ON THE INTEGRABLE DYNAMICAL SYSTEMS IN STATISTICAL MECHANICS

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For mum and dad
I would like to send my biggest gratitude to my parents, to whom I am forever indebted, for giving me complete support and freedom in pursuing my dreams and passions, for respecting and trusting my own decisions no matter how unrealistic it may sound, for giving me life to see this beautiful crazy world. You are the dawn light in my heart guiding me through all obstacles. No words are enough to describe the beauty of those joyful moments with you. Mom and dad, I love you.

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And finally Beijing, the city where my heart beats.

Now let our journey begin..
I hereby declare that this submission is produced by my own intellectual efforts and completely written by me. It contains no materials taken straight from thesis previously published or accepted for the award of a degree at any institution, except for the explicitly indicated academic references, which are studied by me in details and taken into context using my own understanding. Any contribution to this thesis, including discussion and peer advice, is acknowledged accordingly.

Abstract

Mathematical details of stochastic process are reviewed, before one-dimensional Ising model is introduced and solved statistical mechanically by partition function, quantum mechanically by Bethe ansatz and algebraic Bethe ansatz, and stochastically by master equation. Bethe ansatz are also applied to mass transport models including asymmetric simple exclusion process and zero range process. Several two-dimensional surface growth models and their corresponding universality classes are discussed.

[ We cannot solve our problems with the same thinking we used when we created them. ] Albert Einstein

1 Introduction

The Integrability or Solvability refers to the ability of systems to have exact solutions. There are numerous problems solvable in classical mechanics, while very few in statistical mechanics or relativistic quantum field theory. This scarcity of solvable models in those areas is due to the large number of particles that the system contains where each particle can interact directly or indirectly with others, in contrast to classical mechanics where only few particles of interest appear in the problems. However, it is the purpose of statistical mechanics to study large number of particles and help us gain insight into the macroscopic characteristics of stochastic particle systems. In this thesis we unveil the many faces of integrable systems in the context of statistical mechanics and try to solve them exactly under the given assumptions by various methods. We will focus on the non-equilibrium systems in statistical mechanics and see how the microscopic interactions influence the macroscopic properties of their corresponding long-time-limit stationary states.

In section 2 we review some of the essential formulations of stochastic processes that are required by later sections, especially the discrete and continuous time evolutions of the probability density functions (master and Fokker-Planck equations respectively).

In section 3 we introduce the Ising model and solve for its exact expectations and correlation functions in the one-dimensional case by using the partition functions.

In section 4 we use a quantised version of the Ising chain, namely the Heisenberg spin chain and solve it using the powerful tool of the Bethe ansatz, including coordinate and algebraic Bethe ansatz, and apply this principle to the asymmetric simple exclusion process and the zero range process.

In section 5 instead of solving the Ising model by algebraic means we employ the stochastic methods from section 2 to determine its expectation and correlation function. We also introduce and analyse multiple types of surface growth models such as the single-step model, the Edwards-Wilkinson model and the ballistic deposition model, which can be mapped onto the stochastic Ising chain, and solved exactly for their critical exponents. Then we derive the EW equation and the KPZ equation by the lattice transition rules and the limiting procedure. The exact and approximating Hopf-Cole solutions to the KPZ equation are then introduced with the sharp wedge initial conditions.

2 Stochastic Process

Stochastic Process is defined as a sequence of the stochastic variables \( \{ x(t) \} \), where \( t \) represents the time which maybe integer or real valued. Although the way we write the variable seems to already assume the sole dependency on time, it is legitimate to be dependent on other arguments as well, for instance the spatial position \( r \). In our study of the stochastic dynamics of the integrable systems, we will be predominately dealing with those stochastic processes depending only on time. It should be noted that just like time, the stochastic variables can also be discrete (gambling wins) or continuous (the motion of Brownian particle).

There are two ways in which we can describe the process: by modelling the time evolution of the probability density function (PDF) of stochastic variables, which leads to the master equation and the Fokker-Planck equation; or by developing a differential equation for the stochastic variables, which leads to the stochastic differential equations. In this section we will attempt a detailed look at the stochastic processes in these two ways, before we apply the techniques to the integrable systems in the next section.

Deterministic dynamical processes which we see so far determines the state at a later time given the states of the
system in the previous time steps. There can be no probabilistic variations to the predicted outputs of the state. Stochastic processes, however, can only be specified by the probability of finding the system at a given state. There can be more than one possible future states of the system, which we cannot determine beforehand. Each of the outcomes is associated with a probability. If the future state depends only on the previous state, but not the ones further away, then the stochastic process is called Markov Process. Markov processes are significantly simpler than other stochastic processes and we will be concentrating on them here.

A mathematical description of the Markov processes involves PDF \( P(x_1, t_1; \ldots; x_n, t_n) \), which is the probability of the system being in state \( x_i \) at time \( t_i \), \( 1 \leq i \leq n, i \in \mathbb{Z} \), and the conditional PDF \( P(x_m, t_m; \ldots; x_{n+1}, t_{n+1}|x_n, t_n; \ldots; x_1, t_1) \), which is the probability of the system at the state \( x_i \) at the time \( t_i \), \( n + 1 \leq i \leq m, i \in \mathbb{Z} \) given previously it was at state \( x_j \) at time \( t_j, 1 \leq i \leq n, i \in \mathbb{Z} \). Since the state of the system is only dependent on the immediate past, the entire history of the system previous to the immediate past can be forgotten and the PDF is only conditional on the most recent time step.

\[
P(x_m, t_m; \ldots; x_{n+1}, t_{n+1}|x_n, t_n; \ldots; x_1, t_1) = P(x_m, t_m; \ldots; x_{n+1}, t_{n+1}|x_n, t_n)
\]

(1)

All PDFs can be defined by \( P(x, t) \), which is the probability of the system at a given state \( x \) and a given time \( t \), and \( P(x', t'|x, t) \), which is the Transition Probability from state \( x \) at time \( t \) to state \( x' \) at time \( t' \), by the following relations:

\[
P(x_2, t_2) = \int dx_1 P(x_2, t_2|x_1, t_1)P(x_1, t_1)
\]

(2)

\[
P(x_3, t_3|x_1, t_1) = \int dx_2 P(x_3, t_3|x_2, t_2)P(x_2, t_2|x_1, t_1)
\]

(3)

Equation (3) is referred to as the Chapman-Kolmogorov Equation.

Proof of the Chapman-Kolmogorov equation:

\[
P(x_{m+n}, t_{m+n}|x_1, t_1) = P([L_n(x_{m+n}, t_{m+n}; x_n, t_n)]|x_1, t_1)
\]

(4)

\[
= \sum_{n} P(x_{m+n}, t_{m+n}; x_n, t_n|x_1, t_1)
\]

(5)

\[
= \sum_{n} P(x_{m+n}, t_{m+n}|x_n, t_n; x_1, t_1)P(x_n, t_n|x_1, t_1)
\]

Equation \( = (1) \sum_{n} P(x_{m+n}, t_{m+n}|x_n, t_n)P(x_n, t_n|x_1, t_1) \)

(6)

2.1 Markov Chain

We start with the simplest class of the Markov processes: the so-called Markov chains, where both of time and state spaces are discrete. It was first investigated for finite number of states by [Markov (1906)] and for an infinite number of states by [Kolmogorov (1936)].

When the states are discrete, we denote them by \( n \) rather than \( x \), which we reserve for the continuous case to avoid confusion. Two equations (2) and (3) governing the Markov processes thus read:

\[
P(n_2, t_2) = \sum_{n_1} d_n P(n_2, t_2|n_1, t_1)P(n_1, t_1)
\]

(7)

\[
P(n_3, t_3|n_1, t_1) = \sum_{n_2} d_{n_2} P(n_3, t_3|n_2, t_2)P(n_2, t_2|n_1, t_1)
\]

(8)

We confine our discussion to an even simpler case where the process is stationary. A Stationary Process is one where the conditional PDF \( P(n', t'|n, t) \) depends only on the time difference \( (t' - t) \). This property is also called temporal homogeneity in some textbook, which enables us to write \( P(n', t + k|n, t) \) in a more straightforward form as \( p_{n'}^{(k)} \).

The Chapman-Kolmogorov equation then reads:

\[
p_{n'}^{(2)} = \sum_k p_{n'}^{(1)}p_{k}^{(1)}
\]

(9)

This is equivalent to the matrix multiplication of \( p^{(1)} \) with itself. It can be deduced that \( p^{(k)} = (p^{(1)})^k \). We denote \( p^{(1)} \) as \( P \), whose entries are non-negative and sum up to one in each column.

\[
\sum_{n'} p_{n'n'} = \sum_{n'} P(n', t + 1|n, t) = 1
\]

(10)
Those matrices are called **Stochastic Matrices**, which stands for the transition probabilities of the Markov chains. By induction it can be shown that if \( \mathcal{P} \) is stochastic, then \( \mathcal{P}^k \) is also stochastic.

The Markov chain is then defined in terms of matrices as:

\[
P(n, t + 1) = \sum_{n'} p_{n'n} P(n', t)
\]

\[
\mathbf{P}(t + 1) = \mathcal{P}\mathbf{P}(t)
\]

\[
\mathbf{P}(t) = \mathcal{P}\mathbf{P}(t - 1) = \ldots = \mathcal{P}^k\mathbf{P}(0)
\]

where \( P(n, t) \) is written in the vector form \( \mathbf{P}(t) \). So with the initial state of the system \( \mathbf{P} \) given, we are equipped to find the state at any time \( t \).

Now we are interested in observing the behaviours of the Markov chains as time goes to infinity. For the case of a non-trivial stationary state \( P_{st}(n) \), we have the following relation:

\[
P_{st} = \mathcal{P}P_{st}
\]

where \( P_{st} \) is a right eigenvector of \( \mathcal{P} \) with unit eigenvalue. Solving exactly for the eigenvectors, if mathematically possible at all, gives us the distribution of the stationary state. The eigenvectors for the Ehrenfest urn have proven to be solvable exactly [Krafft, Schaefer (1993)].

### 2.2 Master Equation

The master equation is a Markov chain in the limit when the time has infinitesimally small steps and becomes continuous. Its purpose is to describe the time evolution of the PDF of the state of the system. We derive the equation by first referring to the Chapman-Kolmogorov equation:

\[
P(n', t + \Delta t|n_0, t_0) = \sum_n P(n', t + \Delta t|n, t)P(n, t|n_0, t_0)
\]

Since we are considering temporally homogeneous stationary processes, which depends only on time difference, we might as well set \( t_0 = 0 \) without loss of generality and remember that \( P(n', t + \Delta t|n, t) \) is also independent of \( t \). Define \( T(n'|n) \) to be the **Transition Rate**. We assume that:

\[
P(n', t + \Delta t|n, t) = T(n'|n) \Delta t
\]

This assumption is reasonable because the transition probabilities are proportional to the time difference, which means that the longer we wait, the more likely the system undergoes transition, while at short time difference the system is likely to remain at its previous state. Substitute (12) into (11) and we calculate the rate of change of the transition probabilities (note that \( \sum_n P(n', t + \Delta t|n, t) = 1 \)):

\[
\frac{dP(n', t)}{dt} = \sum_n \left[ T(n'|n)P(n, t) - \sum_n T(n'|n')P(n', t) \right]
\]

\[
\frac{dP(n', t)}{dt} = \sum_n \left[ T(n'|n)P(n, t) - \sum_n T(n|n')P(n', t) \right]
\]

Take the limit of \( \Delta t \to 0 \) and we obtain the **Master Equation in Continuous Time** (14) which describes how the PDF of the state of the system changes with time. It is also valid for the continuous state space if we change the summation into an integral.

\[
\frac{dP(n', t)}{dt} = \sum_n \left[ T(n'|n)P(n, t) - \sum_n T(n|n')P(n', t) \right]
\]

The master equation shows that the time derivative of a particular state is the difference of those transitioning into it and those transitioning out of it, which makes intuitive sense.

If the transitions take place between states whose labels differ only by one, which means that \( T(n|n') = 0 \) and \( T(n'|n) = 0 \) unless \( n = n' + 1 \) or \( n = n' - 1 \). Then we call them **One-Step Processes** and reformulate the master equation in a simpler form:

\[
\frac{dP(n', t)}{dt} = T(n'|n' + 1)P(n' + 1, t) + T(n'|n - 1)P(n' - 1, t) - [T(n'|n) + T(n' - 1|n')]P(n', t)
\]

Define \( g_n = T(n + 1|n) \) and \( r_n = T(n - 1|n) \). Replace all \( n' \) in (14) with \( n \) and we have:

\[
\frac{dP(n, t)}{dt} = r_{n+1}P(n + 1, t) + g_{n-1}P(n - 1, t) - (r_n + g_n)P(n, t)
\]

Whether or not a stationary state of the system following the master equation exists depends on the boundary conditions of the system. Two most important examples are the reflecting boundaries and he absorbing boundaries.
In the former case the probability current vanishes at the boundaries (there are two probability currents of opposite directions at a reflecting boundary and the net current is zero) so the system has conserved probability. In the latter case the probability itself vanishes at the boundaries so it leaks out of the system.

A stationary process cannot happen within the absorbing boundaries because the probability leaks out of the system and as time goes to infinity there will be no probability left to define the stationary process. So we assume a one-step process lies within two reflecting boundaries. Define the **Probability Current** \( J(n,t) \) as the net flow of probability from state \( n \) to state \( n+1 \):

\[
J(n,t) = g_n P(n,t) - r_{n+1} P(n+1,t) \tag{17}
\]

And the master equation (16) can be rewritten as:

\[
\frac{dP(n,t)}{dt} = J(n-1,t) - J(n,t) \tag{18}
\]

For a stationary state, the PDF is time invariant, which makes the left hand side of (18) zero. Since the currents are time invariant as well, \( J(n-1) = J(n) \) for all \( n \) equals to a constant. The current vanishing at the boundaries sets this constant to zero. Thus we have by (17) \( r_{n+1} P_{st}(n+1) = g_n P_{st}(n) \) for all \( n \). Suppose one boundary is at \( n = 0 \) and the other is at \( n = N \), then by the recurrent relation we can easily express the stationary states as follows:

\[
P_{st}(n) = \frac{g_{n-1}...g_0}{r_{n-1}...r_1} P_{st}(0) \tag{19}
\]

where the constant \( P_{st}(0) \) can be determined by normalisation:

\[
\sum_{n=0}^{N} P_{st}(n) = P_{st}(0) + \sum_{n=1}^{N} P_{st}(n) = 1 \tag{20}
\]

\[
P_{st}(0) = \left(1 + \sum_{n=1}^{N} \frac{g_{n-1}...g_0}{r_{n-1}...r_1}\right)^{-1} \tag{21}
\]

The discrete version of master equation can be found even more easily. First note that \( T'(n|n') = T(n|n') \Delta t \) is the transition probability and it sums up to one over \( n' \). Assume the time step is \( \Delta t \) and we start from the continuous version of master equation:

\[
\frac{\Delta P(n',t)}{\Delta t} = \sum_n \left[ T(n'|n) P(n,t) \right] - \sum_n \left[ T(n|n') P(n',t) \right] \tag{22}
\]

\[
\Delta P(n',t) = \sum_n \left[ T(n'|n) P(n,t) \right] - \sum_n \left[ T(n|n') \Delta t \right] P(n',t) \]

\[
= \sum_n \left[ T(n'|n) \Delta t \right] P(n,t) - P(n',t) \tag{22}
\]

\[
P(n',t + \Delta t) = \Delta P(n',t) + P(n',t) = \sum_n \left[ T(n'|n) \Delta t \right] P(n,t) \tag{23}
\]

The discrete master equation (23) makes intuitive sense because the probability function is decomposed into a sum of its previous probability functions weighted by their respective transition probabilities.

### 2.3 Fokker-Planck Equation

The master equation deals with the time evolution of the PDF of the Markov processes with discrete state space and continuous time steps, while the Fokker-Planck equation aims to extend our description of the time evolution of the PDF to continuous stochastic variables. We first derive the Kramers-Moyal expansion of the master equation, before truncate it to obtain a second-order partial differential equation, namely Fokker-Planck equation [Fokker (1914)] [Planck (1917)].

We define the **Jump Moments** for the system, which stands for the expectation of the moments of jump of the stochastic variable at two different times:

\[
M_l(x,t,\Delta t) = \int d\xi (\xi - x)^l P(\xi,t + \Delta t|x,t) \tag{24}
\]

which can also be written in terms of the stochastic process \( X(t) \) using the bracket notations for the expectation:

\[
M_l(x,t,\Delta t) = \langle (\xi - x)^l \rangle = \langle (X(t + \Delta t) - X(t))^l \rangle \tag{25}
\]

We start from Chapman-Kolmogorov equation (3) with continuous time steps and state space, in which we also drop the dependence on the initial conditions. Also define \( \Delta x = x - x' \), which is independent of \( x \) and \( x' \), and only dependent on their difference.
moments (24) that full probability, it follows from the definition of the jump
the system can only assume one state at a given time with
the Fokker-Planck Equation
orders of the jump moments can be neglected, and obtain
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series expansion. We truncate the Kramers-Moyal expan-
Absorbinussign into the integral from \(-\infty\) to \(\infty\)
We assume jump moments take the following form for
(28) is the Kramers-Moyal Expansion obtained by
nothing more than the Markov property and the Taylor
series expansion. We truncate the Kramers-Moyal expansion at the second order in some cases, where the higher orders of the jump moments can be neglected, and obtain the Fokker-Planck Equation:

\[
\frac{\partial P(x,t + \Delta t)}{\partial \tau} = \int dx' P(x,t + \Delta t|x',t)P(x',t)
\]

\[
= \int dx' P([x + \Delta x] - x, t + \Delta t|x - x, t)P(x - x, t)
\]

Taylor expansion at \(x + \Delta x\)

\[
\int dx' \sum_{l=0}^{\infty} \frac{(-\Delta x)^l}{l!} \frac{\partial^l}{\partial x^l} \left\{ P(x + \Delta x, t + \Delta t|x, t)P(x, t) \right\}
\]

\[
= \sum_{l=0}^{\infty} \frac{(-1)^l}{l!} \int dx' (\Delta x)^l \frac{\partial^l}{\partial x^l} \left\{ P(x + \Delta x, t + \Delta t|x, t)P(x, t) \right\}
\]

\[
= \sum_{l=0}^{\infty} \frac{(-1)^l}{l!} \frac{\partial^l}{\partial x^l} \left\{ \int dx' (\Delta x)^l P(x + \Delta x, t + \Delta t|x, t)P(x, t) \right\}
\]

Substitute \(M_l\) in and let \(\xi = x + \Delta x, d\xi = dx'\)

\[
\int dx' \sum_{l=0}^{\infty} \frac{(-\Delta x)^l}{l!} \frac{\partial^l}{\partial x^l} \left\{ P(x + \Delta x, t + \Delta t|x, t)P(x, t) \right\}
\]

\[
= \sum_{l=0}^{\infty} \frac{(-1)^l}{l!} \frac{\partial^l}{\partial x^l} \left\{ M_l(x, t, \Delta t)P(x, t) \right\}
\]

(26)

Since \(P(\xi, t|x, t) = \delta(\xi - x)\), which is reasonable because the system can only assume one state at a given time with full probability, it follows from the definition of the jump moments (24) that \(\lim_{\Delta t \to 0} M_l(x, t, \Delta t) = 0\) for \(l \geq 1\) and \(M_0(x, t, \Delta t) = 1\).

We assume jump moments take the following form for \(l \geq 1\):

\[
M_l(x, t, \Delta t) = D^{(l)}(x,t) \Delta t + o(\Delta t)
\]

(27)

Sustituting (27) into the previous result for \(P(x, t + \Delta t)\), dividing by \(\Delta t\) and taking the limit \(\Delta t \to 0\) give:

\[
\frac{\partial P(x,t)}{\partial \tau} = \sum_{l=0}^{\infty} \frac{(-1)^l}{l!} \frac{\partial^l}{\partial x^l} \left\{ M_l(x, t, \Delta t)P(x, t) \right\}
\]

(28)

which can be integrated by introducing an integrating factor to give the PDF for the stationary process:

\[
P_{st}(x) = \frac{C}{B(x)} \exp \left\{ \int x ds' A(s') B(s') \right\}
\]

(33)

Interestingly, we can transform the Fokker-Planck equation to a Schrödinger-like equation by \(P(x,t) = P_{st}(x) \frac{1}{\sqrt{2\pi}} \psi(x,t) = \frac{C}{B(x)} \exp \left\{ \int x ds' A(s') \right\} \psi(x,t)\), under the circumstances of a time independent \(A\) and a constant \(B\):

\[
-B \frac{\partial \psi}{\partial t} = - \frac{B^2}{2} \frac{\partial^2 \psi}{\partial x^2} + U(x) \psi
\]

(34)

where \(U(x) = A(x)^2 + \frac{B}{2} \frac{dA}{dx}\).

So a one dimensional stationary process under some given restraints is equivalent to the time evolution of the wave function in quantum mechanics with imaginary time, while \(B\) bears the role of the Planck’s constant.

An example for the Fokker-Planck equation would be the Ornstein-Uhlenbeck Process defined by:
\[
\frac{\partial P}{\partial t} = \frac{\partial}{\partial x}(axP) + D\frac{\partial^2 P}{\partial x^2}, \quad a > 0 \tag{35}
\]

where the potential \( U(x) = (a^2 x^2 - 2aD)/2 \). Correspondingly, \( A(x) = -ax \) and \( B = 2D \). This process is equivalent to a one-dimensional simple harmonic oscillator in quantum mechanics (remember its analogy to the potential of a spring system), with an energy shift represented by the constant term.

### 2.4 Stochastic Differential Equation (Langevin Equation)

So far we have discussed the time evolution of the PDF of the stochastic variables. Now we will be continuing on describing the system in terms of the time evolution of stochastic variables themselves. The example we use is the **Langevin Equation** for the velocity of a Brownian particle:

\[
m \frac{d^2 x}{dt^2} = -\alpha \frac{dx}{dt} - \frac{dV}{dx} + F(t) \tag{36}
\]

where \( m \) is the mass of a small macroscopic particle immersed in a liquid of temperature \( T \). Its velocity \( v(t) \) fluctuates due to the random collisions with the molecules of the liquid. The motion in this model is confined to be one dimensional. \( \alpha \) is the friction constant and \( V(x) \) is the potential of the interaction between the particle and the external forces. \( F(t) \) represents the random force due to the collisions with molecules. In order to solve this differential equation, we give the particle an initial position \( x(0) = x_0 \) and an initial velocity \( v(0) = v_0 \). The random force are defined to be Gaussian white noise such that:

(a) \( \langle F(t) \rangle = 0 \), which means that no direction is favoured in the motion.

(b) \( \langle F(t)F(t') \rangle = 2D\delta(t-t') \). The **Correlation Function**, which describes the average tendency of the correlation between the variables, is approximated by a delta function. This indicates that after a few collision times the correlation between \( F \) at its present value and its previous value is zero, so \( F(t) \) no longer depends on its previous value. We will discuss more about the importance of the correlation function in the next section.

(c) \( F(t) \) is considered to be Gaussian distributed, for simplicity, and also because we expect the collisions with large number of molecules will lead to a Gaussian distribution, by central limit theorem.

