\sigma}) - \sum_{\vec{\sigma}} W(\vec{\tau} \to \vec{\sigma}) P_N(\vec{\tau}) = 0$$

Note the sum is over $\vec{\sigma}$, while $\vec{\tau}$ is given.

How does one go about finding a solution for this?

The most well-known trick is to hope that the the equation also holds without the sum over $\vec{\sigma}$. The solution is determined by

$$\frac{P_N(\vec{\tau})}{P_N(\vec{\sigma})} = \frac{W(\vec{\sigma} \to \vec{\tau})}{W(\vec{\tau} \to \vec{\sigma})}$$

An overcomplete set of equations, which has solution in equilibrium only. It requires that for any cyclic sequence of states the forward probability is equal to the backward.

$$\prod_{k=1}^{m} W(\vec{\sigma}_m \to \vec{\sigma}_{m+1}) = \prod_{k=1}^{m} W(\vec{\sigma}_m \to \vec{\sigma}_{m-1})$$

Very useful approach is called the
Matrix Ansatz or **Matrix Product Method**
(Derrida, Evans, Hakim and Pasquier, 1993).
But an essential ingredient is a recursion in the system size.
(Derrida, Domany, Mukamel, Schütz, 1992)

First we write the equation for the stationary state more explicitly.

Consider the motion between the sites i and $i + 1$.

The contribitions to the steady state equation (gain - loss $= 0$)

for $\qquad \{\tau_i, \tau_{i+1}\} = \{1, 0\} \qquad q P_N(\ldots, 0, 1, \ldots) - p P_N(\ldots, 1, 0, \ldots)$

for $\qquad \{\tau_i, \tau_{i+1}\} = \{0, 1\} \qquad p P_N(\ldots, 1, 0, \ldots) - q P_N(\ldots, 0, 1, \ldots)$

and if $\tau_i = \tau_{i+1}$ there are not contributions.

These contributions can be written as a matrix multiplication:

$$\sum_{\sigma_i, \sigma_{i+1}} B(\tau_i, \tau_{i+1}; \sigma_i, \sigma_{i+1}) \, P_N(\ldots, \tau_{i-1}, \sigma_i, \sigma_{i+1}, \tau_{i+2}, \ldots)$$

This should be summed over i in the steady state equation, and complemented with the left and right boundary terms

$$\sum_{\sigma_1} L(\tau_1; \sigma_1) P_N(\sigma_1, \tau_2, \ldots) + \sum_{\sigma_N} R(\tau_N; \sigma_N) P_N(\ldots, \tau_{N-1}, \sigma_N)$$

It is (boldly) proposed that up to normalization

$$\sum_{\sigma_i, \sigma_{i+1}} B(\tau_i, \tau_{i+1}; \sigma_i, \sigma_{i+1}) P_N(\ldots \tau_{i-1}, \sigma_i, \sigma_{i+1}, \tau_{i+2} \ldots) =$$

$$- (2\tau_i - 1) P_{N-1}(\ldots, \tau_{i-1}, \tau_{i+1}, \tau_{i+2}, \ldots)$$

$$+ (2\tau_{i+1} - 1) P_{N-1}(\ldots, \tau_{i-1}, \tau_i, \tau_{i+2}, \ldots)$$

This satisfies the obvious properties of the LHS that it vanishes when $\tau_i = \tau_{i+1}$, and that it changes sign as $\tau_i \leftrightarrow \tau_{i+1}$.

And it solves the steady state equation,
because the two terms cancel one with the previous and the other with the next term in the sum over i.

For the whole steady state equation we also need

$$\sum_{\sigma_1} L(\tau_1; \sigma_1) P_N(\sigma_1, \tau_2, \ldots) = +(2\tau_1 - 1) P_{N-1}(\tau_2, \tau_3, \tau_4, \ldots)$$

and

$$\sum_{\sigma_N} R(\tau_N; \sigma_N) P_N(\ldots, \tau_{N-1}, \sigma_N) = -(2\tau_N - 1) P_{N-1}(\ldots, \tau_{N-1})$$

One might wonder why to believe the proposal. But the steady state admits only one solution. If we find it by means of a proposal however bold, the proposal is correct.

A further proposal
(which gave the method its name **Matrix product ansatz**)
is that the statonary state can be written as an element of a
product of matrices:

$$P_N(\ldots, 0, 1, 1, 0, 0, 1, \ldots) = \langle W | \ldots EDDEED \ldots | V \rangle$$

the matrix E for an empty site and D for a particle. Formally we
could write

$$P_N(\vec{\tau}) = \frac{1}{Z_N} \langle W | \prod_{i=1}^{N} M_{\tau_i} | V \rangle$$

with $M_0 = E$ and $M_1 = D$, and with normalization

$$Z_N = \langle W | \prod_{i=1}^{N} (D + E) | V \rangle$$

This proposal is reasonable, as long as the matrices are free.