Unfortunately Langevin equation does not define a Markov process because the involvement of the second derivative suggests that \( x(t + \Delta t) \) not only depends on its former step \( x(t) \) but also on \( x(t - \Delta t) \), which is two steps away. So we introduce another stochastic variable \( v(t) \) velocity and transform the second order differential equation into two first order differential equations:

\[
\frac{dx}{dt} = v \tag{37}
\]

\[
m \frac{dv}{dt} = -\alpha v - \frac{dV}{dx} + F(t) \tag{38}
\]

To make it easier for our analysis, we assume that there are no external forces acting on the particle, so \( \frac{dv}{dt} = 0 \). We can then write (38) as:

\[
\frac{dv}{dt} = -\gamma v + F'(t); v(0) = v_0 \tag{39}
\]

with \( \gamma = \alpha/m \) and \( F'(t) = F(t)/m \). Since \( F'(t) \) is a random variable, solving the Langevin equation will give \( v(t) \) as a random variable instead of a definite expression. It is therefore referred to as **Stochastic Differential Equation**. \( F'(t) \) is often called the **Noise**, or **White Noise** because the Fourier transform of a delta function is a constant.

Solving equation (39) by multiplying an integrating factor and substituting in the initial condition, we have:

\[
v(t) = v_0 e^{-\gamma t} + e^{-\gamma t}\int_0^t dt' F'(t')e^{\gamma t'} \tag{40}
\]

The direct solution also contains a stochastic variable. In order to have a better description of the solution, we can also find the associated differential equation of the PDE using the Fokker-Planck equation. Taking the average of \( v(t) \) (remember that \( \langle F(t) \rangle = 0 \) by assumption), we find \( \langle v(t) \rangle = v_0 e^{-\gamma t} \). We then square \( v(t) \) and calculate \( \langle v(t)^2 \rangle \):

\[
\langle v(t)^2 \rangle = \langle v_0^2 e^{-2\gamma t} \rangle + 2v_0 \langle F'(t') \rangle \\
+ e^{-2\gamma t}\int_0^t \int_0^t dt' dt'' \langle F'(t')F'(t'') \rangle e^{\gamma(t'+t'')}
\]

\[
= v_0^2 e^{-\gamma t} + e^{-2\gamma t}\frac{2D}{m^2} \int_0^t \int_0^t dt' dt'' \delta(t'-t'') e^{\gamma(t'+t'')}
\]

\[
= v_0^2 e^{-\gamma t} + e^{-2\gamma t}\frac{2D}{m^2} \int_0^t dt' e^{2\gamma t'}
\]

\[
= v_0^2 e^{-\gamma t} + \frac{D}{\alpha m} \left[ 1 - e^{-2\gamma t} \right] \tag{41}
\]

As \( t \to \infty \), \( \lim_{t \to \infty} \langle v(t)^2 \rangle = \frac{D}{\alpha m} \). On the other hand, the Brownian particle will be in thermal equilibrium: \( \frac{1}{2}mv_0^2 = \frac{1}{2}kT \) and \( v_0^2 = \frac{D}{\alpha m} \). This gives us the expression of \( D \) in terms of the friction constant and the temperature of the liquid:
which is known as the **Einstein-Smoluchowski Relation**, an early example of the **Fluctuation-Dissipation Theorem**, which states that when there is a process of dissipating energy and turning it into heat, there is a reverse process of thermal fluctuation. In our example of the Brownian particles, the friction that the particle experiences dissipates energy into heat. And in return the heat caused thermal fluctuation, which corresponds to the Brownian motion of the particles. This brownian motion turns heat back into kinetic energy. The molecules of the liquid is acting as a heat bath for the particle system.

It is worth noting that [Zwanzig (1973)] has given another derivation of the Langevin equation where the starting point is a Hamiltonian that contains three terms: the system, the heat bath and the interaction between the two.

An example of Langevin equation is the **Overdamped Brownian Motion**, where the inertial term \( m \frac{d^2x}{dt^2} \) is negligible compared to the damping force \(-\alpha v\). We erase this term from left hand side of (36) and scale time by \( \alpha \) to arrive at the equation governing the overdamped Brownian motion:

\[
\frac{dx(t)}{dt} = -\frac{dV(x)}{dx} + F(t); \quad x(0) = x_0
\]  

(43)

And due to the scaling of time,

\[
\langle F(t) \rangle = 0; \quad \langle F(t)F(t') \rangle = 2\tilde{D}\delta(t-t'); \quad \tilde{D} = \frac{D}{\alpha}
\]  

(44)

A well-known case is when the particle is moving in a harmonic potential \( V(x) = \frac{ax^2}{2} \). (43) becomes:

\[
\frac{dx(t)}{dt} = -ax + F(t); \quad x(0) = x_0
\]  

(45)

Since (45) is linear and \( F(t) \) follows the Gaussian distribution, \( x(t) \) is also distributed in a Gaussian fashion. Comparing (45) with (39), we find that they are very similar in the structure except one has \( x(t) \) as variable while the other has \( v(t) \), a difference that does not restrain us from using the previous results (40) and (41) and obtain \( \langle x(t) \rangle = x_0e^{-\alpha t} \) and \( \langle x(t)^2 \rangle = x_0^2e^{-2\alpha t} + \frac{\tilde{D}}{\alpha}(1 - e^{-2\alpha t}) \). Also the standard deviation \( \sigma^2 \) of \( x(t) \) is simply \( \langle x(t)^2 \rangle - \langle x(t) \rangle^2 = \frac{\tilde{D}}{\alpha}(1 - e^{-2\alpha t}) \). The PDF for the Gaussian distribution of \( x(t) \) is thus given by:

\[
P(x,t|x_0,0) = \sqrt{\frac{a}{2\pi\tilde{D}(1-e^{-2\alpha t})}} \exp \left\{ -\frac{a(x-x_0e^{-\alpha t})^2}{2\tilde{D}(1-e^{-2\alpha t})} \right\}
\]  

(46)

It is straightforward to see this PDF agree with the Fokker-Planck equation for the Ornstein-Uhlenbeck process (35), which was formulated to describe the overdamped Brownian particles.

The Langevin equations with the Gaussian white noise \( F(t) \) are equivalent to the Fokker-Planck equations. The jump moments can be calculated easily from (25). We take the Langevin equation for the overdamped Brownian particles (43) as an example:

\[
\Delta x(t) = x(t+\Delta t) - x(t) = \int_t^{t+\Delta t} dt'\dot{x}(t')
\]  

\[
= -\int_t^{t+\Delta t} dt'\frac{dV(x(t'))}{dx} + \eta(t)
\]  

(47)

where \( \eta(t) = \int_t^{t+\Delta t} dt'F(t') \). Equation (44) suggests that \( \langle \eta(t) \rangle = 0 \) and furthermore \( \langle \eta(t)^n \rangle = 0 \) for \( n \) being odd.

\[
\langle \eta(t)^2 \rangle = \int_t^{t+\Delta t} dt'\int_t^{t+\Delta t} dt''\langle F(t')F(t'') \rangle = 2\tilde{D}\Delta t \quad \text{(48)}
\]

(\( \langle \eta(t)^n \rangle \) is at least of order \( (\Delta t)^2 \) for \( n \geq 4 \) and even.

By referring to the definition of the jump moments (25) we have:

\[
M_1(x,t,\Delta t) = \left\langle \frac{\int_t^{t+\Delta t} dt'\left(-\frac{dV(x(t'))}{dx}\right)}{\Delta t} \right\rangle
\]  

mean value theorem, \( \exists t = O(\Delta t) \) \( \left\langle -\frac{dV(x(t+\Delta t))}{dx}\right\rangle \Delta t \)

Taylor expansion at \( t \) \( \left\langle \frac{dV(x(t))}{dx} + O(\Delta t) \Delta t \right\rangle \Delta t \)

\[
= -\frac{dV(x(t))}{dx}\Delta t + O((\Delta t)^2)
\]  

(49)

with moments of order \( (\Delta t)^2 \) or higher for \( l > 2 \). Now we can express the Fokker-Planck equation (29) with the first two jump moments we just found :

\[
\frac{\partial P}{\partial t} = \frac{\partial}{\partial x}\left[ \frac{dV(x)}{dx} P \right] + \frac{\partial^2 \tilde{D}P}{\partial x^2}
\]  

(50)

From (33), the stationary distribution is given by

\[
P_{st}(x) = C \exp \left\{ -\frac{V(x)}{\tilde{D}} \right\} \quad (42),(44) = C \exp \left\{ -\frac{V(x)}{kT} \right\}
\]  

(51)
It is worth noting that in the example the noise term can be decomposed as \( F(t) = gN(t) \) where \( g \) is a multiplicative term describing the strength of the noise, possibly depending on \( x \). While \( N(t) \) is an orthonormal noise term satisfying \( \langle N(t) \rangle = 0 \) and \( \langle N(t)N(t') \rangle = \delta(t-t') \). If \( g \) is dependent on \( x \), then the question arises as to whether the \( x \) used in \( g(x) \) is taken before or after the impact of the noise. Even when the time step is infinitesimal, the values of \( x \) at two end points of the time step can still be drastically apart, in the case of the extreme noise. There are two different perspectives in interpreting the situation, one is the Itô convention and the other is the Stratonovich convention [van Kampen (1980)].

Consider a general form of the multiplicative Langevin equation (38):

\[
\frac{dx}{dt} = f(x) + gN(t)
\]

(52)

If \( g \) does not depend on \( x \), then the Fokker-Planck equation can be found by (50) by substituting \( f(x) = -\nabla V(x) / \partial x \) and \( D = \frac{1}{2}g^2 \):

\[
\frac{\partial P}{\partial t} = \frac{\partial}{\partial x} f(x)P + \frac{1}{2} g^2 \frac{\partial^2 P}{\partial x^2}
\]

(53)

For the case of \( g \) depending on \( x \), in the Itô Convention, we use the value of \( x \) before the noise strikes, the value at the starting point of the ongoing time step \( x = x(t) \). The Fokker-Planck equation is then:

\[
\frac{\partial P}{\partial t} = \frac{\partial}{\partial x} f(x)P + \frac{1}{2} g^2 \frac{\partial^2 P}{\partial x^2} g(x)^2 P
\]

(54)

In Stratonovich Convention the value of \( x \) in \( g(x) \) takes the average before and after the noise \( x = \frac{1}{2}x(t) + \frac{1}{2}x(t+dt) \). The Fokker-Planck equation is then:

\[
\frac{\partial P}{\partial t} = \frac{\partial}{\partial x} f(x)P + \frac{1}{2} \frac{\partial}{\partial x} g(x) \frac{\partial}{\partial x} g(x)P
\]

(55)

Since both of statistical mechanics and finance deal with a large-scale stochastic system and their theoretics share a lot in common, those two interpretations have an interesting application in the Black-Schosles option pricing [Perelló et al (2000)]. Though Itô convention is more convenient in finance because in this case \( \langle gN(t) \rangle = 0 \) and a deterministic equation for the expectation of the option price can be obtained.

### 2.5 Multi-Dimensional Stochastic Differential Equation

Up to now in our treatment of the stochastic processes we have been focusing on one variable. The construction of the Fokker-Planck equation from the Langevin equation follows a similar way for the \( n \)-dimensional processes \( x = (x_1, ..., x_n) \). Their jump moments are:

\[
\langle \Delta x_i(t) \rangle_{x(t) = x} = D_{i1, ..., in}(x,t) \Delta t + o(\Delta t), \quad i \in \{1, ..., n\}
\]

(56)

where \( \Delta x_i = x_{i_o}(t + \Delta t) - x_{i_o} \). The Fokker-Planck equation according to the expansion (28) is then:

\[
\frac{\partial P}{\partial t} = \sum_{l=0}^{\infty} \frac{(-1)^l}{l!} \frac{\partial^l}{\partial x_{i_1}...\partial x_{i_l}} \{D_{i_1...i_l}(x,t)\}
\]

(57)

The Langevin equation for the Brownian motion (38) is a good verification of this generalization to \( n \) dimensions. In this case the variables \( x(t) \) and \( v(t) \) together make the Brownian system two dimensional. In terms of their jump moments, we have \( D_{v1} \Delta t = \langle \Delta v(t) \rangle = \gamma v \Delta t - m^{-1}V(x) \Delta t \) and \( D_{v2} \Delta t = \langle (\Delta v(t))^2 \rangle \) ignore \( O((\Delta t)^2) \) terms:

\[
m^{-2}(\eta(t))^2 \]

(48)

Take those results into (57):

\[
\frac{\partial P}{\partial t} = -\frac{\partial}{\partial x} \left\{D_{x1}P\right\} - \frac{\partial}{\partial v} \left\{D_{v1}P\right\} + \frac{\partial^2}{\partial v^2} \left\{D_{v2}P\right\}
\]

\[
= -\frac{\partial}{\partial x} \left\{vP\right\} - \frac{\partial}{\partial v} \left\{\left(\gamma v + \frac{1}{m} \frac{dV(x)}{dx}\right)P\right\} + \frac{D}{m^2} \frac{\partial^2}{\partial v^2} \left\{P\right\}
\]

(42)

\[
= \frac{d}{dt} \frac{\partial}{\partial x} \left\{vP\right\} - \frac{\partial}{\partial v} \left\{\left(\gamma v + \frac{1}{m} \frac{dV(x)}{dx}\right)P\right\} + \frac{\gamma kT}{m} \frac{\partial^2}{\partial v^2} P
\]

(58)

(58) is called Kramer’s Equation. Its stationary solution is \( P_{st}(x,v) = C \exp \left\{-\frac{E}{kT}\right\} \) where \( E = \frac{1}{2}mv^2 + V(x) \).

Now we want to generalise the dimension from 2 to arbitrary \( n \) and find the Fokker-Planck equation equivalent to the general set of the Langevin equations:

\[
\dot{x}_i = A_i(x,t) + \sum_{\alpha=1}^{m} g_{i\alpha}(x,t)N_\alpha(t); \quad i \in \{1, ..., n\}
\]

(59)

where \( \zeta(t) \) is a Gaussian white noise with:

\[
\langle N_\alpha(t) \rangle = 0
\]

\[
\langle N_\alpha(t)N_\beta(t') \rangle = \delta_{\alpha\beta} \delta(t-t')
\]

(60)
In accordance with (54) and (55), the Fokker-Planck equation in the Itô and Stratonovich conventions are:

\[
\frac{\partial P}{\partial t} = -\sum_{i=1}^{n} \frac{\partial}{\partial x_i} \left[ A_i(x, t)P(x, t) \right] + \frac{1}{2} \sum_{i,j=1}^{n} \sum_{\alpha=1}^{m} \frac{\partial^2}{\partial x_i \partial x_j} \left[ g_{i\alpha}(x, t) g_{j\alpha}(x, t) P(x, t) \right] - \sum_{i,j=1}^{n} \sum_{\alpha=1}^{m} \frac{\partial^2}{\partial x_i \partial x_j} \left[ g_{i\alpha}(x, t) \frac{\partial}{\partial x_j} \left( g_{j\alpha}(x, t) P(x, t) \right) \right]
\]

(61)

\[
\frac{\partial P}{\partial t} = -\sum_{i=1}^{n} \frac{\partial}{\partial x_i} \left[ A_i(x, t)P(x, t) \right] + \frac{1}{2} \sum_{i,j=1}^{n} \sum_{\alpha=1}^{m} \frac{\partial^2}{\partial x_i \partial x_j} \left[ g_{i\alpha}(x, t) \frac{\partial}{\partial x_j} \left( g_{j\alpha}(x, t) P(x, t) \right) \right] + \sum_{i,j=1}^{n} \sum_{\alpha=1}^{m} \frac{\partial}{\partial x_i} \left[ g_{i\alpha}(x, t) \frac{\partial}{\partial x_j} \right] \left[ g_{j\alpha}(x, t) P(x, t) \right]
\]

(62)

\[P[x] \propto \exp \left(-\frac{1}{4D} \int dt (\dot{x} + V'(x))^2 + \frac{1}{2} \int dt V''(x) \right)
\]

(65)

With the PDF in hand, we are able to calculate all quantities of interest such as the expectations and the correlation functions. For example, the conditional probability density is given by:

\[
P(x, t|x_0, t_0) = \langle \delta(x - x(t)) \rangle_{x_0 = x_0} = \int_{x_0 = x_0} Dx \delta(x - x(t)) P[x]
\]

(66)

\[S[x] \text{ is an action functional, which is also an important ingredient in quantum field theory and contains all the information of the physical processes and also appears in the Feynman’s formulation of quantum mechanics. It is the quantum analogy to the action in classical mechanics. For a } n\text{-dimensional process in the form of (59) but without the multiplicative term, the action functional can be generalised as:}
\]

\[
S[x] = \int dt \left[ \frac{1}{2} \sum_{i,j} (\dot{x}_i - A_i(x))^2 D^{-1}_{ij}(\dot{x}_j - A_j(x)) + \frac{1}{2} \sum_i \frac{\partial A_i}{\partial x_i} \right]
\]

(67)

\[2.6 \text{ Nonlinear Stochastic Process and Path Integral}
\]

Now we have focused on linear stochastic processes, but there is no nonlinear term in Langevin equation. Otherwise it can be solved exactly like we did before. We can, however, borrow some techniques from the functional integrals and write the solutions in terms of the path integrals to get around the nonlinear terms [Feynman, Hibbs (1965)]. Take the overdamped Brownian motion (43) as an example, where the noise (44) is assumed to be Gaussian. We can represent \( F \) by a Gaussian PDF:

\[
P[F]DF \propto \exp \left(-\frac{1}{4D} \int dt F^2(t) \right) DF
\]

(63)

where \( DF \) is a functional measure. The PDF for the \( x \) variable can be found by mapping \( F \) to \( x \):

\[
P[x] = P[F]_{F=\dot{x}+V'(x)} J[x]
\]

\[
\propto \exp \left(-\frac{1}{4D} \int dt (\dot{x} + V'(x))^2 \right) J[x]
\]

(64)

where \( J[x] = det[\frac{\delta F}{\delta x}] \) is the Jacobian of the transformation. The explicit expression for the Jacobian is found to be \( J[x] \propto \exp(\theta \int dt V''(x)) \). \( \theta \) depends on the interpretation we choose. \( \theta = 0 \) for the Itô, and \( \theta = 1/2 \) for the Stratonovich (or the mid-point rule, which is more favoured in physics). Under the mid-point rule, substitute the Jacobian into (58) and we have:

\[df(W_t, t) = \partial_w f(W_t, t) dW_t + \frac{1}{2} \frac{\partial^2}{\partial w^2} f(W_t, t) dt + \partial_t f(W_t, t) dt
\]

(69)
Integrate Itô’s lemma from $t = a$ to $t = b$ we have the theorem of Itô’s lemma:

$$f(W_b, b) - f(W_a, a) = \int_a^b \partial_w f(W_t, t) dW_t$$

$$+ \int_a^b \left( \frac{1}{2} \partial^2_{ww} f(W_t, t) + \partial_t f(W_t, t) \right) dt$$

(70)

**Proof of Itô’s Lemma:**

We will prove (70) under the assumption that $f$ is a differentiable function up to third derivatives and all mixed partial derivatives up to third order exist and are bounded. The idea is to make a discrete approximation of the total change in $f$ and take a continuous limit. We use the following notational conventions to make the writing easier: $\Delta t = 2^{-m}$; $t_j = j\Delta t$; the change in any quantity from $t_j$ to $t_{j+1}$ is $\Delta(j**)$; subscript $j$ stands for $t_j$. Then we represent the left hand side of (70) by a telescoping sum:

$$f(W_b, b) - f(W_a, a) \approx \sum_{a \leq t_j \leq b} \Delta f_j$$

(71)

When $\Delta t$ and $\Delta w$ are small, we can make a Taylor expansion of $\Delta f_j$ with leading orders forming the right hand side of (70) while the remaining terms go to zero as $\Delta t \to 0$. Let $\Delta f = f(w + \Delta w, t + \Delta t) - f(w, t)$, then the Taylor expansion is:

$$\Delta f = \partial_w f(w, t) \Delta w + \frac{1}{2} \partial^2_{ww} f(w, t) \Delta w^2 + \partial_t f(w, t) \Delta t$$

$$+ O(|\Delta w|^3) + O(|\Delta w| \times |\Delta t|) + O(|\Delta t^2|)$$

(72)

The error terms correspond to the highest order neglected terms in the Taylor expansion, which are $\partial^2_{ww} f(w, t) \Delta w^3$, $\partial_w \partial_t f(w, t) \Delta w \Delta t$ and $\partial^2_t f(w, t) \Delta t^2$. Big-O notation $O(|*|)$ means a quantity $Q$ such that there exists a constant $C$ that leads to $|Q| \leq C |*|$. The sum on the right hand side of (71) now breaks into six terms corresponding to the right hand side of (72):

$$\sum_{a \leq t_j \leq b} \Delta f_j = S_1 + S_2 + S_3 + S_4 + S_5 + S_6$$

(73)

We consider those summation terms one by one and show that they converge in the continuous limit of the time step. The first is:

$$S_3 = \sum_{a \leq t_j \leq b} \partial_t f(W_j, t_j) \Delta t$$

$$m \to \infty, \Delta t \to 0 \implies \int_a^b \partial_t f(W_s, s) dW_s$$

(74)

The third one is:

$$S_3 = \sum_{a \leq t_j \leq b} \partial_t f(W_j, t_j) \Delta t$$

$$m \to \infty, \Delta t \to 0 \implies \int_a^b \partial_t f(W_s, s) dW_s$$

(75)

Since this is random, let us evaluate its expectation, with the knowledge that $\Delta W_j^2$ is connected to $\Delta t$ and so $E[|\Delta W_j^2|] = \Delta t^{3/2}$.

$$E[|S_4|] \leq C_4 \sum_{a \leq t_j \leq b} \Delta t^{3/2} = C_4 \Delta t^{1/2} \sum_{a \leq t_j \leq b} \Delta t$$

(76)

The second error goes a similar way, since $E[|\Delta W_j| \times \Delta t]$ also scales as $\Delta t^{3/2}$.

The last term error is:

$$|S_6| \leq C_6 \sum_{a \leq t_j \leq b} \Delta t^2 = C_6 (b-a) \Delta t$$

(78)

Now we are only left with the second term:

$$S_2 = \sum_{a \leq t_j \leq b} \frac{1}{2} \partial^2_{ww} f(W_j, t_j) \Delta W_j^2$$

(79)

which can be rewritten with respect to the connection $\Delta W_j^2 = \Delta t + R_j$:

$$S_2 = \sum_{a \leq t_j \leq b} \frac{1}{2} \partial^2_{ww} f(W_j, t_j) \Delta t + \sum_{a \leq t_j \leq b} \frac{1}{2} \partial^2_{ww} f(W_j, t_j) R_j$$

$$= \sum_{a \leq t_j \leq b} S_{2,1} + \sum_{a \leq t_j \leq b} S_{2,2}$$

(80)

with the random process $\{R_j\}$ satisfying $E[R_j | F_j] = 0$ and $E[R_j^2 | F_j] = 2\Delta t^2$. $S_{2,1}$ converges to the Riemann integral $\int_a^b (1/2) \partial^2_{ww} f(W_s, s) dW_s$, while $S_{2,2}$ converges to zero almost surely. To see this, we calculate $E[S_{2,2}^2]$, which is a
double sum over \( t_j \) and \( t_k \). The off-diagonal terms where \( j \neq k \) vanish:
\[
\mathbb{E} \left[ \left( \frac{1}{2} \partial_t^2 f(W_j, t_j) R_j \right) \left( \frac{1}{2} \partial_t^2 f(W_k, t_j) R_k \right) \right] = 0
\]
(81)

The diagonal terms are:
\[
\frac{1}{4} \mathbb{E} \left[ \left( \partial_t^2 f(W_j, t_j) \right)^2 \right] = \frac{1}{4} \mathbb{E} \left[ \left( \partial_t^2 f(W_j, t_j) \right)^2 \Delta t^2 \right]
\]
(82)

which are bounded since the second-order partial derivatives are bounded by assumption. Then the second term of (80) converges almost surely by the Borel Cantelli Lemma, which states that if \( S_n \) is a family of random variables with \( \sum_{n=1}^{\infty} \mathbb{E}[S_n^2] < \infty \), then \( S_n \to 0 \) as \( n \to \infty \) almost surely.

Now substituting all six terms in the continuous time limit into (73) and equating the result to (71) and we have the Itô’s lemma (70).

Upon Feynman’s reformulation of the quantum theory in terms of path integrals, Kac came up with a similar representation for the solution to the heat equation, which is known as Feynman-Kac formula [Kac (1949)]. Itô’s lemma will be applied in its proof.

Consider the simplest heat equation with a non-negative and continuous cooling term \( K \):
\[
\frac{\partial u}{\partial t} = \frac{1}{2} \frac{\partial^2 u}{\partial x^2} - K(x)u
\]
(83)

**Feynman-Kac Formula** states that the bounded solution to (83) with the initial condition:
\[
u(x, 0) = \lim_{(y,t) \to (x,0)} u(y, t) = f(x)
\]
(84)

where \( f \) is a bounded and continuous function, is given by:
\[
u(x, t) = \mathbb{E}_x \left[ \exp \left\{ - \int_0^t K(W_s) ds \right\} f(W_t) \right]
\]
(85)

where the process \( \{W_t\}_{t \geq 0} \) is a Brownian motion started at \( x \).

**Proof of Feynman-Kac Formula:**

Fix \( t > 0 \) and consider the stochastic process:
\[
Y_s = e^{-R(s)} u(W_s, t - s)
\]
where \( R(s) = \exp \left\{ - \int_0^s K(W_r) dr \right\} \)
(86)

Since \( u(x, t) \) is a solution to the heat equation (83), it is continuously differentiable once in \( t \) and twice in \( x \). Since \( u \) is bounded, so is the process \( \{Y_t\} \). By Itô’s lemma,
\[
dY_s = -K(W_s)e^{-R(s)}u(W_s, t - s)ds - u_0(W_s, t - s)e^{-R(s)}ds
+ u_x(W_s, t - s)e^{-R(s)}dW_s + \frac{1}{2}u_{xx}(W_s, t - s)e^{-R(s)}ds
\]
(87)

Since \( u \) satisfies the heat equation (83), the \( ds \) terms sum up to zero. This leaves us with:
\[
dY_s = u_x(W_s, t - s)e^{-R(s)}dW_s
\]
(88)

This proves that \( Y_s \) is a martingale up to time \( t \). By the conservation of expectation law for martingales, it follows that:
\[
u(x, t) = Y_0 = \mathbb{E}_x[Y_t] = \mathbb{E}_x[e^{-R(t)}u(W_t, 0)] = \mathbb{E}_x[e^{-R(t)}f(W_t)]
\]
(89)

The Feynman-Kac formula will be used later in the Hopf-Cole solution to KPZ equation in section 5.

### 3 A Statistical Mechanical Introduction to Integrable Models

Statistical mechanics is a branch of physics with a long history and but still has the vitality that draws the attention of many physicists. It concerns with finding the average behaviour of large-scale mechanical systems by applying probability theory. There are generally three approaches to tackle the problem, one is the **Fundamental Approach** which aims to derive the physical properties by rigorous mathematical methods; one is **Phenomenological Approach** which makes use of experiments to explain the results; the last one, which we will be relying on throughout this thesis, is the **Model Building Approach** which takes advantage of simple models to gain insight into the physical phenomena. Because of the large number of particles in statistical mechanical systems, the exactly solved models are hard to come by. But luckily some simple models in the
lower dimensional space have proven to be integrable and the most famous one of all has to be the Ising Model. This section follows the treatment of the Ising model from [McCoy, Wu (2014)].

3.1 Statistical Mechanics

The model introduced by [Ising (1925)] consists of a lattice of spin variables $\sigma_j$, which only take values from $\{1, -1\}$. By convention, the spin pointing upwards corresponds to the positive value. Any two spins have a mutual interaction energy $-J(j, k)\sigma_j\sigma_k$. The interpretation would be that their mutual interaction energy is $-J(j, k)$ for spins of the same orientation, while the mutual energy is $J(j, k)$ for spins pointing towards the opposite directions. In addition, a spin may interact with an external magnetic field $H$ with the energy $-H\sigma_j$ (note that the magnetic field here has unit of energy, it really means the magnetic energy).

In all of our discussion of the Ising model here, we only consider Nearest Neighbour Interaction, which means that $J(j, k)$ vanishes for all locations except when $j$ and $k$ are nearest neighbours on the lattice (their indices differ by 1). This assumption is essential for two dimensional Ising models to be solved exactly [Onsager (1944)], while not for the one dimensional case, where explicit computations have been carried out for interactions including non-nearest neighbours.

Before describing the Ising model using the partition function, we will have some review of basic technical details of statistical mechanics. In order to avoid unnecessary mathematical difficulties, we restrict our attention only to the systems with discrete energies.

Because the interpretation of statistical mechanics requires the system to possess a reasonably large number of particles, it is impossible to define an isolated Ising model with a small number of sites. So we will consider a large number of $N$ of identical Ising models of $M$ rows and $N$ columns by infinitely weak forces that allows the models to exchange energy but the force itself does not contribute to the total energy of the system. We are focusing on only one of those identical Ising models and the others help to define the temperature. Such a collection of systems is called an Ensemble.

Let $\sigma^{(n)}$ be the set of variables for the $n$th Ising model, $E^{(n)}(\sigma^{(n)})$ be the energy of $n$th Ising model and $E_{tot}$ be the total energy of the configuration of the Ising models we are constructing. The constraint imposed on the possible values of energy each Ising model can take is that the whole ensemble has a total energy of $E_{tot}$. The fundamental postulate of statistical mechanics in discrete energies says that all possible configurations $\sigma^{(1)}, ..., \sigma^{(N)}$ of Ising models have to add up to the total energy of the ensemble and each configuration is equally probable. In mathematical terms, we have:

$$P(\sigma^{(1)}, ..., \sigma^{(N)}; E_{tot}) = \frac{\delta_{E_{tot}, E_{tot}}}{\Omega(E_{tot})}$$ (90)

where $\Omega(E_{tot}) = \sum_{\sigma^{(1)}} ... \sum_{\sigma^{(N)}} \delta_{E_{tot}, E_{tot}}$ counts the number of all configurations having the total energy of $E_{tot}$.

In other words, the number of ways the total energy may be distributed among $N$ Ising models.

Since we are only interested in one particular Ising model $\sigma^{(1)}$ out of many, we sum up all probabilities of configurations corresponding to $\sigma^{(1)}$:

$$P(\sigma^{(1)}; E_{tot}) = \frac{\sum_{\sigma^{(1)}} ... \sum_{\sigma^{(N)}} \delta_{E_{tot}, E_{tot}}}{\Omega(E_{tot})}$$ (91)

As $N \to \infty$, the collection of the Ising models is known as Canonical Ensemble. By going through some complex analysis, which we will not be presenting here, the probability function for a canonical ensemble (91) can be written in a more compact form:

$$P(\sigma^{(1)}; E_{tot}) = \frac{e^{-\beta E(\sigma^{(1)})}}{Z(\beta)}(1 + O(N^{-1}))$$ (92)

where the Partition Function $Z(\beta)$ is defined in terms of the average energy of the ensemble:

$$Z(\beta) = \sum_{\sigma} e^{-\beta E(\sigma)}$$ (93)

$\beta$ is a parameter, or as some prefer to call it, the Thermodynamic Beta, which only makes sense when the system is large enough. It is determined as:

$$\bar{E} = \frac{E_{tot}}{N} = -\frac{\partial}{\partial \beta} \ln Z(\beta)$$ (94)

And associated with the temperature (in kelvin) by:

$$\beta = \frac{1}{kT}$$ (95)

With the probability function of $\sigma^{(1)}$ we are well equipped to study any function of the Ising model that depends on $\sigma^{(1)}$. In particular, the expectation value of $f$ in a large system of the Ising models with $M$ rows and $N$ columns:

$$\langle f \rangle_{M,N} = \lim_{N \to \infty} \sum_{\sigma} f(\sigma)P(\sigma; E_{tot}) = \frac{\sum_{\sigma} f(\sigma)e^{-\beta E(\sigma)}}{Z(\beta)}$$ (96)
The probability distribution of an Ising model allows us to study its properties in the thermal equilibrium. We will introduce several thermodynamic concepts. In addition to Internal Energy $E$ (previously calculated by $E = E_{\text{tot}}/N$, denoting the energy contained within the system excluding the kinetic and potential contributions. In the case of the Ising model ensemble, where the weak interaction between models do not contribute to the energy of the system, the internal energy is computed as the average value of the total energy of ensemble), there are also magnetisation, heat capacity, entropy and Helmholtz free energy, which are all related by the law of thermodynamics.

**Heat** is defined as the work done on the system by external forces, which are not accounted for the Interaction Energy caused by the interactions between particles or between particles and external fields (interaction energy and internal energy together make up the total energy). So if we fix the external magnetic field $H$, the change in the heat $\delta Q$ is related to the change in the internal energy $dE$ by:

$$dE = \delta Q \quad (97)$$

The Heat Capacity is defined by the partial derivative of internal energy with respect to temperature, while holding the interaction energy constant:

$$C = \left. \frac{\delta Q}{\delta T} \right|_{\delta H=0} = \left. \frac{\partial E}{\partial T} \right|_{H} \quad (98)$$

The Total Magnetisation or the total spin of a two dimensional Ising model of $M$ rows and $N$ columns is:

$$\sum_{j,k} \sigma_{j,k} \quad (99)$$

The Average Total Magnetisation of the Ising model in a canonical ensemble is then:

$$\bar{M} = \langle \sum_{j,k} \sigma_{j,k} \rangle = \frac{\sum \sigma_{j,k} e^{-\beta E(\sigma)}}{Z(\beta)} \quad (100)$$

Define $E = -H(\sum_{j,k} \sigma_{j,k}) \beta^{-1} \frac{\partial \ln Z(\beta)}{\partial H}$

If we consider an ensemble in equilibrium and change the external magnetic field from $B$ to $B + \Delta B$, while thermally isolating it, then the work done per Ising model is:

$$dE = -\bar{M}dH \quad (101)$$

Since the only external forces acting on the Ising model come from the external magnetic field and the heat bath, the total change in the internal energy is:

$$dE = \delta Q - \bar{M}dH \quad (102)$$

This is the **First Law of Thermodynamics**.

For our ensemble of $N$ identical Ising models and total energy $E_{\text{tot}}$, the Entropy $S_{\text{tot}}$ is defined as:

$$S_{\text{tot}} = k \ln \Omega(E_{\text{tot}}) \quad (103)$$

It is characterised by the number of possible microscopic configurations in a thermodynamic system given certain macroscopic properties. It is a measure of the disorder within a macroscopic system.

As $N \to \infty$ we define the entropy per Ising model $\bar{S}$ to be:

$$\bar{S} = \lim_{N \to \infty} S_{\text{tot}} / N = k[\beta \bar{E} + \ln Z(\beta)] = \frac{1}{T} \bar{E} + k \ln Z(\beta) \quad (104)$$

Note that in order to make sure a clear presentation of the notations, we adopt the following abbreviations $\frac{\partial}{\partial B} \mid_{B} = \frac{\bar{E}}{\beta}$, $\frac{\bar{E}}{\beta} \mid_{B} = \frac{\bar{E}}{\beta}$ and $\frac{\partial}{\partial T} \mid_{B} = \frac{\beta}{\bar{E}}$.

Finally we define the Helmholtz Free Energy $A$ by:

$$Z(\beta) = \bar{E} - T\bar{S} = e^{-\beta A} \quad (105)$$

It represents the energy needed to create a system once the spontaneous energy transferred from the environment is accounted for. It is the maximum amount of the work obtainable from a closed system.

In our canonical ensemble of Ising models, we assume an $N \to \infty$ number of Ising models to ensure precise measurements. In each Ising model, we also assume a large number of spins where its dimension $MN \to \infty$ and investigate the per-spin value of those properties we mentioned earlier in the limit of an infinite dimension. This limit is called **Thermodynamic Limit**.

The free energy per spin (in the thermodynamic limit we will call it "free energy" hereafter and the same convention goes for other properties) is defined by:

$$F = \lim_{M \to \infty, N \to \infty} A / MN \quad (106)$$

Internal energy $u$, magnetisation $M$, entropy $S$ and specific heat $c$ can be defined similarly.
Another useful property of the spin system is the Magnetic Susceptibility defined as:

\[ \chi = \lim_{M \to \infty, N \to \infty} \frac{\partial M}{\partial H} \]  

(107)

In order to gain insight into the behaviour of the Ising model, we also study the Spin Correlation Function, defined as the expectation value of a pair of spins. They indicate on the average the tendency of the pair of spins to be correlated.

\[ \langle \sigma_{M,N} \sigma_{M',N'} \rangle = \lim_{M \to \infty, N \to \infty} \frac{\sum_{\sigma_{M,N}} e^{-\beta \mathcal{E}(\sigma)}}{Z(\beta)} \]  

(108)

### 3.2 One-Dimensional Ising Model

A one-dimensional Ising model with nearest-neighbour interactions does not undergo a phase transition while in two dimensions it does. Still it is useful to examine the one-dimensional case first where both the free energy and the spin correlation function can be solved for exactly in closed forms with an external magnetic field.

#### 3.2.1 Partition Function

In a one-dimensional lattice with \( N \) spins, there are two possible boundary conditions. One is cyclic where the spin chain forms a closed ring, and the other is free where the end points of spin chain do not join.

1. **Cyclic.** The spin chain is deformed into a closed ring and site 1 is connected to site \( N \) by a bond of strength \( J \). The interaction energy is:

\[ \mathcal{E}_C = -J \sum_{k=1}^{N} \sigma_k \sigma_{k+1} - H \sum_{k=1}^{N} \sigma_k \]  

(109)

where \( \sigma_{N+1} = \sigma_1 \).

The partition function under the cyclic boundary condition is:

\[ Z_C^N = \sum_{\sigma_1} \cdots \sum_{\sigma_N} \exp \left\{ \beta \left[ J \sum_{k=1}^{N} \sigma_k \sigma_{k+1} + H \sum_{k=1}^{N} \sigma_k \right] \right\} \]  

(110)

2. **Free.** The spin arrangement in this case is a linear chain. The corresponding interaction energy is:

\[ \mathcal{E}_F = -J \sum_{k=1}^{N-1} \sigma_k \sigma_{k+1} - H \sum_{k=1}^{N} \sigma_k \]  

(111)

Its partition function is:

\[ Z_F^N = \sum_{\sigma_1} \cdots \sum_{\sigma_N} \exp \left\{ \beta \left[ J \sum_{k=1}^{N-1} \sigma_k \sigma_{k+1} + H \sum_{k=1}^{N} \sigma_k \right] \right\} \]  

(112)

To calculate the partition functions explicitly, we employ a matrix formalism introduced by [Kramers, Wannier (1941)].

Define the spin states in terms of vectors:

\[ |\sigma = 1\rangle = |\uparrow\rangle = \left( \begin{array}{c} 1 \\ 0 \end{array} \right) \]

\[ |\sigma = -1\rangle = |\downarrow\rangle = \left( \begin{array}{c} 0 \\ 1 \end{array} \right) \]  

(113)

The vector \( V \) is defined to be:

\[ V = \begin{pmatrix} e^{\frac{1}{2} \beta H} \\ e^{-\frac{1}{2} \beta H} \end{pmatrix} \]  

(114)

The matrix \( T \) (which is called Transfer Matrix) is defined to be:

\[ T = \begin{pmatrix} T(\uparrow, \uparrow) & T(\uparrow, \downarrow) \\ T(\downarrow, \uparrow) & T(\downarrow, \downarrow) \end{pmatrix} = \begin{pmatrix} e^{\beta(J+H)} & e^{-\beta J} \\ e^{-\beta J} & e^{\beta(J-H)} \end{pmatrix} \]  

(115)

So that we can easily check the following relations:

\[ \langle \sigma|T|\sigma' \rangle = \exp \left\{ \beta \left[ J \sigma \sigma' + \frac{1}{2} H (\sigma + \sigma') \right] \right\} \]  

(116)

\[ \langle \sigma|V = e^{\beta H \sigma/2} \]

\[ V^T|\sigma \rangle = e^{\beta H \sigma/2} \]  

(117)

We may write the magnetic contribution to the interaction energy in a more symmetric form:
\[
-H \sum_{k=1}^{N} \sigma_k = -\frac{1}{2} H \sum_{k=1}^{N} \sigma_k - \frac{1}{2} H \sum_{k=1}^{N} \sigma_k
= -\frac{1}{2} H \sum_{k=1}^{N} \sigma_k - \frac{1}{2} H \sum_{k=0}^{N-1} \sigma_{k+1}
\]

Similarly, \(N_F\) can be written in terms of transfer matrix \(N_C\):

\[
\sum_{\sigma_N} \langle \sigma_1 | T | \sigma_2 \rangle \ldots \langle \sigma_{N-1} | T | \sigma_N \rangle \langle \sigma_N | T | \sigma_1 \rangle
= \sum_{\sigma_1} \langle \sigma_1 | T \left( \sum_{\sigma_2} \langle \sigma_2 | \sigma_2 \rangle \ldots \right) \langle \sigma_N | \sigma_N \rangle | T | \sigma_1 \rangle
= \sum_{\sigma_1} \langle \sigma_1 | T \sum_{\sigma_2} \langle \sigma_2 | \sigma_2 \rangle | T | \sigma_1 \rangle
= \sum_{\sigma_1} \langle \sigma_1 | T^N | \sigma_1 \rangle
= tr(T^N)
\]

Similarly, \(Z_N^F\) can be written in terms of \(T\) and \(V\):

\[
Z_N^F = \sum_{\sigma_1} \ldots \sum_{\sigma_N} V^T | \sigma_1 \rangle \langle \sigma_1 | T | \sigma_2 \rangle \ldots \langle \sigma_{N-1} | T | \sigma_N \rangle \langle \sigma_N | V
= \sum_{\sigma_1} \ldots \sum_{\sigma_N} V^T | \sigma_1 \rangle \langle \sigma_1 | T \sum_{\sigma_2} \langle \sigma_2 | \sigma_2 \rangle | T \sum_{\sigma_N} \langle \sigma_N | \sigma_N \rangle | V
= V^T T^{N-1} V
\]

Since \(T\) is a symmetric matrix, it can be diagonalised by a similarity transformation with a matrix \(U\):

\[
U^{-1} T U = \begin{pmatrix} \lambda_+ & 0 \\ 0 & \lambda_- \end{pmatrix}
\]

where the eigenvalues \(\lambda_+\) and \(\lambda_-\) satisfy the characteristic equation:

\[
\det(T - \lambda I_2) = 0
\]

which is a simple quadratic equation and can be solved easily:

\[
\lambda \pm = e^{J} \left[ \cosh \beta H \pm \left( \cosh^2 \beta H - 2e^{-2\beta J} \sinh 2\beta J \right)^{1/2} \right]
= e^{J} \left[ \cosh \beta H \pm \left( \sinh^2 \beta H + e^{-4\beta J} \right)^{1/2} \right]
\]

One possible choice for matrix \(U\) can be obtained by setting \(U_{12} = U_{21} = 1\) and substituting those into (121):

\[
U = \begin{pmatrix} -e^{J} \left( e^{J-H} - \lambda_+ \right) & 1 \\ 0 & -e^{J} \left( e^{J-H} - \lambda_- \right) \end{pmatrix}
\]

with \(U^{-1}\) obtained by taking the inverse of \(U\):

\[
U^{-1} = U \begin{pmatrix} -(\det U)^{-1} & 0 \\ 0 & -(\det U)^{-1} \end{pmatrix}
\]

Now we can express the partition functions with the eigenvalues of the diagonal matrix:

\[
Z_N^C = tr(T^N) = tr[U^{-1} T U]^N
= tr \left( \lambda_+^N \begin{pmatrix} 0 & 0 \\ 0 & \lambda_-^N \end{pmatrix} \right)^N
= \lambda_+^N + \lambda_-^N = \lambda_+^N \left( 1 + \left( \frac{\lambda_-}{\lambda_+} \right)^N \right)
\]

Similar computations can be done for the free boundary condition:

\[
Z_F^C = V^T T^{N-1} V
= V^T (U \begin{pmatrix} \lambda_+ & 0 \\ 0 & \lambda_- \end{pmatrix} U^{-1})^N V
= V^T U \begin{pmatrix} \lambda_+^N & 0 \\ 0 & \lambda_-^N \end{pmatrix} U^{-1} V
= \lambda_+^{N-1} \left[ \cosh \beta H + (\sinh^2 \beta H + e^{-2\beta J})(\sinh^2 \beta H + e^{-4\beta J})^{1/2} \right]
+ \left( \frac{\lambda_-}{\lambda_+} \right)^{N-1} \left[ \cosh \beta H - (\sinh^2 \beta H + e^{-2\beta J}) \right] \times (\sinh^2 \beta H + e^{-4\beta J})^{1/2}
\]
From (123) it is trivial to see that, given our assumption that $H$ is real and $\beta$ is finite and positive,

$$\lambda_+ > \lambda_- \quad (128)$$

Therefore by the definitions of free energy (105) and (106):

$$\lim_{N \to \infty} N^{-1} \ln Z_N^C = \lim_{N \to \infty} N^{-1} \ln Z_N^C = \ln \lambda_+ = -\beta F \quad (129)$$

So in the thermodynamic limit, the free energy with cyclic boundary condition is the same as the free energy with free boundary condition. Just as we expect, the boundary condition becomes unimportant when the the scale of Ising model is infinitely large.