Now we combine the proposals:

$$\sum_{\sigma_i, \sigma_{i+1}} B(\tau_i, \tau_{i+1}; \sigma_i, \sigma_{i+1}) P_N(\ldots \tau_{i-1}, \sigma_i, \sigma_{i+1}, \tau_{i+2} \ldots) =$$

$$- (2\tau_i - 1) P_{N-1}(\ldots, \tau_{i-1}, \tau_{i+1}, \tau_{i+2}, \ldots)$$

$$+ (2\tau_{i+1} - 1) P_{N-1}(\ldots, \tau_{i-1}, \tau_i, \tau_{i+2}, \ldots)$$

yields

$$pDE - qED = D + E$$

And the boundary terms

$$(\beta D - \delta E)|V\rangle = |V\rangle$$

$$\langle W|(\alpha E - \gamma D) = \langle W|$$

The matrix formulation gives a convenient approach to correlation functions, e.g.

$$\rho_i = \langle \tau_i \rangle = \frac{1}{Z_N} \langle W| \ldots C^{i-1} D C^{N-i} \ldots |V\rangle$$

where $C = E + D$.

It still requires some manipulation to actually get explicit answer from these matrix products.

But consider

$$\langle J_i \rangle = \langle p\tau_i(1 - \tau_{i+1}) - q\tau_{i+1}(1 - \tau_i)\rangle =$$

$$\frac{1}{Z_N}\langle W| \ldots C^{i-1}(pDE - qED)C^{N-i-1} \ldots |V\rangle =$$

$$\frac{1}{Z_N}\langle W| \ldots C^{i-1}(D + E)C^{N-i-1} \ldots |V\rangle = \frac{Z_{N-1}}{Z_N}$$

This may not be explicit, but we find that it is independent of i as it should. It also promises that once one is able to calculate Z_N, the phase diagram for $J(\alpha, \beta)$ is recovered, with explicit softening of the boundaries for finite sizes.

Such observables can be computed exactly. For instance in the case $q = \gamma = \delta = 0$, it is found that

$$Z_N = \sum_{k=0}^{N} \frac{k(2N-k-1)!}{N!(N-k)!} \frac{\alpha^{-k-1} - \beta^{-k-1}}{\alpha^{-1} - \beta^{-1}}$$

Similar expressions can be found for the density profile and other observables.

This can be obtained from using the algebraic relations between E, D, $|V\rangle$ and $\langle W|$, or by constructing an explicit (but infinite dimensional) representation of these objects.

The approach has been generalized to numerous variations, multiple species with particular passing rules, non conserved particles, one exceptional particle. In all cases (so far) the method is limited to the stationary state.

Bethe Ansatz

When one is interested in time-dependence, the study of the stationary state does not suffice. We now aim for the complete diagonalization of the transition matrix. A formidable task.

But similar to statistical mechanics (transfer matrix) and quantum mechanics (Hamiltonian).

Back to the Master equation:

$$\frac{\partial}{\partial t}P_N(\vec{\tau};t) = \sum_{\vec{\sigma}}W(\vec{\sigma}\to\vec{\tau})\,P(\vec{\sigma};t) - \sum_{\vec{\sigma}}W(\vec{\tau}\to\vec{\sigma})\,P(\vec{\tau};t)$$

We could formally write this as

$$\frac{\partial}{\partial t}P_N = -\mathcal{H}\cdot P_N$$

then $\mathcal{H}$ is a stochastic (probability conserving) operator.
Its spectrum controls how transient contributions to the states will decay in time.

Bethe proposed a form for the eigenstates of the Heisenberg chain, now called the **Bethe Ansatz**, which works also in this case. (Gwa and Spohn, 1992)

I will expose it for periodic boundary conditions (number of particles conserved).

We denote P_N as function of τ, by Ψ as function of the position of the particles.

In the sector with one particle:

$$E\Psi(x) = (p+q)\Psi(x) - p\Psi(x-1) - q\Psi(x+1)$$

proposal for eigenvector $\Psi(x) = z^x$ (plane wave), then

$$Ez^x = (p+q)z^x - pz^{x-1} - qz^{x+1}$$

so clearly $E = p(1 - z^{-1}) + q(1 - z)$,
hile periodicity requires that $z^N = 1$.

Bethe proposed that also with more particles, the solutions consist of plane waves, as long as the particles do not overlap.

$$\Psi(x_1, x_2) = z_1^{x_1} z_2^{x_2}$$

When the particles are far apart, they can move freely, as if they are alone. This requires that

$$E = p(1 - z_1^{-1}) + q(1 - z_1) + p(1 - z_2^{-1}) + q(1 - z_2)$$

But if we exchange the z_i, the energy remains the same. Therefore we propose that

$$\Psi(x_1, x_2) = A \, z_1^{x_1} \, z_2^{x_2} + B \, z_2^{x_1} \, z_1^{x_2}$$

for $x_1 < x_2$, and with this work out the eigenvalue equation.