Now with the partition function solved, we are ready to find the explicit forms of the thermodynamic properties of the system. Organise (129) a bit and we find the free energy $F$:

$$F = -\beta \ln \lambda_+ \quad (123)$$

$$-J - \beta^{-1} \ln \{ \cosh \beta H + (\sinh^2 \beta H + e^{-4\beta J})^{1/2} \} \quad (130)$$

The internal energy $u$ is:

$$u \quad (94), (106) \frac{\partial \beta F}{\partial \beta} = -H \sinh \beta H (\sinh^2 \beta H + e^{-4\beta J})^{1/2}$$

$$- J \coth 2\beta J + J e^{-2\beta J} \cosh 2\beta J \cosh \beta H$$

$$\times (\sinh^2 \beta H + e^{-4\beta J})^{-1/2} \quad (131)$$

The specific heat $c$ is:

$$c \quad (98) \frac{\partial u}{\partial T} = k \frac{\partial u}{\partial \beta} = k \frac{\partial u}{\partial \beta} = -k^2 \frac{\partial u}{\partial \beta}$$

$$= k^2 \left\{ H e^{-4\beta J} [H \cosh \beta H + 2J \sinh \beta H] \right.$$

$$\times (\sinh^2 \beta H + e^{-4\beta J})^{-3/2} - 2J^2 \cosh^2 \beta H$$

$$+ 2J^2 \cosh^2 2\beta J \cosh \beta H (\sinh^2 \beta H + e^{-4\beta J})^{-1/2}$$

$$- [JH \sinh \beta H (e^{-4\beta J}) - 1] + 2J^2 e^{-4\beta J} \cosh \beta H (e^{-2\beta J}) \cosh 2\beta J$$

$$\times (\sinh^2 \beta H + e^{-4\beta J})^{-3/2} \right\} \quad (132)$$

The magnetisation is:

$$M \quad (100), (106) \frac{\partial F}{\partial H} = \sinh \beta H [\sinh^2 \beta H + e^{-4\beta J}]^{-1/2} \quad (133)$$

**3.2.2 Spin Correlation Function**

Spin correlation functions can be computed by the same matrix formalism. Consider cyclic boundary condition and for $N' \leq N$, we have

$$\langle \sigma_{N'} \sigma_N \rangle_N^C = (Z_N^C)^{-1} \sum_{\sigma} \sigma_N \sigma_N \exp \left \{ \beta \left[ J \sum_{k=1}^N \sigma_k \sigma_{k+1} + H \sum_{k=1}^N \sigma_k \right] \right \} \quad (119)$$

$$= (Z_N^C)^{-1} \sum_{\sigma} \sigma_N \sigma_N \langle \sigma_1 | \sigma_2 | \cdots | \sigma_{N-1} | \sigma_N | T | \sigma_{N'} | T | \sigma_{N'+1} \rangle \langle \sigma_{N-1} | T | \sigma_N | T | \sigma_{N+1} + \langle \sigma_{N-1} | T | \sigma_N | T | \sigma_{N'+1} \rangle \quad (134)$$

[continuing from (134)]

$$= (Z_N^C)^{-1} \sum_{\sigma_1} \langle \sigma_1 | T \left[ \prod_{l=2}^{N-1} \sum_{\sigma_l} \langle \sigma_l | T \right] \left[ \sum_{\sigma_{N'}} \sigma_N | \sigma_{N'} \right] T \langle \sigma_{N'-1} | \sigma_{N'} \rangle N' \langle \sigma_{N'-1} \rangle N' \left( 1 \ 0 \right) T^{N-N'} \left( 1 \ 0 \right) T^{N-N+1} | \sigma_1 \rangle \quad (135)$$

[continuing from (135)]

$$= (Z_N^C)^{-1} \text{tr} \left\{ T^{N-N'} \left( 1 \ 0 \right) T^{N-N'} \left( 1 \ 0 \right) T^{N-N+1} \right\} \quad (136)$$

In order to evaluate the trace, we diagonalise the transfer matrix $T$ (121):

$$\langle \sigma_{N'} \sigma_N \rangle_N^C = (Z_N^C)^{-1} \text{tr} \left\{ U \left( \frac{\lambda_+}{\lambda_-} \right)^{N-(N-N')} U^{-1} \left( 1 \ 0 \right) \right\} \quad (137)$$
By using the explicit expression of $U$ in (124), we obtain the spin correlation function with cyclic boundary condition:

$$\langle \sigma_{N'} \sigma_N \rangle_{\mathcal{N}}^C = (\sinh^2 \beta H + e^{-4\beta J})^{-1} \times [\sinh^2 \beta H + (\lambda_+^{N-N} \lambda_-^{N-N'}) + \sum_{k=0}^{N-1} \lambda_+^k \lambda_-^{N-k-1} e^{-4\beta J}]$$

(138)

The thermodynamic limit can be found by keeping $N - N'$ fixed and let $\mathcal{N} \rightarrow \infty$:

$$\langle \sigma_{N'} \sigma_N \rangle_{\mathcal{N}}^C = (\sinh^2 \beta H + e^{-4\beta J})^{-1} \times [\sinh^2 \beta H + (\lambda_-/\lambda_+)^{N-N'} e^{-4\beta J}]$$

(139)

Particularly, for the case of an absent magnetic field ($H = 0$):

$$\langle \sigma_{N'} \sigma_N \rangle_{\mathcal{N}}^C |_{H=0} = (\tanh \beta J)^{N-N'}$$

(140)

We define the Long Range Order, which describes the correlation of infinitely distant spins within a physical system, as follows:

$$\lim_{N-N' \rightarrow \infty} \langle \sigma_{N'} \sigma_N \rangle_{H=0} = \begin{cases} 1 & \text{if } T = 0 \ (\beta = \infty) \\ 0 & \text{otherwise} \end{cases}$$

(141)

When $T = 0$, the system is in the ground energy level with all the spins pointing towards the same direction. So the correlation function is 1 for any two spins in the system. For $T > 0$, the system goes beyond the ground state and gets excited. But due to the large degeneracy of excited states (large number of configurations corresponding to the same energy level), there is no correlation between distant spins and the long range order is 0.

The case with free boundary condition can be treated in a similar fashion with (134):

$$\langle \sigma_{N'} \sigma_N \rangle_{\mathcal{N}}^F = (Z_N^F)^{-1} \sum_{\sigma} \langle \sigma_{N'} \sigma_N \rangle \exp \left\{ \beta \left[ J \sum_{k=1}^{N} \sigma_k \sigma_{k+1} + H \sum_{k=1}^{N} \sigma_k \right] \right\}$$

$$= (Z_N^F)^{-1} V^T U \left( \begin{array}{cc} \lambda_+ & 0 \\ 0 & \lambda_- \end{array} \right)^{N-1} U^{-1} \left( \begin{array}{cc} 1 & 0 \\ 0 & -1 \end{array} \right)$$

$$\times U \left( \begin{array}{cc} \lambda_+ & 0 \\ 0 & \lambda_- \end{array} \right)^{N-N'} U^{-1} \left( \begin{array}{cc} 1 & 0 \\ 0 & -1 \end{array} \right) U \left( \begin{array}{cc} \lambda_+ & 0 \\ 0 & \lambda_- \end{array} \right)^{N-N'} U^{-1} V$$

(142)

(142) can be evaluated by direct substitution:

$$\langle \sigma_{N'} \sigma_N \rangle_{\mathcal{N}}^F = (\sinh^2 \beta H + e^{-4\beta J})^{-1} \times [\sinh^2 \beta H + (\lambda_-/\lambda_+)^{N-N'} e^{-4\beta J}]$$

(143)

[continuing from (143)]

$$\times \left[ \lambda_+^{-1} [\cosh \beta H (\sinh^2 \beta H + e^{-4\beta J})^{1/2} + \sinh^2 \beta H + e^{-2\beta J}] + (\lambda_-/\lambda_+)^{N-N'} [\cosh \beta H (\sinh^2 \beta H + e^{-4\beta J})^{1/2} - \sinh^2 \beta H + e^{-2\beta J}] \right]^{-1}$$

$$\times \lambda_+^{-1} [\cosh \beta H (\sinh^2 \beta H + e^{-4\beta J})^{1/2} + \sinh^2 \beta H + e^{-2\beta J}] + (\lambda_-/\lambda_+)^{N-N'} [\cosh \beta H (\sinh^2 \beta H + e^{-4\beta J})^{1/2} - \sinh^2 \beta H + e^{-2\beta J}]$$

(144)

[continuing from (144)]

$$\times \lambda_+^{-1} [\cosh \beta H (\sinh^2 \beta H + e^{-4\beta J})^{1/2} + \sinh^2 \beta H + e^{-2\beta J}] + (\lambda_-/\lambda_+)^{N-N'} [\cosh \beta H (\sinh^2 \beta H + e^{-4\beta J})^{1/2} - \sinh^2 \beta H + e^{-2\beta J}]$$

(145)

This monstrous expression of correlation function with free boundary condition is the reason why we prefer to work with cyclic boundary condition in statistical mechanical problems. Since this expression depends on $N$ and $N'$ separately, in order to take the thermodynamic limit, we let $N \rightarrow \infty$ and $N' \rightarrow \infty$ separately and let $\mathcal{N} \rightarrow \infty$.
\[\langle \sigma_N \sigma_N \rangle^F = (\sinh^2 \beta J + e^{-4\beta J})^{-1} \left\{ \sinh^2 \beta H + e^{-4\beta J} \langle \sigma_N \sigma_N \rangle^F \right\}
- 4 \sinh^2 \beta J e^{-4\beta J} \sinh^2 \beta J \langle \sigma_N \sigma_N \rangle^F \langle \sigma_{N-N'} \sigma_{N-N'} \rangle^F \]

(146)

If we consider taking the limit as previously described but also take \( N - N' \to \infty \) and \( N' - N \to \infty \) (meaning that the two correlated spins are infinitely far away from the boundaries), which is called Bulk Limit, then we find that \( \langle \sigma_N \sigma_N \rangle^F \) is exactly the same as the thermodynamic limit for cyclic boundary condition (139). So the bulk properties of the Ising model is indifferent to boundary conditions.

### 4 Quantum Integrable Models

An intuitive definition of Quantum Integrability is that the system is exactly solvable, in the sense that a full set of eigenstates can be constructed explicitly. This is a correspondence with the action-angle variables in classical system. A more rigorous definition has been proposed by [Caux and Mossel (2010)] to tackle the many technical ambiguities that has been surrounding the topic, and also to give a clearer classification of quantum integrable models, where different classes exhibit distinguishable behaviours. But we will not bother ourselves too much here with the definition that is still in debate. Let us illustrate quantum intergrability by an example.

#### 4.1 Heisenberg Spin Chain

The example we choose to illustrate quantum intergrability is Heisenberg Spin Chain, which is similar in configuration to the one-dimensional Ising model that we discussed earlier, except this time we treat the system in a quantum context and look for the eigenvalues of the Hamiltonian. For the spectrum of the Hamiltonian by a technique called Bethe Ansatz, invented by [Hans Bethe (1931)] for the exact purpose of dealing with the Heisenberg model. By introducing some algebraic tools, we can obtain a modified version of Bethe Ansatz, namely Algebraic Bethe Ansatz, which will help us analyse the spin system in a more theoretical nature.

##### 4.1.1 Bethe Ansatz

The Heisenberg Spin Chain is a closed one-dimensional model of spin-\( \frac{1}{2} \) particles that have nearest-neighbour spin interactions. The closed boundaries make the chain into a ring. The spin chain consists of \( N \) sites with only one particle on each site. The spin states are quantised and denoted as \( | \uparrow \rangle \) and \( | \downarrow \rangle \). Any linear combination of the two is possible. The total Hilbert space the spin states live in is a tensor product of quantum spaces \( \mathbb{C}^2 \).

\[ H = - \sum_{\alpha = x, y, z} \sum_{i=1}^{N} J_{\alpha} S_i^\alpha S_{i+1}^\alpha \]

(148)

If the exchange coupling constant \( J \) is the same in all directions, then the spin model is called XXX \( 1/2 \). If it is the same for \( x \) and \( y \) directions, then the name is XXZ \( 1/2 \). We look at the former case only.

The energy shift constant \( J N \) is added to the Hamiltonian of XXX \( 1/2 \) to make sure the ground state energy is zero and completely up for choice. It can be further rewritten using raising and lowering operators \( S^\pm = S^x \pm i S^y \).

\[ H = \frac{J N}{4} - \frac{J}{2} \sum_{i} (S_i^+ S_{i+1}^- + S_i^- S_{i+1}^+ + 2S_i^z S_{i+1}^-) \]

(149)

The actions of those operators on the spin states are defined as follows:

\[ S^+ | \uparrow \rangle = 0 \quad S^+ | \downarrow \rangle = | \uparrow \rangle \]
\[ S^- | \uparrow \rangle = | \downarrow \rangle \quad S^- | \downarrow \rangle = 0 \]
\[ S^z | \uparrow \rangle = \frac{1}{2} | \uparrow \rangle \quad S^z | \downarrow \rangle = -\frac{1}{2} | \downarrow \rangle \]

The size of the Hamiltonian is \( 2N \times 2N \) and its eigenvalues are impossible to be solved for large systems by brute force, especially when it comes to the thermodynamic limit \( N \to \infty \). We need analytical techniques to deal with the problem and this is when Bethe Ansatz steps in as the solution. Consider a ground state where all spins are up or down and then flip some spins to go up in energy level. Those spins behave like quasi-particles called Magnons.

Let us define the ground state, also called Ferromagnetic Vacuum, to be:

\[ | 0 \rangle = | \uparrow \uparrow \ldots \uparrow \rangle \]

(150)

The ground energy as an eigenvalue can be easily found to be exactly \( JN/4 \) by applying Hamiltonian (149) to \( | 0 \rangle \).
Consider the case when a total number of $M$ spins are flipped by acting with $S_n^-$ on the vacuum:

$$|n_1, ..., n_M\rangle = S_{n_1}^- ... S_{n_M}^- |0\rangle$$  \hspace{1cm} (151)

An eigenstate with $M$ flipped spins is of the form:

$$|\psi\rangle = \sum_{1 \leq n_1 < ... < n_M \leq N} f(n_1, ..., n_M) |n_1, ..., n_M\rangle$$  \hspace{1cm} (152)

The coefficients satisfy the boundary condition:

$$f(n_2, ..., n_M, n_1 + N) = f(n_1, ..., n_M)$$  \hspace{1cm} (153)

Now let only one spin flip at site $n$. The system can be regarded as having a particle with momentum $p$ at site $n$. We denote the wavefunction as $|p\rangle$. The Bethe Ansatz postulates that the eigenstate is of plain-wave type, which is also a Fourier transform from position space to momentum space:

$$|p\rangle = \sum_n e^{ipn} S_n^- |0\rangle = \sum_n e^{ipn} |n\rangle$$  \hspace{1cm} (154)

The boundary condition tell us that $e^{ipN} = 1$:

$$|p\rangle = \sum_n e^{i(p(n+N)} S_{n+N}^- |0\rangle = e^{ipN} \sum_n e^{ipn} S_n^- |0\rangle$$  \hspace{1cm} (155)

Substitute the Ansatz (154) into the Hamiltonian (149) and we find:

$$H |p\rangle = 2J \sin^2 \frac{p}{2} |p\rangle$$  \hspace{1cm} (156)

Hence the flipped spin at site $n$ behaves like a particle with momentum $p$ and energy $2J \sin^2 \frac{p}{2}$.

Now imagine we have two magnons (two flipped spins) in the system. If they are well-separated we expect them to behave as two single magnons. Only when they are situated together does the system become non-trivial.

The Bethe Ansatz says that the wave function for two magnons is:

$$|p_1, p_2\rangle = \sum_{n_1 < n_2} \left[ A' e^{i(p_1 n_1 + p_2 n_2)} + A e^{i(p_2 n_1 + p_1 n_2)} \right] S_{n_1}^- S_{n_2}^- |0\rangle$$

$$= \left[ \sum_{n_1 < n_2} A' e^{i(p_1 n_1 + p_2 n_2)} + \sum_{n_2 < n_1} A e^{i(p_2 n_2 + p_1 n_1)} \right] S_{n_1}^- S_{n_2}^- |0\rangle$$  \hspace{1cm} (157)

The wave function is comprised of two terms, the first magnon to the left of the second one and the other way around. Let the Hamiltonian act on a system state. When two magnons are not next to each other ($|n_1 - n_2| > 2$), the system behaves like two disjoint one-magnon states and the eigenvalue of the Hamiltonian is simply the total energy of two magnons $2J \sin^2 \frac{p}{2} + 2J \sin^2 \frac{p}{2}$.

When two magnons are next to each other ($|n_1 - n_2| = 2$), the only non-vanishing terms after Hamiltonian action are $|\cdots \uparrow \downarrow \uparrow \cdots\rangle$, $|\cdots \uparrow \downarrow \downarrow \cdots\rangle$ and $|\cdots \uparrow \uparrow \downarrow \cdots\rangle$. Let Hamiltonian act on this eigenstate and we have:

$$\frac{A'}{2} \left[ e^{i(p_1 (n+1) + p_2 (n+1))} - 2 e^{i(p_1 n + p_2 (n+1))} + e^{i(p_1 n + p_2 (n+2))} \right]$$

$$+ \frac{A}{2} \left[ e^{i(p_2 (n-1) + p_1 (n+1))} - 2 e^{i(p_2 n + p_1 (n+1))} + e^{i(p_2 n + p_1 (n+2))} \right]$$

$$= \left[ 2J \sin^2 \frac{p_1}{2} + 2J \sin^2 \frac{p_2}{2} \right]$$

$$\times \left( A' e^{i(p_1 n + p_2 (n+1))} + A e^{i(p_2 n + p_1 (n+1))} \right)$$  \hspace{1cm} (158)

We can compute the ratio of $A$ and $A'$ easily from this relation:

$$\frac{A}{A'}(p_1, p_2) = \frac{\cot(p_1/2) - \cot(p_2/2) - 2i}{\cot(p_1/2) - \cot(p_2/2) + 2i} = e^{i\theta_{12}}$$  \hspace{1cm} (159)

$A/A'$ is called S-Matrix describing the scattering of two magnons, which satisfies:

$$\frac{A}{A'}(p_1, p_2) = \frac{A}{A'}(p_2, p_1) = 1$$  \hspace{1cm} (160)

By imposing boundary conditions (153) on (157), we obtain the Bethe Equations:

$$\frac{A}{A'}(p_1, p_2) = e^{i p_2 N} \frac{A}{A'}(p_2, p_1) = e^{i p_1 N}$$  \hspace{1cm} (161)

The Bethe equations can be transformed into a set of polynomial equations by Rapidity $u = 2 \cot(p/2)$:

$$\begin{bmatrix} \frac{u_1 + \frac{i}{2}}{u_1 - \frac{i}{2}} \end{bmatrix}^N = \begin{bmatrix} u_1 - u_2 + i \n \frac{u_1 - u_2 - i} \end{bmatrix}$$

$$\begin{bmatrix} \frac{u_2 + \frac{i}{2}}{u_2 - \frac{i}{2}} \end{bmatrix}^N = \begin{bmatrix} u_2 - u_1 + i \n \frac{u_2 - u_1 - i} \end{bmatrix}$$  \hspace{1cm} (162)

The generalisation of Bethe equation to multiple magnons is given by:
The energy of individual magnon can be expressed in terms of the rapidity by substituting momentum in (156):

\[ E_i = \frac{2J}{4 + u_i^2} \]  

(164)

So the spectrum of the Hamiltonian can be exactly represented by solving the Bethe equations for the rapidities and sum up all the corresponding energies.

### 4.1.2 Algebraic Bethe Ansatz

Now we adopt a different approach, which is a modified version of Bethe Ansatz with significant algebraic elements, to study the XXX Heisenberg model in details [Faddeev (1995)].

The basic tool of the algebraic Bethe Ansatz is the **Lax Operator** \( L_{n,a} : V_n \otimes V_a \rightarrow V_n \otimes V_a \), where \( V_a = \mathbb{C}^2 \) is an **Auxiliary Space** (interpreted as the space which specifies the matrix structure of the lax operator):

\[
L_{n,a}(u) = uI_n \otimes I_a + i \sum_{\alpha=x,y,z} S_n^{\alpha} \otimes \sigma^\alpha
\]

(165)

where \( u \) is the **Spectral Parameter** taking complex values, and \( \sigma^\alpha \) are Pauli matrices:

\[
\sigma^x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma^y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma^z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}
\]

(166)

which are related to the spin operators by \( S_n^\alpha = \frac{1}{2} \sigma^\alpha, \alpha \in \{x,y,z\} \).

Lax operators expressed in matrix form are:

\[
L_{n,a}(u) = \begin{pmatrix} u + i S_n^z & i S_n^- \\ i S_n^+ & u - i S_n^z \end{pmatrix}
\]

(167)

The **Permutation Operator**, which permutes the tensor product of vectors in \( \mathbb{C}^2 : \forall x, y \in V, P(x \otimes y) = y \otimes x \), is defined as:

\[
P_{n,a} = \frac{1}{2} \left( I_n \otimes I_a + \sum_{\alpha=x,y,z} \sigma_n^\alpha \otimes \sigma_a^\alpha \right) = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}
\]

(168)

It is trivially symmetric: \( P_{n,a} = P_{a,n} \), as when we are permuting two elements, it does not matter which one comes first.

The lax operator can be rewritten with respect to permutation operator:

\[
L_{n,a}(u) = \left( u - \frac{i}{2} \right) I_n \otimes I_a + iP_{n,a}
\]

(169)

Consider two lax operators \( L_{n,a_1} \) and \( L_{n,a_2} \) with auxiliary spaces \( V_{a_1} \) and \( V_{a_2} \). Their commutation relation can be established by an operator \( R_{a_1,a_2} : V_{a_1} \otimes V_{a_2} \rightarrow V_{a_1} \otimes V_{a_2} \) called **Quantum R-matrix** defined as:

\[
R_{a_1,a_2}(u_1, u_2) = u_1 I_{a_1} \otimes I_{a_2} + iP_{a_1,a_2} = \begin{pmatrix} u_1 + i & 0 & 0 & 0 \\ 0 & u_2 & i & 0 \\ 0 & i & u_2 & 0 \\ 0 & 0 & 0 & u_1 + i \end{pmatrix}
\]

(170)

The commutation relation of the Lax operators (also named **Fundamental Commutation Relation (FCR)**) is formulated as:

\[
R_{a_1,a_2}(u_1 - u_2)L_{n,a_1}(u_1)L_{n,a_2}(u_2) = L_{n,a_2}(u_2)L_{n,a_1}(u_1)R_{a_1,a_2}(u_1 - u_2)
\]

(171)

which can be easily checked by substituting in the lax operator and R-matrix (169) and (170) and making use of the commutation relation of permutation matrix:

\[
P_{n,a_1}P_{n,a_2} = P_{a_2,a_1}P_{n,a_1} = P_{n,a_2}P_{a_1,a_2}
\]

(172)

These can be proved easily by applying the operators to a test matrix \( m \otimes x \otimes y \) from \( V_n \otimes V_{a_1} \otimes V_{a_2} \). For example:

\[
P_{n,a_1}P_{n,a_2}(m \otimes x \otimes y) = P_{n,a_1}(y \otimes x \otimes m) = x \otimes y \otimes m
\]

\[
P_{a_1,a_2}P_{n,a_1}(m \otimes x \otimes y) = P_{a_1,a_2}(x \otimes m \otimes y) = x \otimes y \otimes m
\]

\[
\rightarrow P_{n,a_1}P_{n,a_2} = P_{a_1,a_2}P_{n,a_1}
\]

(173)

It should be noted that the FCR is only valid for Lax operators on the same site \( n \). Two Lax operators on different sites simply commute with each other because they are independent. The Lax operator \( L_{n,a} \) is interpreted as the transport from site \( n \) to site \( n + 1 \) along the spin chain.

We can construct product of a string of Lax operators to transport from site 1 to \( N + 1 \):
The monodromy matrix at $i \frac{1}{2}$ is thus:

$$T_{N,a}(i\frac{1}{2}) = i^N P_{N,a} ... P_{2,N}$$

The last step can be proved by induction using the easily verified property $P_j,a P_{j-1,a} = P_{j-1,j} P_{j,a}$ of permutation matrix.

Take the trace and we have transfer matrix at $i \frac{1}{2}$:

$$F_N(i\frac{1}{2}) = i^N P_{1,2} ... P_{N-1,N} tr_a[P_{N,a}]$$

$$= i^N P_{1,2} ... P_{N-1,N}$$

Differentiate $T_{N,a}$ with respect to $u$ at $u = i \frac{1}{2}$:

$$\frac{d}{du} T_{N,a}(u)|_{u=i\frac{1}{2}} = i^{N-1} \sum_n P_{N,a} ... P_{N+1,a} P_{N-1,a} ... P_{1,a}$$

same trick as (181)

$$= i^{N-1} \sum_n P_{1,2} ... P_{N-1,n+1} ... P_{N-1,N} P_{N,a}$$

Let us examine $F_N$ in the neighbourhood of $u = i \frac{1}{2}$. By the definition of the Lax operator (169):

$$L_{n,a}(i\frac{1}{2}) = iP_{n,a}$$

The commutative property of $F_N$ makes $Q_i$ commutative as well. So $F_N$ defines a family of commuting operators $Q_i$. We can show that the Hamiltonian is one of them, so that by diagonalising transfer matrix and computing its eigenstates, we automatically obtain the spectrum of the Hamiltonian. And along with it the spectrum of all conserved commuting charges $Q_i$. 

$F_N(u) = 2u^N + \sum_{l=0}^{N-2} Q_l u^l$

$F_N(u) = 2u^N + \sum_{l=0}^{N-2} Q_l u^l$
Hamiltonian (148) can be represented by a sum of permutation matrices as well:

$$\mathcal{H} = -\frac{J}{4} \sum_{\alpha=x,y,z} \sum_{n=1}^{N} \sigma_n^\alpha \sigma_{n+1}^\alpha$$

(186)\[ \quad (187) \]

Hence the Hamiltonian indeed can be constructed from the transfer matrix and is one of the commuting operators $Q_i$. This proves the integrability of our model.

Now let us find the eigenstates of the transfer matrix in order to solve for the energy spectrum. We start by substituting the explicit expressions of the R-matrix (170) and the monodromy matrix (175) into the commutation relation for the monodromy matrices (176):

$$\begin{bmatrix} u_1 - u_2 + i & 0 & 0 & 0 \\ i & u_1 - u_2 & i & 0 \\ 0 & 0 & 0 & u_1 - u_2 + i \\ 0 & i & u_1 - u_2 & 0 \end{bmatrix}$$

(188)

Carrying out the matrix multiplication on each side and equating two resulting matrices row by row, we obtain the commutation relations between operators $A_{N}$, $B_{N}$ and $D_{N}$:

$$B_{N}(u_1)B_{N}(u_2) = B_{N}(u_2)B_{N}(u_1)$$

(189)

$$A_{N}(u_1)B_{N}(u_2) = u_1 - u_2 - i \frac{B_{N}(u_2)A_{N}(u_1)}{u_1 - u_2} + i \frac{B_{N}(u_1)A_{N}(u_2)}{u_1 - u_2}$$

(190)

$$D_{N}(u_1)B_{N}(u_2) = u_1 - u_2 - i \frac{B_{N}(u_2)D_{N}(u_1)}{u_1 - u_2} - i \frac{B_{N}(u_1)D_{N}(u_2)}{u_1 - u_2}$$

(191)

From the form of the Lax operator (167), we can interpret the operator $B_{N}$ as the magnon creation operator (since it flips spin down). The algebraic Bethe Ansatz specifies the state of the system in terms of the spectral parameter:

$$|v_1, ..., v_M\rangle = B_{N}(v_1)...B_{N}(v_M)|0\rangle$$

(192)

where $|0\rangle$ is the ground state, in which all the spins are pointing upwards. In particular,

$$A_{N}(u)|0\rangle = \prod_{n=1}^{N} (u + iS^z_n)|0\rangle = (u + \frac{i}{2})^N|0\rangle$$

(193)

$$D_{N}(u)|0\rangle = \prod_{n=1}^{N} (u - iS^z_n)|0\rangle = (u - \frac{i}{2})^N|0\rangle$$

(194)

Now we want to find the eigenstate of the transfer matrix (which in turn is also the eigenstate of Hamiltonian) by acting it on the Ansatz state. This can be done component-wise by applying $A_{N}$ and $D_{N}$ respectively.

$$A_{N}(u_1)|v_1, ..., v_M\rangle = A_{N}(u_1)B_{N}(v_1)...B_{N}(v_M)|0\rangle$$

repetitively applying (190) and when $A_{N}$ reaches $|0\rangle$ use (193)

$$\left(u_1 + \frac{i}{2}\right)^N \prod_{n=1}^{M} \frac{u_1 - v_n - i}{u_1 - v_n} |v_1, ..., v_M\rangle$$

$$+ \sum_{n=1}^{M} \frac{i(v_n + \frac{i}{2})^N}{u_1 - v_n} \prod_{j=1, j \neq n}^{M} \frac{v_n - v_j - i}{v_n - v_j} |v_1, ..., v_M\rangle$$

(195)

Similarly,

$$D_{N}(u_1)|v_1, ..., v_M\rangle$$

$$\left(u_1 - \frac{i}{2}\right)^N \prod_{n=1}^{M} \frac{u_1 - v_n - i}{u_1 - v_n} |v_1, ..., v_M\rangle$$

$$- \sum_{n=1}^{M} \frac{i(v_n - \frac{i}{2})^N}{u_1 - v_n} \prod_{j=1, j \neq n}^{M} \frac{v_n - v_j + i}{v_n - v_j} |v_1, ..., v_M\rangle$$

(196)

Hence $|v_1, ..., v_M\rangle$ is an eigenstate of the transfer matrix $F_{N}(u_1) = A_{N}(u_1) + D_{N}(u_1)$ with the following eigenvalue:

$$\left(u_1 + \frac{i}{2}\right)^N \prod_{n=1}^{M} \frac{u_1 - v_n - i}{u_1 - v_n} + \left(u_1 - \frac{i}{2}\right)^N \prod_{n=1}^{M} \frac{u_1 - v_n - i}{u_1 - v_n}$$

(197)
When the other two terms cancel out, which means that:

\[
\sum_{n=1}^{M} \frac{i(v_n + \frac{i}{2})^N}{u_1 - v_n} \prod_{j=1,j\neq n}^{M} \frac{v_n - v_j - i}{v_n - v_j} \\
- \sum_{n=1}^{M} \frac{i(v_n - \frac{i}{2})^N}{u_1 - v_n} \prod_{j=1,j\neq n}^{M} \frac{v_n - v_j + i}{v_n - v_j} \\
\rightarrow \left[ \frac{v_n + \frac{i}{2}}{v_n - \frac{i}{2}} \right]^N = \prod_{j=1,j\neq n}^{M} \frac{v_n - v_j + i}{v_n - v_j - i}
\]

This is exactly the Bethe equations (163) we obtained using Bethe Ansatz. The spectral parameters are naturally identified with the rapidities. Having the eigenvalue of the transfer matrix in place, the energy spectrum of the Hamiltonian can be calculated by substituting it into (187).

### 4.2 Asymmetric Simple Exclusion Process (ASEP)

Now that we have presented how to use the Bethe Ansatz to solve the Heisenberg spin chain, we would like to apply the method again to get a better understanding of the Bethe wave functions, this time in the context of the Asymmetric Simple Exclusion Process, which is an example of Mass Transport Models that comprise of a class of dynamical lattice models, where mass (or particle) is transported stochastically from site to site.

**Simple Exclusion Process**, first introduced as an example of the interacting Markov process by [Spitzer (1970)](spitzer1970interacting), is a Markov process on \( \{0,1\}^N \), \( N \in \mathbb{Z}^+ \) on a one-dimensional lattice with at most one particle per site. Every particles waits an exponentially distributed amount of time to jump to its neighbouring site in the positive direction with probability \( p \) and to that in the negative direction with probability \( q \), provided the neighbouring site is vacant. For the case of \( p \neq q \), the process is called **Asymmetric Simple Exclusion Process (ASEP)** and there is a relative drift of the particle system towards the direction whose associated jumping probability is higher. If all particles are restricted to jump to the positive direction, then it is called **Totally Asymmetric Simple Exclusion Process** (TASEP).

#### 4.2.1 Bethe Ansatz for ASEP with Closed Boundaries

ASEP is the first and most explored application of the Bethe ansatz in one-dimensional stochastic processes [Derrida (1998)]. Consider a closed ASEP on a homogeneous ring of \( N \) particles and \( L \) sites, where they jump to vacant neighbouring sites on the left with rate \( p \) and on the right with rate \( q \). The configuration of the system can be specified by the positions of particles \( 1 \leq x_1, \ldots, x_N \leq L \). The equation of eigenstate of the system is:

\[
E \psi(x_1, \ldots, x_N) = p \sum_{i,x_{i-1}+1<x_i} \left[ \psi(x_1, \ldots, x_{i-1} - 1) - \psi(x_1, \ldots, x_N) \right] + q \sum_{i,x_{i-1}+1<x_i} \left[ \psi(x_1, \ldots, x_i + 1) - \psi(x_1, \ldots, x_N) \right] 
\]

(199)

Note that the summation is strictly over indices where the neighbouring sites are vacant.

- **Single Particle**

For \( N = 1 \), the equation of eigenstate becomes:

\[
E \psi(x) = p \psi(x - 1) + q \psi(x + 1) - (p + q) \psi(x)
\]

(200)

which is a linear recursive equation whose solution is in the form of \( \psi(x) = A z^x + B z^{-x} \). \( r = z \) are two roots of the characteristic equation \( qr^2 - (E + p + q)r + p = 0 \). The boundary condition is \( \psi(x + L) = \psi(x) \), which implies \( z^L = 1 \). So \( z \) has to be a root of unity. Since \( z_+ z_- = p/q \), for the asymmetric case \( p \neq q \), \( z_+ z_- > 1 \) or \( z_+ z_- < 1 \). Thus only one root can meet the boundary condition \( z^L = 1 \) and we neglect the other one. The general solution is thus:

\[
\psi(x) = Az^x, \quad z = e^{2k\pi i/L}, \quad i \in \mathbb{Z}
\]

(201)

This is a simply a plane wave with momentum \( 2k\pi/L \). Energy eigenvalue can be obtained by substituting the wave solution into (200):

\[
E = \frac{p}{z} + qz - (p + q)
\]

(202)

- **Two Particles**

For \( N = 2 \), we need to be aware of some jumps that are impossible without a vacant neighbouring site. If two particles are separated by at least one empty site, then there are no restrictions to their jumps and the equation of eigenstate is:

\[
E \psi(x_1, x_2) = p[\psi(x_1 - 1, x_2) + \psi(x_1, x_2 - 1)] + q[\psi(x_1 + 1, x_2) + \psi(x_1, x_2 + 1)] - 2(p + q) \psi(x_1, x_2)
\]

(203)

Since two particles jumps independently, the eigenstate can be written as a product of two plane waves:
\[ \psi(x_1, x_2) = A z_1^{x_1} z_2^{x_2} \]  

with the energy eigenvalue:

\[ E = E_1 + E_2 = p(z_1^{-1} + z_2^{-1}) + q(z_1 + z_2) - 2(p + q) \]  

If two particles are located adjacent (without loss of generality let \( x_2 = x_1 + 1 \)), the exclusion condition forbids two particles to jump towards each other. So the terms \( p[\psi(x_1, x_1) - \psi(x_1, x_1 + 1)] \) and \( q[\psi(x_1 + 1, x_1 + 1) - \psi(x_1, x_1 + 1)] \) have to cancel out, this gives us the cancellation boundary condition:

\[ p\psi(x_1, x_1) + q\psi(x_1 + 1, x_1 + 1) - (p + q)\psi(x_1, x_1 + 1) = 0 \]  

The equation of eigenstate only comprises of terms regarding two particles jumping away from each other:

\[ E\psi(x_1, x_1 + 1) = p\psi(x_1 - 1, x_1 + 1) + q\psi(x_1, x_1 + 2) - (p + q)\psi(x_1, x_1 + 1) \]  

The eigenstate cannot be obtained from two independent plane waves this time due to the exclusion condition. But from (205), we observe that the eigenvalue is invariant by a permutation \( z_1 \leftrightarrow z_2 \). There are two plane waves \( A z_1^{x_1} z_2^{x_2} \) and \( B z_1^{x_1} z_2^{x_2} \) corresponding to the same energy. So we try a linear combination of those two waves

\[ \psi(x_1, x_2) = A_{12} z_1^{x_1} z_2^{x_2} + A_{21} z_1^{x_1} z_2^{x_2} \]  

The coefficients \( A_{12} \) and \( A_{21} \) can be chosen to meet the cancellation condition. So we substitute (208) into (206) and get the following ratio of amplitudes:

\[ \frac{A_{21}}{A_{12}} = -\frac{qz_1 z_2 - (p + q)z_2 + p}{qz_1 z_2 - (p + q)z_1 + p} \]  

Now we impose the periodic boundary condition on the wave solution:

\[ \psi(x_1, x_2) = \psi(x_3, x_1 + L) \]
\[ A_{12} z_1^{x_1} z_2^{x_2} + A_{21} z_1^{x_1} z_2^{x_2} = A_{12} z_1^{x_1} z_2^{x_1 + L} + A_{21} z_2^{x_2} z_1^{x_1 + L} \]
\[ \Rightarrow A_{12} = A_{21} = z_2^{L} = z_1^{-L} \]  

Equating two expressions for the ratio of amplitudes and we obtain the Bethe equation for \( N = 2 \):

\[ z_1^{L} = -\frac{qz_1 z_2 - (p + q)z_1 + p}{qz_1 z_2 - (p + q)z_2 + p} \]
\[ z_2^{L} = -\frac{qz_1 z_2 - (p + q)z_2 + p}{qz_1 z_2 - (p + q)z_1 + p} \]  

By solving two Bethe equations with two unknowns, we are able to construct the solution to the eigenstate equation.

- Three Particles

For \( N = 3 \), the case where all three particles have vacant neighbouring sites and can jump independently is similar to the previous case in which the eigenstate is the product of three single-particle waves and the eigenvalue is the sum of three single-particle energies.

The adjacent case is more complicated. Consider first the Two-Particle Collisions where two particles are next to each other while the third one is far apart. This corresponds to two scenarios: \( x_1 \) and \( x_2 \) adjacent while \( x_3 \) apart \((x_1 = x < x + 1 = x_2 << x_3)\), and \( x_2 \) and \( x_3 \) adjacent while \( x_1 \) apart \((x_1 << x_2 = x < x + 1 = x_3)\). Cancellation conditions are again the terms corresponding to jumps of the adjacent particles towards each other:

\[ p\psi(x, x, x_3) + q\psi(x + 1, x + 1, x_3) - (p + q)\psi(x, x + 1, x_3) = 0 \]
\[ p\psi(x_1, x, x) + q\psi(x_1 + 1, x + 1, x) - (p + q)\psi(x_1, x + 1, x) = 0 \]  

Now consider Three-Particle Collisions, where all three particles are adjacent \((x_1 = x, x_2 = x + 1, x_3 = x + 2)\). The cancellation condition is:

\[ p[\psi(x, x, x + 2) + \psi(x, x + 1, x + 1)] \]
\[ +q[\psi(x + 1, x + 1, x + 2) + \psi(x, x + 2, x + 2)] \]
\[ -2(p + q)\psi(x, x + 1, x + 2) = 0 \]  

which can be seen as a linear combination of the two-particle collisions (212).

As discussed the eigenvalue for the case where all particles are located far away from each other is:

\[ E = E_1 + E_2 + E_3 \]
\[ = p(z_1^{-1} + z_2^{-1} + z_3^{-1}) + q(z_1 + z_2 + z_3) - 3(p + q) \]  

which is invariant if we permute the wave functions \( z_1 \leftrightarrow z_2 \leftrightarrow z_3 \).
So we try a Bethe wave function incorporating all the permutations of \( z_i \):

\[
\psi(x_1, x_2, x_3) = A_{123}z_1 z_2 z_3 + A_{132}z_1 z_3 z_2 + A_{213}z_2 z_1 z_3 + A_{231}z_2 z_3 z_1 + A_{312}z_3 z_1 z_2 + A_{321}z_3 z_2 z_1
\]

\[
= \sum_{\sigma \in \mathcal{S}_3} A_{\sigma} z_{\sigma(1)} z_{\sigma(2)} z_{\sigma(3)}
\]

(215)

Now we can fix ratios of amplitudes by the Two-Particle collisions. We say that ASEP can be decomposed into several two-particle collisions. Since all multi-particle collisions can be decomposed into several two-particle collisions, we say that ASEP can be diagonalised by the Bethe Ansatz.

In summary:

**Bethe Wave Function:**

\[
\psi(x_1...x_N) = \sum_{\sigma \in \mathcal{S}_N} A_{\sigma} z_{\sigma(1)}...z_{\sigma(N)}
\]

(216)

**Eigenvalues:**

\[
E = p \sum_{i=1}^N z_i^{-1} + 1 + \sum_{i=1}^N z_i - N(p + q)
\]

(217)

**Periodic Condition:**

\[
\psi(x_1, x_2...x_N) = \psi(x_2...x_N, x_1 + L)
\]

(218)

**Bethe Ansatz Equations:**

\[
z_i^L = (-1)^{N-1} \prod_{j=1, j\neq i}^N q z_i z_j - (p + q) z_i + p q z_i z_j - (p + q) z_j + p
\]

(219)

Interestingly, for the symmetric case \((p = q = \frac{1}{2})\), if we make the identification between the wave function \( z_i \) and the rapidity \( u_i \), which is introduced for the XXX\(1/2\) Heisenberg spin chain, by \( z_i = e^{u_i/2} \), then Bethe equations above become:

\[
\left[ u_i + i/2 \right]^L = (-1)^{N-1} \prod_{j=1, j\neq i}^N \frac{u_n - u_j + i}{u_n - u_j - i}
\]

(220)

which is exactly the Bethe equations (163) up to a constant term \((-1)^{N-1}\), depending on the parity of the number of particles. Hence we can expect that for odd number, particle jumps in the ASEP behave the same way as magnons in the Heisenberg spin chain, sharing same Bethe equations. While for even number, their behaviours are not trivial due to the extra minus sign in the Bethe equations.

### 4.2.2 Matrix Product Method for Stationary TASEP with Open Boundaries

TASEP with open boundaries can be solved by the matrix product method, but only in its stationary state [Derrida (1998)]. Clearly Bethe ansatz has an advantage in the possibility of solving for time-dependent quantities and is not limited to the stationary state. But we would still like to introduce the matrix method.

The configuration of TASEP with \( L \) sites and \( N \) particles is specified by associating value 1 to occupied sites and value 0 to empty sites. Let \( a_i \) denote the occupation number at site \( i \). Its evolution during a time interval \( dt \) is given by:

\[
a_i(t + dt) = \begin{cases} 
  a_i(t) & \text{with probability } (1 - 2dt) \\
  a_{i-1}(t) + a_i(t) - a_{i-1}(t)a_i(t) & \text{with probability } dt \\
  a_i(t)a_{i+1}(t) & \text{with probability } dt 
\end{cases}
\]

(221)

The first line corresponds to no interaction. The second line corresponds to particle interactions between sites \( i \) and \( i - 1 \). The third line corresponds to particle interactions between \( i \) and \( i + 1 \). It is easy to check that those rules satisfy the exclusion condition.

By taking the average we find the time evolution of the expectation of occupation number:

\[
\frac{d \langle a_i \rangle}{dt} = \langle a_{i-1} \rangle - \langle a_i \rangle - \langle a_{i-1}a_i \rangle + \langle a_ia_{i+1} \rangle
\]

(222)

In the case of open boundary, the evolution at boundary points have to be modified accordingly. Assume at site 1 particle enters with probability \( \alpha dt \) and at site \( N \) particle leaves with probability \( \beta dt \). The corresponding time evolutions of the average occupation number become:
\[
\frac{d(a_1)}{dt} = \alpha(1 - a_1) - \langle a_1(1 - a_2) \rangle
\]
\[
\frac{d(a_L)}{dt} = \langle a_L - 1(1 - a_L) \rangle - \beta(a_L)
\]

(223)

Now the stationary state PDF of a given configuration \(\{a_1, ..., a_L\} \) can be written as:

\[
P_{st}(a_1, ..., a_L) = Z^{-1} \langle W \prod_{i=1}^{L} a_i D + (1 - a_i) E \rangle V
\]

(224)

where \(D\) and \(E\) are matrices, where \(D\) appears whenever a site is occupied while \(E\) appears whenever a site is empty, and \(\langle W \rangle \) and \(|V|\) are vectors. \(Z\) is a normalisation factor given by:

\[
Z = \sum_{a_1=0,1} \sum_{a_L=0,1} \langle W \prod_{i=1}^{L} a_i D + (1 - a_i) E \rangle V
\]

\[
= \langle W \rangle (D + E)^L |V|
\]

(225)

[Derrida et al (1993)] showed that (224) and (225) do provide a valid description of the stationary state of the ASEP when the following rules are met:

\[
DE = D + E, \quad \langle W | E = \frac{1}{\alpha} \langle W |, \quad D | V = \frac{1}{\beta} | V
\]

(226)

Once stationary PDF is known, we can calculate all the stationary state properties. For example, the average occupation at site \(i\) is:

\[
\langle a_i \rangle = \sum_{a_1=0,1} \sum_{a_N=0,1} a_i P_{st}(a_1, ..., a_N)
\]

(227)

\[
= \frac{\langle W | (D + E)^{i-1} D (D + E)^{N-i} | V \rangle}{\langle W | (D + E)^N | V \rangle}
\]

4.3 Zero-Range Process (ZRP)

Zero-Range Process (ZRP) is also an example of the mass transport models, which is similar in configuration to the ASEP except each lattice site can hold an integer number of indistinguishable particles, not limited to only one particle. It was first introduced as an example of the interacting Markov processes by [Spitzer (1970)] as well.

Consider a one-dimensional lattice ring of \(L\) sites and \(N\) particles in total. The occupation number at each site \(i\) is \(n_i\). We assume a totally asymmetric homogeneous ZRP, where particles only jump to the right one step at a time to its nearest neighbour with jumping rates \(u(n)\) as a function of the number of particles at the site of departure but independent of the site itself. Note that the jumping rate \(u(n)\) here is the rate per all particles at departure site. The rate per one particle would simply be \(u(n)/n\).

- Factorised Stationary State

An important feature of the continuous-time ZRP is that its stationary state can be factorised into a product \([\text{Evans (2000)}]\). It means that the joint probability \(P(\{n_i\})\) of finding the system in the configuration \(\{n_i\}\) is given by a product of one-site factors \(f(n_i)\) (which is also called probability weight \(W\)):

\[
P(\{n_i\}) = \frac{1}{Z(L, N)} \prod_{i=1}^{L} f(n_i)
\]

(231)

where \(Z(L, N)\) is a normalisation term to make sure the probabilities of all the configurations sum up to one. \(f(n)\) is given by:

\[
f(n) = \begin{cases} 
\prod_{n=1}^{\infty} \frac{1}{n^{1/3}} & \text{for } n \geq 1 \\
1 & \text{for } n = 0
\end{cases}
\]

(232)

and determined up to a multiplicative constant. To prove this, we assume (231) and consider the fact that in the stationary state the probability current (17) for particles jumping out of a configuration is equal to the probability current for jumps into the configuration:
Here the Heaviside function, which is 1 for non-negative arguments and 0 for negative arguments, is to ensure that the jumps can only occur if there is at least one particle at the departure site. By equating summations on both sides component-wise we obtain:

\[
\sum_i \theta(n_i - 1)u(n_i)P(n_1..n_{i-1}..n_L) = \sum_i \theta(n_i - 1)u(n_i - 1 + 1)P(n_1..n_i-1 + 1, n_i - 1..n_L)
\]

\[\text{(233)}\]

Choose \(f(0) = 1\) and iterate

\[
\sum_{n} = \prod_{n=1}^{L} \frac{1}{u(n)} f(n-1)
\]

\[\text{(234)}\]

The factorisation (232) works for the case of the inhomogeneous ZRP as well, where the jumping rate is site-dependent.