The eigenvalue follows from the cases that $x_2 > x_1 + 1$, but when $x_2 = x_1 + 1 = x + 1$, we have an extra requirement:

Eigenvalue $\times \Psi$ = sum of allowed processes.

$$(2p + 2q - pz_1^{-1} - qz_1 - pz_2^{-1} - qz_2)(z_1z_2)^x (Az_2 + Bz_1) =$$

$$(z_1z_2)^x \left[Az_2(p + q - pz_1^{-1} - qz_2) + Bz_1(p + q - pz_2^{-1} - qz_1) \right]$$

This results in

$$A\, z_2\,(p + q - pz_2^{-1} - qz_1) + B\, z_1\,(p + q - pz_1^{-1} - qz_2) = 0$$

or

$$\frac{B}{A} = -\frac{p\,z_2 + q\,z_2 - p - q\,z_1\,z_2}{p\,z_1 + q\,z_1 - p - q\,z_1\,z_2}$$

So for this choice of the coefficients A and B, the eigenvalue also applies to the configurations where the particles are adjacent.

Periodicity now requires that

$$Az_2^N = B \qquad \text{and} \qquad Bz_1^N = A$$

Eliminating the coefficient we find

$$z_1^N = -\frac{pz_1 + qz_1 - p - qz_1z_2}{pz_2 + qz_2 - p - qz_1z_2} \quad \text{and} \quad z_2^N = -\frac{pz_2 + qz_2 - p - qz_1z_2}{pz_1 + qz_1 - p - qz_1z_2}$$

Before we proceed to more than two particles, we pause to look at

$$A\, z_2\, (p + q - pz_2^{-1} - qz_1) \;+\; B\, z_1\, (p + q - pz_1^{-1} - qz_2) \;=\; 0$$

This equation gives a ratio between A and B unless

$$(p + q - pz_2^{-1} - qz_1) = (p + q - pz_1^{-1} - qz_2) = 0$$

that is unless $z_1 = z_2 = 1$.

In that case the ration is undetermined but also meaningless.

This exception we have to keep in mind.

Now for more particles, we propose:

$$\Psi(x_1, x_2, \ldots, x_n) = \sum_\sigma A_\sigma \prod_{i=1}^{n} z_{\sigma(i)}^{x_i}$$

where $\{\sigma(1), \sigma(2), \ldots, \sigma(n)\}$ is a permutation of $\{1, 2, 3, \ldots, n\}$.

Clearly this proposal works while all particles are well separated. But when two are adjacent, we obtain a requirement on the coefficients A_σ:

$$\frac{A_{\ldots,\mu,\nu,\ldots}}{A_{\ldots,\nu,\mu,\ldots}} = -\frac{(p+q)\, z_\mu - p - q\, z_\mu\, z_\nu}{(p+q)\, z_\nu - p - q\, z_\mu\, z_\nu}$$

again unless both z_μ and z_ν are equal to 1.

This leads to the so called Bethe Ansatz equations:

$$z_i^N = -\prod_{j=1}^{n} -\frac{(p+q)\, z_j - p - q\, z_i\, z_j}{(p+q)\, z_i - p - q\, z_i\, z_j}$$

These equations can be used to find numerically exact solution. These are non-linear coupled equations, but there are only n, while the matrix $\mathcal{H}$ is $\begin{pmatrix} N \\ n \end{pmatrix} \times \begin{pmatrix} N \\ n \end{pmatrix}$: exponential in n.

In the thermodynamic limit more is possible, but not without pain.

When $q = 0$ or $q = p$ there are significant simplifications.

The ground state for generic p and q all $z_j = 1$, a distribution in which all states are equally probable.

In order to find out how fast a system will decay into this state one needs to calculate the first higher state, presumably one in which one $z \neq 1$.

Let A_k be the coefficient for the k-th particle carrying the non-zero momentum. Then

$$\frac{A_k}{A_k - 1} = -\frac{(p+q) - p - qz}{(p+q)z - p - qz} = \frac{q}{p}$$

Therefore z is the solution of

$$z^N = -\left(\frac{p}{q}\right)^{n-1}$$

so that

$$z = \left(\frac{p}{q}\right)^{(n-1)/N} \exp((1+2m)i\pi/N)$$

The corresponding gap in the eigenvalue follows from

$$E = q(1-z) + p(1-z^{-1})$$

- **Mean Field**: very flexible, very easy, powerful for qualitative understanding

- But uncontrolled approximation

- **Matrix product**: exact description of steady state.

- also quite flexible, but requiring advanced combinatorics

- **Bethe Ansatz**: Exact spectrum and eigenstates

- Efficient way to obtain spectrum of finite system numerically

- in principle acces to time dependence