\* Mapping to ASEP

An exact mapping from ZRP to ASEP can be constructed by considering the particles in the ZRP as empty sites in the ASEP.

The idea, as shown in figure 4.3(1), is to first refigure each vertical cluster of particles in the ZRP onto the one-dimensional lattice in the ASEP while add an empty site between two nearest horizontal clusters of particles. Note that the mapping changed the size of lattice from \(L\) to \(L + N\). This configuration can be further considered as a jump of empty site towards the opposite direction with the same jumping rate as the particle cluster, which depends on the number of particles in front. So particles can feel each other’s presence and this makes long-range interaction possible.

Just like ASEP, the integrability of ZRP with totally asymmetric dynamics can also be investigated by the Bethe ansatz method.

4.3.1 Continuous-Time ZRP with One Parameter

The Bethe solution of a totally asymmetric ZRP on a ring with continuous time steps can be determined with one parameter [Povolotsky (2004)], by solving the eigenvalue problem for the master equation in continuous time (14) of ZRP. It might be better categorised as a stochastic integrable models for the next section but we still include it here to demonstrate the use of the Bethe ansatz.

The probability \(P(n_1..n_L; t)\) for the occupation numbers \(n_1..n_L\) on \(L\) sites at time \(t\) obeys the master equation in continuous time (14):

\[
\frac{\partial P(n_1..n_L; t)}{\partial t} = \sum_{k=1}^{L} \left\{ u(n_k - 1 + 1)P(n_k-1 + 1, n_k - 1..n_L) - u(n_k)P(n_1..n_L; t) \right\}
\]

\[\text{(235)}\]

with periodic condition \(n_1 = n_{L+1}\). Remember \(u(n)\) is the jumping rate (transition rate) defined in (232).

It turns out that using the coordinates of \(N\) particles \(\{x_i\} = \{x_1..x_N\}\) to specify the system configuration instead of occupation numbers is easier for us to derive the analytical solution via Bethe ansatz. We do this by applying the Bethe ansatz to \(P^0(x_1..x_N; t)\) which is related to the solution of the master equation by \(P(x_1..x_N; t)\) by:

\[
P(x_1..x_N; t) = W(\{n_i\})P^0(x_1..x_N; t)
\]

\[\text{(236)}\]

where \(W(\{n_i\})\) is the weight given by the product factors in (231):

\[
W(\{n_i\}) = \prod_{i=1}^{L} f(n_i)
\]

\[\text{(237)}\]
\(P^0(x_1, x_N; t)\) is the solution to the master equation of a ZRP with non-interacting particles (also called free equation), which means that the jumping rate is independent of the occupation number.

**Two Particles**

Consider the case when \(N = 2\) and generalise to arbitrary \(N\). Without loss of generality we assume \(1 \leq x_1 \leq x_2 \leq L\) and define the jumping rate as follows:

\[
u(1) = 1 \quad \nu(2) = u\]

(238)

In the free equation, we set \(\nu(n) = 1\) for all \(n \geq 1\). Now we are going to show that the solution \(P^0(x_1, x_2; t)\) of the free equation is related to the solution \(P(x_1, x_2; t)\) to master equation of the ZRP by (236), provided the former satisfies some constraint, on which we will apply the Bethe ansatz and obtain the Bethe equations.

Since particles do not interact in the free equation, it is simply the master equation (235) with jumping rate 1, where the occupation numbers are replaced by the particle coordinates as arguments:

\[
\frac{\partial P^0(x_1, x_2; t)}{\partial t} = P^0(x_1 - 1, x_2; t) + P^0(x_1, x_2 - 1; t) - 2P^0(x_1, x_2; t)
\]

(239)

We need the free equation (242) to coincide with the following master equation of ZRP at \(x_1 = x_2 = x\):

\[
\frac{\partial P(x, x; t)}{\partial t} = P(x - 1, x; t) - uP(x, x; t)
\]

(243)

This can be achieved by redefining the unwanted term \(P^0(x, x - 1; t)\) to be the difference of (242) and (243):

\[
P^0(x, x - 1; t) = (u - 1)P^0(x, x; t) - (u - 2)P^0(x, x; t)
\]

(244)

This is the constraint we have for the solution to the free equation, in which we can use the Bethe ansatz to represent the eigenfunction:

\[
P^0(x_1, x_2; t) = e^{\lambda t}(A_{12}z_1^{-x_1}z_2^{-x_2} + A_{21}z_1^{-x_2}z_2^{-x_1})
\]

(245)

Compared with the Bethe ansatz (216), it has an extra term \(e^{\lambda t}\) in the wave function to allow for the time dependence. Substitute (245) into the free equation (239) and we find:

\[
\lambda = z_1 + z_2 - 2
\]

(246)

Substitute the ansatz (245) together with the relation (246) into the constraint (244) and we obtain the ratio of amplitudes:

\[
\frac{A_{12}}{A_{21}} = \frac{(2 - u) - (1 - u)z_2 - z_1}{(2 - u) - (1 - u)z_1 - z_2}
\]

(247)

Take this ratio into the cyclic boundary condition \(P^0(x_1, x_2; t) = P^0(x_2, x_1 + L; t)\) and we obtain the Bethe equations for \(N = 2\):

\[
z_1^{-L} = \frac{(2 - u) - (1 - u)z_2 - z_1}{(2 - u) - (1 - u)z_1 - z_2}
\]

(248)

\[
z_2^{-L} = \frac{(2 - u) - (1 - u)z_1 - z_2}{(2 - u) - (1 - u)z_2 - z_1}
\]

**N Particles**

The way we solve the two-particle ZRP can be generalised to arbitrary number of particles. Consider the configuration with two neighbouring coordinates \(x\) and \(x + 1\) having \(m\) and \(n\) particles respectively. The master equation corresponding to this part of the configuration in terms of coordinates is:
The master equation basically says that rate of change of a particular configuration is the difference of those transitioning into it and those transitioning out of it.

Transform this master equation in terms of free solution $P^0(x_1..x_N)$ by (236):

\[
\frac{\partial P^0(x_n, (x+1)^n, t)}{\partial t} = .. + u(n) \left[ P^0(x_n, (x+1)^n, t) - P^0(x_n, (x+1)^n, t) \right] + ..
\]

(250)

Since the jumping rate in (250) does not depend on the occupation number at departure site, we can set $m = 0$.

The free equation is this case is:

\[
\frac{\partial P^0(x_n, (x+1)^n, t)}{\partial t} = .. + \left[ P^0(x_n, (x+1)^n, t) - nP^0(x_n, (x+1)^n, t) \right] + 
\]

(251)

\[+ \sum_{j=2}^{n} P^0(x_n, (x+1)^{j-1}, t) + .. \]

where $\sum_{j=2}^{n} P^0(x_n, (x+1)^{j-1}, t)$ are the unphysical terms that go beyond our assumed domain of $x_i \leq x_{i+1}$. Those terms can be cancelled out by equating (250) and (251):

\[(u(n) - 1)P^0(x_n, (x+1)^n, t) - \sum_{j=2}^{n} P^0(x_n, (x+1)^{j-1}, t) = 0 \]

(252)

This is the constraint we obtain for the $N$-particle case. It can be verified to be reducible to (244) by setting $n = 2$.

We can further simplify (252) by applying the two-particle constraint to the unphysical term $P^0(x_n, (x+1)^n, t)$ in the summation and requiring the constraint hold for $u(n - 1)$:

\[(u(n) - 1)P^0(x_n, (x+1)^n, t) - \sum_{j=2}^{n} P^0(x_n, (x+1)^{j-1}, t) = 0 \]

(253)

and we obtain a recurrent formula for the jumping rates:

\[u(n) = 1 - (1 - u)u(n - 1) \quad \text{where} \quad u = u(2) \]

(254)

which can be solved in terms of the Q-Number:

\[u(n) = [n]_q = \frac{1 - q^n}{1 - q} \quad \text{where} \quad q = u - 1 \]

(255)

Hence the jumping rates of the continuous time ZRP can be defined by the q-number as the only parameter.

Q-number appears frequently in the Bethe ansatz solvable models such as Q-Boson Totally Asymmetric Diffusion Model, which is shown to be equivalent to the one-parameter ZRP [Sasamoto, Wadati (1998)], and has profound algebraic implications in relation to the fundamental Yang-Baxter equation.

Now we apply Bethe ansatz for the eigenfunction $P^0(x_1..x_N; t)$:

\[P^0(x_1..x_N; t) = e^{\lambda t} \sum_{\sigma \in S_N} A_{\sigma} \prod_{i=1}^{N} x_i^{-x_i} \]

(256)

Substitute the ansatz into the free equation (251) and we have a similar relation to (246) for the eigenvalue:

\[\lambda = \sum_{i=1}^{N} \zeta_i - N \]

(257)

The Bethe equations following from cyclic boundary conditions are thus generalised as:

\[\zeta_i - L = (-1)^{N-1} \prod_{j=1}^{N} \frac{(2 - u) - (1 - u)\zeta_j - \zeta_i}{(2 - u) - (1 - u)\zeta_i - \zeta_j} \]

(258)
4.3.2 Discrete-Time ZRP with Two Parameters

A Bethe solution to the ZRP with two-parametric jumping rates in discrete time steps, with the Parallel Update, which means that all particles jump simultaneously and not in a one-by-one fashion, has been studied by [Povolotsky, Mendes (2004)]. Bethe equations can be obtained by solving for the eigenfunctions and eigenvalues of the discrete master equation of the generating function of the distance travelled by particles.

Consider a totally asymmetric one-dimensional periodic ZRP with $L$ sites and $N$ particles that undergoes parallel update in discrete time steps. A particle jumps from an occupied site to the next one with probability $p(n)$, depending on occupation number $n$. Since time is discrete now, we use the jumping probability instead of the jumping rates to characterise the dynamics.

The configuration of the system changes as follows:

$$C = \{n_1, \ldots, n_L\} \rightarrow \{n_1 - k_2 + k_1, \ldots, n_L - k_1 + k_L\}$$

where $k_i \in \{0,1\}$ denotes the number of particles arriving at site $i$. All $k_i$ are independent of each other in parallel update. $k_i$ and $n_j$ can be connected in terms of the probability:

$$P(k_i = 1) = p(n_{i-1}), \quad P(k_i = 0) = 1 - p(n_{i-1})$$

The probability $P(C, t)$ for a system to be in configuration $C$ at time $t$ follows the discrete master equation (23):

$$P(C, t + 1) = \sum_{\{C'\}} T(C|C')P(C', t)$$

where $T(C|C')$ represents the transition probability from $C'$ to $C$. Similar to the factorised stationary state of ZRP in continuous time steps (231) (232), the discrete version of ZRP has also proven to factorisable into a product measure in the stationary state [Evans (1997)]:

$$P_{st}(n_1, \ldots, n_L) = \frac{1}{Z(L, N)} \prod_{i=1}^{L} f(n_i)$$

and the one-site factors are defined as:

$$f(0) = 1 - p(1)$$

$$f(n) = \frac{1 - p(1)}{1 - p(n)} \prod_{i=1}^{n} \frac{1 - p(i)}{p(i)}, \quad 1 \leq n \leq N$$

Now let us introduce the generating function of the total distance travelled by the particles:

$$F(C, t) = \sum_{Y=0}^{\infty} e^{\gamma Y} P(C, Y; t)$$

where $P(C, Y; t)$ is the joint probability of the system being in configuration $C$ while the total distance travelled by particles $Y(t) = Y$, at time $t$. For the case $\gamma = 0$, the generating function coincides with $P(C, t)$. $F(C, t)$ obeys a similar evolution equation to the discrete master equation (261):

$$F(C, t + 1) = \sum_{\{C'\}} e^{\gamma N(C|C')} T(C|C')F(C', t)$$

The term $e^{\gamma N(C|C')}$ accounts for the increase of total distance $Y(t)$, where $N(C|C')$ is the number of jumping particles during the transition from $C'$ to $C$.

The eigenfunctions $F_\Lambda$ of (265), where $\Lambda$ is the eigenvalue, satisfy the following equation:

$$\Lambda(\gamma)F_\Lambda(C) = \sum_{\{C'\}} e^{\gamma N(C|C')} T(C|C')F_\Lambda(C')$$

The evolution of generating function (265) can also be expressed in terms of $k_i$:

$$F(n_1 \ldots n_L; t+1) = \sum_{\{k_i\}} \prod_{i=1}^{L} e^{\gamma k_{i+1}} p(n_i - k_i + k_{i+1})^{k_{i+1}} \times (1 - p(n_i - k_i + k_{i+1})^{1-k_{i+1}}) \times F(n_i - k_i + k_2, \ldots, n_L - k_L + k_1; t)$$

where the total number of jumping particles is represented by the total number of particles arriving at each site $N = \sum_{i=1}^{L} k_{i+1}$. If a particle arrives at site $i + 1$, then it implies that there were $n_i - n_i + 1$ particles in total at site $i$ before jump, the corresponding probability is thus $p(n_i - k_i + 1)$. Similarly if there is no particle jumping to site $i + 1$, then the probability is $1 - p(n_i - k_i)$. Combine those two cases and we have $p(n_i - k_i + k_{i+1})^{k_{i+1}}(1 - p(n_i - k_i + k_{i+1})^{1-k_{i+1}}$ as the jumping probability for site $i+1$. The total probability $T$ can be obtained by multiplying across all sites.

In order to apply the Bethe ansatz, we look for solution of the form which is analogous to (236):

$$F(C, t) = P_{st}(C)F^0(C, t)$$
where \( P_{ni}(C) \) is the stationary probability defined in (262) and \( F^0(C, t) \) is the free generating function for the case of non-interacting particles (where jumping probability is independent of occupation number). Substitute (268) into (267):

\[
\prod_{i=1}^{L} f(n_i) F^0(n_1..n_L; t + 1) = \sum_{\{k_i\}} \left[ \prod_{i=1}^{L} \sum_{x} \gamma^{k_{i+1}} p(n_i - k_i + k_{i+1})^{k_{i+1}} \right] 
\]

(Continuing from (269)) Let \( n'_i = n_i - k_i + k_{i+1} \)

\[
\prod_{i=1}^{L} e^{\gamma^{k_{i+1}} p(n'_i)^{k_{i+1}} (1 - p(n'_i))^{1 - k_{i+1}} f(n'_i)} \times F(n_1 - k_1 + k_2, \ldots, n_L - k_L + k_1; t) 
\]  

(Continuing from (270)) Change \( n'_i \) back to \( n_i \),

\[
\prod_{i=1}^{L} e^{\gamma^{k_{i+1}} p(n_i)^{k_{i+1}} (1 - p(n_i))^{1 - k_{i+1}} f(n_i)} \times F(n_1 - k_1 + k_2, \ldots, n_L - k_L + k_1; t) 
\]

(Continuing from (271)) Cancel \( P_{ni}(n_1..n_L) \) on both sides

\[
F^0(n_1..n_L; t + 1) = \prod_{i=1}^{L} e^{\gamma^{k_{i+1}} p(n_i)^{k_{i+1}} (1 - p(n_i))^{1 - k_{i+1}}} \times F(n_1 - k_1 + k_2, \ldots, n_L - k_L + k_1; t) 
\]

(383) is the free equation whose eigenvalues are what we are striving to solve, provided the eigenfunctions are given by the Bethe ansatz. Now we change the representation of the system configuration from the occupation numbers to the particle coordinates, like we did for the continuous-time ZRP.

**Two Particles**

For the simplest case of two particles with coordinates \( 1 \leq x_1 \leq x_2 \leq L \), when \( x_1 \neq x_2 \), the eigen-equation of the motion follows that for non-interacting particles (272):

\[
\Lambda(\gamma) F^0(x_1, x_2) = e^{\gamma p} F^0(x_1 - 1, x_2) + e^{\gamma p} (1 - p) F^0(x_1 - 1, x_2) + F^0(x_1, x_2 - 1) + (1 - p)^2 F^0(x_1, x_2) 
\]

(273)

When \( x_1 = x_2 \), despite that two particles start interacting, the free equation (273) gives:

\[
\Lambda(\gamma) F^0(x, x) = e^{\gamma p} F^0(x - 1, x - 1) + e^{\gamma p} (1 - p) F^0(x - 1, x) + F^0(x, x - 1) + (1 - p)^2 F^0(x, x) 
\]

(274)

The term \( F^0(x, x - 1) \) is violating our assumption of \( x_1 \leq x_2 \) and so the free eigen-equation requires modification. The correct eigen-equation is:

\[
\Lambda(\gamma) F^0(x, x) = e^{\gamma p} F^0(x - 1, x) + (1 - p) F^0(x, x) 
\]

(275)

Note that in this case the jumping probability becomes \( p(2) \). We reconcile the difference between (274) and (275) by matching those two equation and find a constraint where the unphysical term \( F^0(x, x - 1) \) can be cancelled out, all by simple substitution:

\[
ar F^0(x, x) + b F^0(x, x - 1) + c F^0(x - 1, x) + d F^0(x - 1, x - 1) = 0 
\]

where \( a = e^{\gamma p} (1 - p)^2 \), \( b = e^{\gamma p} (1 - p) \), \( c = e^{\gamma p} (1 - p) - p(2) \), \( d = (1 - p)^2 \)

(276)

Now we make a Bethe ansatz of the eigenfunctions:

\[
F^0(x_1, x_2) = A_{12} z_1^{-x_1} z_2^{-x_2} + A_{21} z_1^{-x_2} z_2^{-x_1} 
\]

(277)

Substitute the Bethe eigenfunction into (275) and we obtain the eigenvalue:

\[
\Lambda(\gamma) = (e^{\gamma p_{x_1}} + (1 - p)) (e^{\gamma p_{x_2}} + (1 - p)) 
\]

(278)

Substitute the Bethe eigenfunction into the constraint (277) and we obtain the ratio of amplitudes:
\[ \frac{A_{12}}{A_{21}} = \frac{a + b z_1 + c z_2 + d z_1 z_2}{a + b z_2 + c z_1 + d z_1 z_2} \quad (279) \]

Now if we impose boundary condition on Bethe eigenfunction (277) and combine with (279), we recover two Bethe equations:

\[ z_1^{-N} = -\frac{a + b z_1 + c z_2 + d z_1 z_2}{a + b z_2 + c z_1 + d z_1 z_2} \quad (280) \]

\[ z_2^{-N} = -\frac{a + b z_2 + c z_1 + d z_1 z_2}{a + b z_1 + c z_2 + d z_1 z_2} \]

\* N Particles

The system with \( N \) particles can be treated similarly. The eigen-equation with non-interacting particles looks like this (we highlight the part corresponding to site \( n \)):

\[ \Lambda(\gamma) \Lambda(\sigma) = \sum_{\{k_i\}} \prod_{i=1}^{N} (e^{\gamma} p)^{k_i} (1-p)^{1-k_i} \times F_\Lambda(x_1-k_1,...,x_N-k_N) \quad (281) \]

In case of \( n \) particles on site \( x \), it becomes:

\[ \Lambda(\gamma) F_\Lambda^0(...x^n,\ldots) = \ldots \times \left[ \sum_{k_1=0}^{1} \ldots \sum_{k_n=0}^{1} (e^{\gamma} p)^{\sum_{i=1}^{n} k_i} (1-p)^{N-\sum_{i=1}^{n} k_i} \times F_\Lambda^0(...x-k_1,\ldots,x-k_N,\ldots) \right] \times \ldots \quad (282) \]

which contains many unphysical terms falling outside the domain of \( 1 \leq x_1 \leq \ldots \leq x_N \leq L \). We redefine those unwanted terms by matching the square bracket in the following corrected free equation:

\[ \Lambda(\gamma) F_\Lambda^0(...x^n,\ldots) = \sum_{\{k_i\}} \prod_{i=1,i\neq x}^{L} (e^{\gamma} p(u_i))^{k_i} (1-p(u_i))^{1-k_i} \times \left[ e^{\gamma p(n)} F_\Lambda^0(...,x-1),x^{n-1},\ldots \right] + (1-p(n)) F_\Lambda^0(...,x^n,\ldots) \quad (283) \]

It can be proved by induction that two terms can indeed be matched up to a \( N \)-particle constraint, which is reducible to the two-particle constraint (276). We assume the equality of two terms to hold for \( p(n-1) \) and require it also holds for \( p(n) \) (refer to a similar process (253)). This results in a recurrent relation between \( p(n) \) and \( p(n-1) \):

\[ p(n) = p + qp(n-1) \quad (284) \]

where \( q = \frac{p(2)}{p} - 1 \)

which can be solved in terms of q-number (255):

\[ p(n) = q \times [n]_q \quad (285) \]

\( p \) and \( q \) here are thus two parameters that characterise the jumping probabilities in the discrete-time ZRP.

Now we use Bethe ansatz to represent generating function:

\[ F_\Lambda^0(x_1,\ldots,x_N;\tau) = \sum_{\sigma \in S_N} A_\sigma \prod_{i=1}^{N} \sigma_a^{-\tau_a(i)} \quad (286) \]

Substitute it into (281) and we have the eigenvalue:

\[ \Lambda(\gamma) = \prod_{i=1}^{N} \left( e^{\gamma p z_i} + (1-p) \right) \quad (287) \]

By substituting the eigenfunction into the two-particle constraint equation and imposing periodic boundary conditions we obtain the generalised Bethe equations for \( N \) particles:

\[ z_i^{-N} = (-1)^{N-1} \prod_{j=1}^{N} \frac{a + b z_i + c z_j + d z_i z_j}{a + b z_j + c z_i + d z_i z_j} \quad (288) \]

4.3.3 Factorised Stationary States in Mass Transport Models

Mass transport models form a general class of lattice models in which mass is transferred stochastically between sites. ASEP and ZRP both belong to such kind of models. Remember that they both have the factorised stationary states. This has been proved not to be a coincidence. Factorised stationary states exist for a wide range of mass transport models provided some condition being satisfied [Evans et al (2004)]. Now we will derive the factorisation in a more general configuration setup than we did for the ASEP and the ZRP. Instead of having particles on a one-dimensional periodic lattice sites, we have mass \( m_i \) on each site \( i \) where the mass variable can take continuous values from 0 to total mass \( M \). The configuration is parallel updated from time \( t \) to \( t+1 \) by chopping off mass \( \mu_i \) from \( m_i \).
and move the chopped mass to \( m_{i+1} \), with the transition probability \( \phi(\mu_i|m_i) \).

The discrete master equation (23) for the unnormalised probability weights \( W(m_1, ..., m_L; t) \) adapted to this case is:

\[
W(m_1, ..., m_L; t + 1) = \prod_{i=1}^{L} \int_{0}^{\infty} d\mu_i \int_{0}^{m'_i} d\mu_i' \phi(\mu_i|m_i') \\
\times \left[ \prod_{j=1}^{L} \delta(m_j - m_j' + \mu_j - \mu_{j-1}) \right] \\
\times W(m'_1, ..., m'_L; t)
\]  

(289)

Notice that a delta function is added to the master equation to ensure the conservation of mass on each site. For instance, on site \( i \) a mass \( m_i' \) receives mass \( \mu_{j-1} \) from site \( i - 1 \) but loses mass \( \mu_i \) to site \( i + 1 \). The resulting mass \( m_i \) has to follow \( m_i' - \mu_i + \mu_{i-1} = m_i \).

The normalisation factor \( Z(M, L) \) is found by integrating the probability weights:

\[
Z(M, L) = \prod_{i=1}^{L} \int_{0}^{\infty} dm_i \delta \left( M - \sum_{i=1}^{L} m_i \right) W(m_1, ..., m_L; t)
\]  

(290)

Again the delta function makes sure the total mass is conserved. Since the normalisation factor is time independent, we can divide (289) by \( Z(M, L) \) and obtain the master equation for the normalised probability \( P(m_1, ..., m_L; t) \).

In the limit \( t \to \infty \), \( W(m_1, ..., m_L; t) \) approaches a stationary state and becomes time independent. Define a Laplace Transform as follows:

\[
G(s_1, ..., s_L) = \prod_{i=1}^{L} \int_{0}^{\infty} dm_i e^{-s_i m_i} W_{st}(m_1, ..., m_L)
\]  

(291)

Laplace transforming (289) at stationary state:

\[
G(m_1, ..., m_L) = \prod_{i=1}^{L} \int_{0}^{\infty} dm_i' \int_{0}^{m'_i} d\mu_i' \phi(\mu_i|m_i') \\
\times e^{-s_i (m'_i - \mu_i + \mu_{i-1})} W_{st}(m'_1, ..., m'_L)
\]  

(292)

Now assume the stationary state can be factorised:

\[
W_{st}(m_1, ..., m_L) = \prod_{i=1}^{L} f(m_i)
\]  

(293)

Take it into (291) and we can represent \( G \) as a factorisation:

\[
G(s_1, ..., s_L) = \prod_{i=1}^{L} g(s_i)
\]  

(294)

where \( g(s_i) = \int_{0}^{\infty} dm f(m) e^{-s_i m} \)

Substitute (293) and (294) into (292):

\[
\prod_{i=1}^{L} g(s_i) = \prod_{i=1}^{L} \left[ \int_{0}^{\infty} dm_i' f(m_i') \int_{0}^{m'_i} d\mu_i' \phi(\mu_i|m_i') \\
\times e^{-s_i (m'_i - \mu_i + \mu_{i-1})} \right]
\]  

(295)

Apply a change variable \( \sigma = m - \mu \), which physically means the mass that remains after chopping off, and define \( R(\mu, \sigma) \) to be:

\[
R(\mu, \sigma) = f(m) \phi(\mu|m)
\]  

(296)

(295) can be rewritten as:

\[
\prod_{i=1}^{L} g(s_i) = \prod_{i=1}^{L} \left[ \int_{0}^{\infty} \int_{0}^{s_i} d\mu_i d\sigma_i R(\mu_i, \sigma_i) \\
\times e^{-s_i (\sigma_i + s_{i+1} \mu_i)} \right]
\]  

(297)

Notice that we change the index of \( s_i \mu_{i-1} \) to \( s_{i+1} \mu_i \). This is possible because all terms on the right hand side of (297) are multiplied together and we can easily interchange \( e^{s_i \mu_{i-1}} \) with \( e^{s_{i+1} \mu_i} \) without causing problems.

A necessary and sufficient condition for (297) to have a solution can be shown to be:

\[
\int_{0}^{\infty} d\mu_i \int_{0}^{s_{i+1}} d\sigma_i R(\mu_i, \sigma_i) e^{-s_i \sigma_i - s_{i+1} \mu_i} = l(s_i)k(s_{i+1})
\]

where \( k(s)l(s) = g(s) \)

(298)

It is straightforward to go from (298) to (297). To prove the other way around, we can take logarithm of (297) and differentiate with respect to \( s_i \) and \( s_{i+1} \).
By Convolution Theorem, there exist two functions $v$ and $w$ such that we can express $f(m)$ as

$$f(m) = [v * w](m) = \int_0^m d\mu \, v(\mu)w(m - \mu)$$

(299)

Substitute into (294):

$$g(s) = \int_0^\infty dm \int_0^m d\mu \, v(\mu)w(m - \mu)e^{-sm}$$

$$\sigma = \mu - \mu \int_0^\infty d\sigma \int_0^\infty d\mu \, v(\mu)w(\sigma)e^{-s\sigma}e^{-s\mu}$$

(300)

$$= \left( \int_0^\infty d\sigma \, w(\sigma)e^{-s\sigma} \right) \left( \int_0^\infty d\mu \, v(\mu)e^{-s\mu} \right)$$

A direct identification can be made by compare (298) and (300):

$$l(s) = \int_0^\infty d\sigma \, w(\sigma)e^{-s\sigma}$$

(301)

$$k(s) = \int_0^\infty d\mu \, v(\mu)e^{-s\mu}$$

Take (301) into (298) and we find:

$$R(\mu, \sigma) = v(\mu)w(\sigma)$$

(302)

By inputing (299) and (302) into (296), we obtain the condition of the transition probability of the mass transport models to be factorised at stationary state (293):

$$\phi(\mu|m) = \frac{v(\mu)w(m - \mu)}{[v * w](m)}$$

(303)

$v$ and $w$ can be reversed to form a dual transition probability $\phi'$:

$$\phi'(\mu|m) = \phi(m - \mu|m) = \frac{w(\mu)v(m - \mu)}{[w * v](m)}$$

(304)

This Duality reverses the mass chopped off and the remaining mass, while preserves the stationary probability weight (293) (since convolution is commutative). If we further perform a Galilean transformation (shifting the lattice by one site) and a parity transformation ($i \leftrightarrow L + 1 - i$), then we can recover the original configuration.

The factorisation of stationary state serves as a crucial step in the derivation of three-parameter ZRP [Povolotsky (2013)], which shares some similarities with the one and two-parameter ZRPs but with more complicated mathematics.

5 Stochastic Integrable Models

It feels natural to continue our exploration of the dynamical systems with stochastic methods (such as master equations), which we have introduced in section 1 and briefly applied to ZRP in section 4, and extend the scope of the integrability to the stochastic realm. After all, probability is at the core of statistical mechanics and we are interested in the time evolution of the system while looking for the exact solution regarding its stationary behaviours as time goes to infinity. We begin the discussion by a simple example of one-dimensional Ising model to set up a theoretical background, and progress into the surface growth models to solve for their dynamical exponents. Then we go from discrete models to continuous universality class equations and introduce the KPZ equation, whose Hopf-Cole solutions can be found in terms of probability distribution.

5.1 One-Dimensional Stochastic Ising Model

The statistical study of the non-equilibrium dynamical systems has motivated theorists to develop simple mathematical models in order to better analyse the physical situation with the hope of obtaining exact solutions. Because there are no physical laws governing those systems. The Boltzmann-Gibbs law suitable for equilibrium systems loses power here. Of course in our adventure of constructing models, the unrealistic simplifications can cause problems in describing the physics, but the exact solutions we obtain are expected to compensate for it with deeper insights into the system. The Ising model has been successful in explaining the ferromagnetic phase transition, which we examined in previous sections. Since in non-equilibrium systems, the PDF undergoes changes constantly with time, we are interested in analysing the time dependent behaviours of the statistical systems and looking for exact solutions with the stochastic methods we studied earlier. Let us review an interesting paper by [Glauber (1963)] on one-dimensional stochastic Ising model whose time-dependent solutions can be computed exactly.

The model we discuss here is a stochastic form of Ising model, whose behaviours can be followed exactly as a function of time. It involves $N$ coupled particles whose spins are represented by the stochastic functions of time $\sigma_j(t)$ for $j \in \{1, ..., N\}$. The spins can only takes values from $\{1, -1\}$ and make transitions between the two values randomly. The transitions happen because of, for instance, an external heat bath applied to the spins. The transition probabilities are assumed to depend on the momentary values of neighbouring spins and also the heat bath. Since every spin is coupled
with its neighbours, we need to treat the whole spin chain as a unit. The spin functions define a Markov process of $N$ discrete random variables with continuous time. Then the behaviour of the system is described by the expectations of the spin functions and their products.

5.1.1 Single-Spin System

The simplest case is a system with only one spin. Its value is affected by the reservoir and thus flips randomly at a known rate. There is no magnetic field present so neither value of spin is preferred. The transition rate from either state to the other one is defined as $\alpha/2$. Applying the master equation (14) to this system we obtain:

$$\frac{dP(\sigma, t)}{dt} = \frac{1}{2}\alpha P(\sigma, t) + \frac{1}{2}\alpha P(-\sigma, t)$$  \hspace{1cm} (305)

The normalisation of the probabilities has to be satisfied at any time: $P(1, t) + P(-1, t) = 1$. Of course we can reduce the master equation to only one variable using the normalisation condition, but a more convenient choice to explore is the difference $q(t)$ of two probabilities, which turns out to be the expectation of the spin value:

$$q(t) = P(1, t) - P(-1, t) = \sum_{\sigma} \sigma P(\sigma, t) = \langle \sigma(t) \rangle$$  \hspace{1cm} (306)

The master equation (305) thus becomes:

$$\frac{dq(t)}{dt} = -\alpha q(t)$$  \hspace{1cm} (307)

with a solution of $q(t) = q(0)e^{-\alpha t}$. It shows that the mean value is always declining to zero regardless of the initial condition. Solve for $P(1, t)$ from (306) and we have:

$$P(\sigma, t) = \frac{1}{2} \left[ 1 + \sigma q(t) \right]$$  \hspace{1cm} (308)

5.1.2 Many-Spin System

In this model $N$ particles are arranged in an evenly spaced linear chain, which can also be closed to form a spin chain. As we mentioned already, the individual spins are not completely independent stochastic functions with time. They are correlated with the momentary values of their neighbouring spins. We consider the linear chain as a whole and introduce a set of $2^N$ probability functions $P(\sigma_1, ..., \sigma_N; t)$ for $\sigma_i \in \{1, -1\}$, $i \in \{1, ..., N\}$.

Let $T_j(-\sigma_j|\sigma_j)$ be the transition rate of $j$th spin flipping from $\sigma_j$ to $-\sigma_j$. The master equation (14) tells us that:

$$\frac{d}{dt}P(\sigma_1, ..., \sigma_N; t) = -\sum_j T_j(-\sigma_j|\sigma_j) P(\sigma_1, ..., \sigma_j, ..., \sigma_N; t)$$

$$+ \sum_j [T_j(\sigma_j|\sigma_j) P(\sigma_1, ..., -\sigma_j, ..., \sigma_N; t)]$$  \hspace{1cm} (309)

Note that since there are only two kinds of spins, we do not need to sum over $\sigma$ in the master equation. But remember that all of $N$ particles are seen as one unit, so we do have to sum over $j$ to reflect this unification.

In case of nearest neighbour interaction, the transition rates $T_j(-\sigma_j|\sigma_j)$ can be chosen to describe the tendency of spins to align themselves with their neighbours in this form:

$$T_j(-\sigma_j|\sigma_j) = \frac{1}{2}\alpha \left[ 1 - \frac{1}{2}\gamma \sigma_j(\sigma_{j-1} + \sigma_{j+1}) \right]$$  \hspace{1cm} (310)

which can only take on three values given all possibilities of $\sigma_{j-1}, \sigma_j$ and $\sigma_{j+1}$. When neighbouring spins are antiparallel (for example $|\uparrow \downarrow \downarrow \downarrow |$), the transition rate is $\frac{1}{2}\alpha$. For $\sigma_j$ parallel to both of its neighbours ($|\uparrow \uparrow \uparrow \downarrow |$), the transition rate takes $\frac{1}{2}\alpha(1 - \gamma)$. Similarly, for $\sigma_j$ antiparallel to both of its neighbours ($|\downarrow \downarrow \downarrow \downarrow |$), the transition rate takes $\frac{1}{2}\alpha(1 + \gamma)$. If $\gamma$ is positive, the parallel configuration is less likely to transit and hence more stable. We call it **Ferromagnetic** case. If $\gamma$ is negative, the antiparallel configuration is less likely to transit and we call it **Antiferromagnetic** case.

At the equilibrium state of the current model we are discussing, $\gamma$ actually quantitatively corresponds to the exchange coupling constant $J$ (the mutual energy aforementioned in the linear Ising model. The Hamiltonian for the linear Ising model, where only nearest neighbour interaction is assumed, is:

$$\mathcal{H} = -J \sum_j \sigma_j \sigma_{j+1}$$  \hspace{1cm} (311)

At the equilibrium state with temperature $T$ in the Ising model, $P_j(\sigma_j)$ is proportional to the **Maxwell-Boltzmann Factor** $\exp(-\mathcal{H}/kT)$. Hence the ratio of probabilities $P_j(-\sigma_j)$ and $P_j(\sigma_j)$ is simply:

$$\frac{P_j(-\sigma_j)}{P_j(\sigma_j)} = \frac{\exp\{-JkT\sigma_j[\sigma_{j-1} + \sigma_{j+1}]\}}{\exp\{JkT\sigma_j[\sigma_{j-1} + \sigma_{j+1}]\}}$$  \hspace{1cm} (312)

We can also write the exponentials in (312) in terms of hyperbolic functions:
tion rates are zero), the system reaches equilibrium where all spins other than $\sigma$ and is not considered the only coupling scheme for the Ising system. So let us break the probability function up into a form that contains the expectation values of interest.

$$
\exp \left\{ \pm \frac{J}{kT} \sigma_j (\sigma_{j-1} + \sigma_{j+1}) \right\}
$$

Checked for $\sigma_j \in \{\pm 1\}$

$$
= \cosh \left[ \frac{J}{kT} (\sigma_{j-1} + \sigma_{j+1}) \right] \pm \sigma_j \sinh \left[ \frac{J}{kT} (\sigma_{j-1} + \sigma_{j+1}) \right]
$$

= $\cosh \left[ \frac{J}{kT} (\sigma_{j-1} + \sigma_{j+1}) \right] \left\{ 1 \pm \sigma_j \tanh \left[ \frac{J}{kT} (\sigma_{j-1} + \sigma_{j+1}) \right] \right\}
$$

Checked for $\sigma_j \in \{\pm 1\}$

$$
= \cosh \left[ \frac{J}{kT} (\sigma_{j-1} + \sigma_{j+1}) \right] \left\{ 1 \pm \frac{1}{2} \sigma_j (\sigma_{j-1} + \sigma_{j+1}) \tanh \frac{2J}{kT} \right\}
$$

And (313) becomes:

$$
P_j(-\sigma_j) = \frac{1 - \frac{1}{2} \sigma_j (\sigma_{j-1} + \sigma_{j+1}) \tanh \frac{2J}{kT}}{1 + \frac{1}{2} \sigma_j (\sigma_{j-1} + \sigma_{j+1}) \tanh \frac{2J}{kT}}
$$

(314)

On the other hand, in the stochastic Ising model, with all spins other than $\sigma_j$ being held fixed (their transition rates are zero), the system reaches equilibrium where

$$
d\frac{dP_\sigma}{dt} = 0
$$

and by (309) we have:

$$
P_\sigma = \frac{T_j(-\sigma_j) |_{\sigma_j} T_j(\sigma_j) |_{-\sigma_j}}{1 - \frac{1}{2} \gamma \sigma_j (\sigma_{j-1} + \sigma_{j+1}) \tanh \frac{2J}{kT}}
$$

(315)

Now a clear correspondence can be seen between (314) and (315) by setting:

$$
\gamma = \tanh(2J/kT)
$$

(316)

It should be pointed out that this identification of $\gamma$ and $J$ is under the simplified assumption of transition rate (310) and is not considered the only coupling scheme for the Ising model.

• Decomposing Probability Function

The probability function $P(\sigma_1, ..., \sigma_N; t)$ contains the dynamics of all the individual spins, which exceeds the amount of information we want to know, since we are predominantly looking for the expectation values of the spins and products of the pairs of spins for the description of the system. So let us break the probability function up into a form that contains the expectation values of interest.

We define the expectation $q_j(t)$ of spin function $\sigma_j(t)$ the same way as we did for the single particle case (306):

$$
q_j(t) = \langle \sigma_j(t) \rangle = \sum_{\{\sigma\}} \sigma_j P(\sigma_1, ..., \sigma_N; t)
$$

(317)

The summation over $\{\sigma\}$ is carried out over a total of $2^N$ values of all the possible combinations of $\{\sigma_1, ..., \sigma_N\}$.

We also define the expectation of the products of spin functions $r_{j,k}(t)$ as:

$$
r_{j,k}(t) = \langle \sigma_j(t) \sigma_k(t) \rangle = \sum_{\{\sigma\}} \sigma_j \sigma_k P(\sigma_1, ..., \sigma_N; t)
$$

(318)

There is an interesting property of $r_{j,k}(t)$ that $r_{j,j}(t) = 1$ because $\sigma_j(t)^2 = 1$ always and the probability function is normalised.

An artificial function can be constructed to relate the probability function to the expectation values of the spins. Consider $\frac{1}{2}(1 + \sigma_j \sigma_j')$ in which $\sigma_j'$ is a value of $j$-th spin that we imagined, it could be of the same value to $\sigma_j$ could be not. $\frac{1}{2}(1 + \sigma_j \sigma_j')$ equals one for $\sigma_j = \sigma_j'$ and zero otherwise. Then we express probability by summing over all the spins $\sigma_j'$:

$$
P(\sigma_1, ..., \sigma_N; t)
$$

$$
= \sum_{\{\sigma\}} \frac{1}{2} (1 + \sigma_1 \sigma_1') \cdots \frac{1}{2} (1 + \sigma_N \sigma_N') P(\sigma_1', ..., \sigma_N'; t)
$$

(319)

This relation makes sense because the only non-zero term in this summation is where $\sigma_j = \sigma_j', j \in \{1, ..., N\}$ and the equation holds trivially. Expand the product using the definitions (317) and (318) and we find the first three terms:

$$
P(\sigma_1, ..., \sigma_N; t)
$$

$$
= \frac{1}{2^N} \left( 1 + \sum_{j} \sigma_j q_j(t) + \sum_{j \neq k} \sigma_j \sigma_k r_{j,k}(t) + ... \right)
$$

(320)

which is the expansion of probability function in terms of the expectation values of the spins. Since the function $1$ and $\sigma$ form a complete orthogonal basis for any function of $\sigma$, (320) is just such an expansion of $N$ independent variable $\sigma_j$. Looking back, (308) is an example for a single spin.

Reduced probability functions, where some individual or pair of spins are held fixed, are defined by a summation of the probability function over all possible values of spins except those fixed. They can also be expressed by $q_j(t)$ and $r_{j,k}(t)$ if the summation is carried out on (319):
\[
P_j(\sigma_j, t) = \sum_{\{\sigma \neq \sigma_j\}} P(\sigma_1, \ldots, \sigma_N; t)
= \frac{1}{2} \left[ 1 + \sigma_j q_j(t) \right]
\]
\[
P_{j,k}(\sigma_j, \sigma_k; t) = \sum_{\{\sigma \neq \sigma_j, \sigma_k\}} P(\sigma_1, \ldots, \sigma_N; t)
= \frac{1}{4} \left[ 1 + \sigma_j q_j(t) + \sigma_k q_k(t) + \sigma_j \sigma_k r_{j,k}(t) \right]
\tag{321}
\]

So by this construction when we are solving for the expectation of the spins, a systematic expansion of the probability function rolls out. How do we solve for those expectations? Remember that probability function satisfies master equation (309), let us multiply both sides of the master equation by \(\sigma_j\) and sum over all values of \(\sigma\). Note that here we break \(\sum_j\) into \(\sum_{j=k}\) and \(\sum_{j\neq k}\) for easier calculation.

\[
d\frac{d}{dt} q_k(t) = -\sum_{\{\sigma\}} \sigma_k T_k(-\sigma_k|\sigma_k) P(\ldots \sigma_k; \ldots; t)
- \sum_{\sigma_k} \sum_{j \neq k \{\sigma \neq \sigma_k\}} T_j(-\sigma_j|\sigma_j) P(\ldots \sigma_j; \ldots; t)
+ \sum_{\sigma_k} T_k(\sigma_k|-\sigma_k)|P(\ldots -\sigma_k; \ldots; t)
+ \sum_{\sigma_k} \sum_{j \neq k \{\sigma \neq \sigma_k\}} T_j(\sigma_j|-\sigma_j)|P(\ldots -\sigma_j; \ldots; t)
\]

Change \(\sigma_k\) into \(-\sigma_k\) in third term; second and fourth terms cancel

\[
= -2 \sum_{\{\sigma\}} \sigma_k T_k(-\sigma_k|\sigma_k) P(\ldots \sigma_k; \ldots; t)
= -2(\sigma_k(t)T_k(-\sigma_k(t)|\sigma_k(t)))
\tag{322}
\]

With the time evolution of the expectation of individual spin given, we are quite ready proceed to solve for the expectation by integrating this ODE either analytically or numerically. The time evolution of the expectation of pair of spins can be calculated in a similar way \((j \neq k)\):

\[
d\frac{d}{dt} r_{j,k}(t) = -2(\sigma_j(t)\sigma_k(t)|T_j(-\sigma_j(t)|\sigma_j(t))
+ T_k(-\sigma_k(t)|\sigma_k(t)))
\tag{323}
\]

If we assume that the transition rate takes the form of (310), then both (322) and (323) can be transformed into recursive systems of differential equations for the expectation values:

\[
d\frac{d}{dt} q_k(t) \tag{317} = -q_k(t) + \frac{1}{2} \gamma [q_{k-1}(t) + q_{k+1}(t)]
\tag{324}
\]

\[
d\frac{d}{dt} r_{j,k}(t) \tag{318} = -2r_{j,k}(t)
+ \frac{1}{2} \gamma [r_{j,k-1}(t) + r_{j,k+1}(t) + r_{j-1,k}(t) + r_{j+1,k}(t)]
\tag{325}
\]

In the following discussions, solving for the expectation values of spins by (324) and (325) will be of primary interest to us for analysing the spin system.

- **Infinite Ring**

  The recursive differential equation is easy to solve for the infinite spin chain \(N \to \infty\). We change the labelling of the spins so that it ranges over all the integers instead of only the positive integers. A generating function is constructed as:

\[
F(\lambda, t) = \sum_{k=-\infty}^{\infty} \lambda^k q_k(t)
\tag{326}
\]

In order to find the time evolution of this generating function, we multiply (324) by \(\lambda^k\) and sum over \(k \in \mathbb{Z}\):

\[
\frac{d}{dt} \sum_{k=-\infty}^{\infty} \lambda^k q_k(t) = -\sum_{k=-\infty}^{\infty} \lambda^k q_k(t)
+ \frac{1}{2} \gamma \left[ \lambda \sum_{k=-\infty}^{\infty} \lambda^{k-1} q_{k-1}(t) + \lambda^{-1} \sum_{k=-\infty}^{\infty} \lambda^{k+1} q_{k+1}(t) \right]
\tag{327}
\]

\[
\rightarrow \frac{d}{dt} F(\lambda, t) = -F(\lambda, t) + \frac{1}{2} \gamma (\lambda + \lambda^{-1})F(\lambda, t)
\]

The solution to this ODE is simply an exponential given the initial condition \(F(\lambda, 0)\):

\[
F(\lambda, t) = F(\lambda, 0) \exp \left\{ -\alpha t + \frac{1}{2} \gamma (\lambda + \lambda^{-1}) \alpha t \right\}
\tag{328}
\]

The solution can be represented by the Bessel functions of imaginary argument \([\text{Watson (1966)}]\):

\[
\exp \left[ \frac{1}{2} \pi \gamma (\lambda + \lambda^{-1}) \right] = \sum_{n=-\infty}^{\infty} \lambda^n I_n(x)
\tag{329}
\]

where \(I_n(x) = i^{-n} J_n(ix)\). We first consider the case where all the spin expectations vanish except for the spin at the origin \(q_k(0) = \delta_{k,0}\), which is equivalent to a single
spin case. So that later we can construct the general solution by linearly combining the results for all spins. This implies that \( F(\lambda, 0) = 1 \).

The generating function becomes:

\[
F(\lambda, t) = e^{-\alpha t} \sum_{k=-\infty}^{\infty} \lambda^k I_k(\gamma \alpha t) \quad (330)
\]

By comparing with (326) it can be seen that the spin expectations are given by:

\[
q_k(t) = e^{-\alpha t} I_k(\gamma \alpha t) 
\]

(331)

The general solution for the spin expectations can thus be obtained by linear superposition with initial conditions \( q_k(0) \):

\[
q_k(t) = e^{-\alpha t} \sum_{m=-\infty}^{\infty} q_m(0) I_{k-m}(\gamma \alpha t) 
\]

(332)

- **Finite Ring**

For a ring of arbitrary \( N \), we seek solutions to the time evolution of the spin expectation (324) in terms of the normal modes:

\[
q_k(t) = A \zeta^k e^{\nu t} 
\]

(333)

where \( A \) is a constant. Take this solution into (324) and we obtain a relation between \( \nu \) and \( \zeta \):

\[
\nu = \alpha \left[ 1 - \frac{1}{2} \gamma (\zeta^{-1} + \zeta) \right] 
\]

(334)

The closure of the particle ring requires that the solution (333) be \( N \)-periodic. So \( q_{k+N}(t) = q_k(t) \), which leads to \( \zeta^N = 1 \). There are \( N \) complex roots for this polynomial:

\[
\zeta_m = \exp \left( \frac{2\pi i m}{N} \right); \ m \in \{0, ..., N - 1\}
\]

(335)

The corresponding eigenvalues for \( \nu_m \) are:

\[
\nu_m = \alpha \left[ 1 - \gamma \cos \left( \frac{2\pi m}{N} \right) \right] 
\]

(336)

The mode functions \( \zeta^k = \exp(2\pi i m k / N) \) form a complete orthogonal basis on the ring. Thus the general solution to (324) can be written as a linear combination of basis:

\[
q_k(t) = \sum_{m=0}^{N-1} A_m e^{\frac{2\pi i m k}{N} - \nu_m t} 
\]

(337)

Particularly:

\[
q_k(0) = \sum_{m=0}^{N-1} A_m e^{\frac{2\pi i m k}{N}} 
\]

(338)

The constants \( A_m \) can be determined by the Fourier’s Trick using the value of \( q_k(0) \). Multiply both sides of (338) by \((s_n^k)^* = \exp(-2\pi i nk/N)\) and sum over \( n \in \{0, ..., N - 1\} \):

\[
\sum_{n=0}^{N-1} \exp \left( -\frac{2\pi in}{N} \right) q_k(0) = \sum_{m=0}^{N-1} A_m \sum_{n=0}^{N-1} e^{\frac{2\pi i (m-n) k}{N}} \\
= \sum_{m=0}^{N-1} A_m N \delta_{m-n,0} \\
= NA_n
\]

(339)

The general solution (337) expressed using the result we just derived for \( A_m \) is then:

\[
q_k(t) \overset{(336),(339)}{=} \frac{1}{N} \sum_{m,n} q_m(0) e^{\frac{2\pi i m (k-n)}{N} - \alpha \left[ 1 - \gamma \cos \left( \frac{2\pi m}{N} \right) \right]} \]

\[
= e^{-\alpha t} \frac{1}{N} \sum_{m,n} q_m(0) e^{\frac{2\pi i m (k-n)}{N}} \left[ e^{\frac{2\pi i \gamma t}{N} + e^{-\frac{2\pi i m}{N}}} \right] 
\]

(328)

\[
= e^{-\alpha t} \frac{1}{N} \sum_{m,n} q_m(0) e^{\frac{2\pi i m (k-n)}{N}} \sum_{j=-\infty}^{\infty} e^{\frac{2\pi i m j}{N}} I_j(\alpha \gamma t) 
\]

(340)

\[
= e^{-\alpha t} \frac{1}{N} \sum_{m,n} q_m(0) \sum_{j=-\infty}^{\infty} e^{\frac{2\pi i N (k-n+j)}{N}} I_j(\alpha \gamma t) 
\]

(328)

\[
= e^{-\alpha t} \frac{1}{N} \sum_{m,n} q_m(0) \sum_{j=-\infty}^{\infty} e^{\frac{2\pi i (m-n+j)}{N}} I_j(\alpha \gamma t) 
\]

let \( j = n-k-N \)

\[
= e^{-\alpha t} \frac{1}{N} \sum_{m,n} q_m(0) \sum_{j=-\infty}^{\infty} e^{\frac{2\pi i m}{N}} I_{n-k-N}(\alpha \gamma t) 
\]

(340)

\[
= e^{-\alpha t} \frac{1}{N} \sum_{m,n} q_m(0) \sum_{j=-\infty}^{\infty} I_{n-k-N}(\alpha \gamma t) 
\]

(340)

A consequence of the solution (340) is that the total magnetisation always decreases to zero exponentially. To see this, we sum up all the spin expectations along the ring at time \( t \) and compare with the initial total expectation:
particular, for differential equations (324) for the infinite ring with the spin at the origin frozen. Without loss of generality, consider permanent magnetisation in the linear Ising model.

When
\[ d \eta = 1 \]

hence makes them inhomogeneous. At equilibrium (that is the recursive solution
\[ \eta^2 \gamma^{-1} - 2 \gamma^{-1} \eta + 1 = 0 \]  

By solving this quadratic equation we can find two solutions, one \( \gamma^{-1}(1 + (1 - \gamma^2)^{1/2}) \) is always greater than 1 given \( |\gamma| \leq 1 \), which does not match the possible range of values the spin expectation can take from \([-1, 1]\). So the correct root is the other solution:

\[ n = \gamma^{-1}(1 - (1 - \gamma^2)^{1/2}) \]  

By substituting in \( \gamma \) for the static Ising model (316), we find the Short-Range Order Parameter of Ising model:

\[ \eta = \tanh \left( \frac{J}{kT} \right) \]  

The solution to the time dependent spin expectation (346) only constitutes a particular solution to the inhomogeneous system. To find the general solution we can add this particular solution to the solution (332) to the homogeneous system of equations where \( q_0(t) \) vanishes. The general solution to the homogeneous system can be obtained by using Method of Images so that the boundary condition \( q_0(t) = 0 \) is satisfied whenever we are modifying the system layout. Consider the requirement that \( q_0(t) = 0 \) splits the ring into two halves that do not interfere with each other. Assume a set of initial values on the positive half of the ring. This is bound to induce a polarisation at the origin. How do we keep the zeroth spin vanishing? We give a set of initial values to the negative half, only this time with opposite values. This will cancel out the influence of positive half on the origin and make sure \( q_0(t) = 0 \) at all times. The set of initial values chosen for the solution is \( q_k(0) - \eta^k \)

for positive half and opposite of that for negative half. The \( \eta^k \) is taken from the initial value to account for the effect of the polarisation cloud in the inhomogeneous system. So the general solution for \( k > 0 \) is:

\[ q_k = \eta^{|k|} \]

This solution suggests that the fixed spin at the origin induces spin on both sides and is surrounded by a \( \text{polarisation cloud\text{}} \). The expectation of the spin decreases exponentially as we go further away from the origin. For ferromagnetic case, the induced spins share the same direction with the fixed one. For antiferromagnetic case opposite sign. Take this solution to the difference equation (343) and we obtain a quadratic equation for \( \eta \):

\[
\begin{align*}
\sum_k q_k(t) & = e^{-\alpha t} \sum_k q_k(0) \sum_{s=-\infty}^{\infty} I_{n-k-Ns}(\alpha \gamma t) \\
& = e^{-\alpha t} \sum_{k=0}^{N-1} q_k(0) \sum_{j=-\infty}^{\infty} I_j(\alpha \gamma t) \\
& = e^{-\alpha(1-\gamma) t} \sum_{k=0}^{N-1} q_k(0)
\end{align*}
\]  

(341)

This indicates the magnetic property of the particle ring wears out over time and corresponds to the absence of the permanent magnetisation in the linear Ising model.

**• Infinite Ring with One Spin Fixed**

Now let us see how the spin system behaves with one of the spins frozen. Without loss of generality, consider the infinite ring with the spin at the origin fixed on value \( \sigma_0 = 1 \), which makes \( q_0(t) = 1 \). Then the recursive differential equations (324) for \( q_k(t) \) still holds for \( k \neq 0 \). In particular, for \( k = 1 \), we have:

\[
\frac{d}{d\alpha t} q_1(t) = -q_1(t) + \frac{1}{2} \gamma (1 + q_2(t))
\]  

(342)

The fact that the spin at the origin is fixed results in a constant \( \frac{1}{2} \gamma \) in the sequence of the differential equations and hence makes them inhomogeneous. At equilibrium (that is when \( \frac{d}{d\alpha t} q_k(t) \)), there is a non-vanishing solution satisfying the recursive solution

\[
q_k(t) = \frac{1}{2} \gamma \left[ q_{k-1}(t) + q_{k+1}(t) \right], \ k \neq 0
\]  

(343)

The solution to this linear Difference Equation can be written as:

\[
q_k = \eta^{|k|}
\]  

(344)

This solution suggests that the fixed spin at the origin induces spin on both sides and is surrounded by a “polarisation cloud”. The expectation of the spin decreases exponentially as we go further away from the origin. For ferromagnetic case, the induced spins share the same direction with the fixed one. For antiferromagnetic case opposite sign. Take this solution to the difference equation (343) and we obtain a quadratic equation for \( \eta \):

\[
\eta^2 - 2 \gamma^{-1} \eta + 1 = 0
\]  

(345)
5.1.3 Spin Correlation Function

Now we turn to the time evolution of the spin correlation functions (or **Instantaneous Spin Correlation Function** in the light that the two spins are taken at the same time), which are described by (325). In order to simplify the problem and get an easier insight into the behaviour of the system, we first assume the initial state of the system is translationally invariant, which means that we know all the spins states equally well and only the distance between two spins matter in determining their correlation. So \( r_{j,k}(0) \) only depends on \( j-l \). Let us define an abbreviation \( r_{j-k} \) of \( r_{j,k} \). By (325) we have:

\[
\frac{d}{dt} r_m(t) = -2r_m(t) + \gamma (r_{m-1}(t) + r_{m+1}(t)), \quad m \neq 0
\]

\[
r_0(t) = 1
\]

(349)

This is precisely the one-spin-fixed problem we have dealt with in previous part. The correlation can be solve for in exactly the same way as for expectation. The general time dependent solution for correlation functions when \( m > 0 \) can then be constructed according to (348):

\[
r_m(t) = \eta^{|m|} + e^{-2\alpha t} \sum_{l=1}^{\infty} (r_l(0) - \eta^l)(I_{m-l}(2\gamma\alpha t) - I_{m+l}(2\gamma\alpha t))
\]

(350)

An example where this formula is applicable is a sudden change of temperature to the spin system from \( T_0 \) to \( T \). Then by (347) the initial values are \( r_l(0) = \tanh(\frac{\mu}{T_0})^l \) and \( \eta = \tanh(\frac{\mu}{T}) \). Then we can calculate the any spin correlation after the temperature change by using this formula.

Now we return to solving the two-index system of differential equations (325) without the assumption of the transational invariance. The system is inhomogeneous because of the condition \( r_{j,j} = 1 \). The equilibrium solution \( r_{k,l} = \eta^{|k-l|} \) can be used as a particular solution to the inhomogeneous system. We also need a general solution to the homogeneous system characterised by \( r_{k,k} = 0 \) as a compliment. Now let us ignore the boundary condition on \( r_{k,k} \) and solve (325) analogous to what we did for \( q_k(t) \) by introducing a two-parameter generating function \( F_r(\lambda, \xi, t) = \sum_{l=1}^{\Lambda} \lambda^l \xi^l r_{k,l}(t) \). The initial condition is given by the vanishing of all spins except \( r_{l,m}(0) \), \( l > m \).

\[
r_{j,k}(0) = \delta_{j,l}\delta_{k,m}
\]

(351)

The solution for \( r_{j,k}(t) \) is similar to (331):

\[
r_{j,k}(t) = e^{-2\alpha t} I_{j-l}(\gamma\alpha t) I_{k-m}(\gamma\alpha t)
\]

(352)

Then we supplement the solution with the requirements for initial values and boundary conditions by linear combination and method of images. Only this time the method of images is applied to a matrix \( r_{j,k} \) instead of a linear sequence \( q_k \). The matrix \( r_{j,k} \) is symmetric because the correlation between two spins should remain regardless of which one we put first. But in order to meet the boundary condition \( r_{j,j}(t) = 0 \), we regard it as antisymmetric. We fix the initial values of matrix elements \( r_{j,k}(0), j > k \), which are half of the matrix below diagonal. To make the diagonal elements all zero, we need the elements above the diagonal \( r_{k,j}, j > k \) to take on the opposite initial values. So that the influence of polarisation induced by the upper matrix elements is balanced out. Also remember to take out the \( \eta^{|l-m}| \) terms from the initial conditions in the general solution to adjust for the inhomogeneity.

Now we are ready to superpose the general solution of the spin correlation function with the particular solution, the modified initial conditions and the general solution for homogeneous system following the logic of (348):

\[
r_{j,k}(t)
= \eta^{|j-k|} + e^{-2\alpha t} \sum_{l=1}^{\infty} (r_l(0) - \eta^l)(I_{j-l}(\gamma\alpha t) - I_{j+l}(\gamma\alpha t))
\]

\[
+ e^{-2\alpha t} \sum_{l=1}^{\infty} (-1)(r_l(0) - \eta^l)(I_{k-l}(\gamma\alpha t) - I_{k+l}(\gamma\alpha t))
\]

\[
\times (I_{j-l}(\gamma\alpha t) I_{k-l}(\gamma\alpha t) - I_{j+l}(\gamma\alpha t) I_{k+l}(\gamma\alpha t))
\]

(353)

### Time-Delayed Spin Correlation Function

As we have explained in the spin system with one spin fixed, the spin at the origin at a given instant can induce a polarisation on the neighbouring spins, not immediately, but after a finite time interval. Hence we decide to analyse the correlation function between two spins separated across a time interval \([t,t+t']\). More technically, the function \( \langle \sigma_j(t)\sigma_k(t+t') \rangle \) : the expectation value of the product of stochastic spin functions \( \sigma_j \) evaluated at \( t \) and \( \sigma_k \) evaluated at \( t+t' \), which we call **Time-Delayed Correlation Function**.

Let spin values at time \( t \) be \( \sigma_1, ..., \sigma_N \) with the probability function \( P(\sigma_1, ..., \sigma_N; t) \) (which satisfies the master equation) and the spin values at time \( t + t' \) be \( \sigma'_1, ..., \sigma'_N \). Since the spin values at time \( t \) are assumed to be known and
regarded as the initial values, we will use conditional probability $P(\sigma_i', ..., \sigma_N'; t + t'|\sigma_i, ..., \sigma_N; t)$ for calculating spin values $\sigma_i', ..., \sigma_N'$.

Hence the correlation function can be found using a slightly different version of (318):

$$\langle \sigma_j(t)\sigma_k(t + t') \rangle = \sum_{\{\sigma\},\{\sigma'\}} \sigma_k' P(\sigma_i, ..., \sigma_N; t)P(\sigma_i', ..., \sigma_N'; t + t'|\sigma_i, ..., \sigma_N; t)$$

(354)

The summation over $\{\sigma'\}$ can be thought of as the spin expectation with the initial values of $q_k(0) = \sigma_k$:

$$\sum_{\{\sigma'\}} \sigma_k' P(\sigma_i', ..., \sigma_N'; t + t'|\sigma_i, ..., \sigma_N; t) = q_k(t')$$

(355)

For an infinite chain, $q_k(t')$ has been calculated to be (332):

$$q_k(t') = e^{-\alpha t'} \sum_{m=-\infty}^{\infty} \sigma_m I_{k-m}(\gamma \alpha t')$$

(356)

Substitute (355) and (356) into (354):

$$\langle \sigma_j(t)\sigma_k(t + t') \rangle = e^{-\alpha t'} \sum_{m=-\infty}^{\infty} I_k-m(\gamma \alpha t') \sum_{\{\sigma\}} \sigma_j \sigma_m P(\sigma_i, ..., \sigma_N; t)$$

(357)

Make another observation that the summation over $\{\sigma\}$ is the instantaneous correlation function $r_{j,m}(t)$ defined by (318). Hence the time delayed correlation function reduces to:

$$\langle \sigma_j(t)\sigma_k(t + t') \rangle = e^{-\alpha t'} \sum_{m=-\infty}^{\infty} I_k-m(\gamma \alpha t') r_{j,m}(t)$$

(358)

The expression for $r_{j,m}(t)$ equation (353) can also be inserted to output a really sophisticated looking result:

$$\langle \sigma_j(t)\sigma_k(t + t') \rangle$$

$$= e^{-\alpha t'} \sum_{m=-\infty}^{\infty} I_k-m(\gamma \alpha t') r_{j,m}(t)$$

$$= e^{-\alpha t'} \sum_{m=-\infty}^{\infty} I_k-m(\gamma \alpha t') \left\{ \eta^{j-m} + e^{-2\alpha t} \sum_{l>v} (r_{l,v}(0) - \eta^{l-v}) \right\}$$

$$\times (I_{j-l}(\gamma \alpha t) I_{m-l}(\gamma \alpha t) - I_{m-l}(\gamma \alpha t) I_{j-l}(\gamma \alpha t))$$

(359)

### 5.1.4 Spin Chain with Magnetic Field

Now with all the technical details of the spin system in hand, we are ready to apply an external magnetic field, which is parallel to the axis of spin, to the spin system. Let us start from the simplest single spin system where the transition rate from $\sigma$ to $-\sigma$ is set to be:

$$T(-\sigma|\sigma) = \frac{1}{2} \alpha (1 - \beta \sigma)$$

(360)

At stochastic equilibrium we have (315):

$$\frac{P(-\sigma)}{P(\sigma)} = \frac{T(-\sigma|\sigma)}{T(\sigma|-\sigma)} = \frac{1 - \beta \sigma}{1 + \beta \sigma}$$

(361)

The Hamiltonian for the single spin in the magnetic field is:

$$\mathcal{H} = -\mu B \sigma$$

(362)

where $\mu$ is the magnetic moment associated with spin and $B$ is the magnetic field. They correspond to the magnetic energy $H$ in previous section by $H = \mu B$.

Statistical mechanics tell us that probability function is proportional to Maxwell-Boltzmann factor $\exp(-H/kT)$ at equilibrium:

$$\frac{P(-\sigma)}{P(\sigma)} = \frac{\exp\{-(\mu B/kT)s\}}{\exp\{\mu B/kT\sigma\}}$$

(363)

$$= \frac{1 - \sigma \tanh(\mu B/kT)}{1 + \sigma \tanh(\mu B/kT)}$$

By correspondence of (361) and (363) we have:

$$\beta = \tanh(\mu B/kT)$$

(364)

The time evolution of the spin expectation is given by (322):

$$\frac{d}{dt} q(t) = -2\{\sigma T(-\sigma|\sigma)\} = -2\left\{ \frac{\sigma}{2} - \frac{1}{2} \beta \sigma^2 \right\}$$

(365)

The magnetic field in the Ising model is treated to be constant but in our stochastic model $\beta$ is free to be time
dependent whenever the magnetic field depends on time, both related by (364).

The solution for the spin expectation is computed via directly integrating (365) from $t_0$ to $t$ by introducing an integrating factor:

$$q(t) = q(t_0)e^{-\alpha(t-t_0)} + \int_{t_0}^{t} e^{-\alpha(t-t')}\alpha \tanh(\mu B(t')/kT)dt'$$

(366)

Then we proceed to a system of spins in a magnetic field. The Hamiltonian of the Ising model is:

$$\mathcal{H} = -\mu B \sum_m \sigma_m - J \sum_m \sigma_m \sigma_{m+1}$$

(367)

The second summation again indicates that only interaction between the nearest neighbours is possible in the model.

If all spins other than $\sigma_j$ are fixed, then when calculating the ratio of equilibrium probabilities, terms regarding all spins except $\sigma_j$ cancel out and we have:

$$P_j(-\sigma_j)/P_j(\sigma_j) = \exp\left(-\frac{1}{kT}J(\sigma_{j-1} + \sigma_{j+1}) + \mu B\right)$$

(312)

$$= \frac{T_j(-\sigma_j|\sigma_j)}{T_j(\sigma_j|-\sigma_j)} \exp\left[-\frac{\mu B}{kT} \sigma_j\right]$$

(313)

Let $T'_j(-\sigma_j|\sigma_j)$ be the transition rate for the spin chain in a magnetic field.

$$\frac{T'_j(-\sigma_j|\sigma_j)}{T'_j(\sigma_j|-\sigma_j)} = \frac{T_j(-\sigma_j)}{P_j}$$

$$= \frac{T_j(-\sigma_j|\sigma_j)}{T_j(\sigma_j|-\sigma_j)} \exp\left[-\frac{\mu B}{kT} \sigma_j\right]$$

(314)

$$= \frac{T_j(-\sigma_j|\sigma_j)}{T_j(\sigma_j|-\sigma_j)} \left[1 - \sigma_j \tanh(\mu B/kT)\right]$$

(315)

(316)

The first step in (316) is related by the master equation in our stochastic model while the second step is derived using the Hamiltonian of the Ising model. In order for our stochastic model to approach the same equilibrium as the Ising model, the two steps have to be matched and we choose:

$$T'_j(-\sigma_j|\sigma_j) = T_j(-\sigma_j|\sigma_j)\left[1 - \sigma_j \tanh(\mu B/kT)\right]$$

(317)

$$= T_j(-\sigma_j|\sigma_j)\left[1 - \sigma_j \mu B/kT\right]$$

(318)

$$= \frac{1}{2} \left[1 - \beta \sigma_j + \frac{1}{2}(\beta - \sigma_j)(\sigma_{j-1} + \sigma_{j+1})\right]$$

(319)

The time evolution of the spin expectation in a magnetic field can then be found by substituting the result for the transition rate into (322):

$$\frac{d}{dt} q_m(t) = -q_m(t) + \frac{1}{2} \gamma [q_{m-1}(t) + q_{m+1}(t)]$$

(320)

$$+ q_{m+1}(t) - \frac{1}{2} \beta \gamma [r_{m-1,m}(t) + r_{m,m+1}(t)]$$

(321)

This differential equation looks particularly difficult to solve for exact solutions but not so in the limit of the weak magnetic fields where $\mu B << kT$. In the weak-field limit, $\mu B/kT$ and the correlation functions $r_{m-1,m}$ and $r_{m,m+1}$ can be found by the zeroth approximation (ignore the summation) in their general expressions (353) : $r_{m-1,m} = r_{m,m+1} = \eta$. That is when the system is in thermal equilibrium to zeroth order of $B$, in other words, the magnetic field only induces small discrepancy from equilibrium.

With those simplifications, (320) reduces to:

$$\frac{d}{dt} q_m(t) = -q_m(t) + \frac{1}{2} \gamma [q_{m-1}(t) + q_{m+1}(t)] + \frac{\mu B(t)}{kT}(1 - \gamma \eta)$$

(322)

$$= -q_m(t) + \frac{1}{2} \gamma [q_{m-1}(t) + q_{m+1}(t)] + \frac{\mu B(t)}{kT}(1 - \gamma \eta)$$

(323)

The differential equation (323) differs from (324) only by an inhomogeneous term $\frac{\mu B(t)}{kT}(1 - \gamma \eta)$. So the general solution is made up of the general solution to the homogeneous equation (332) plus a particular solution corresponding to the extra term. Here we choose a particular solution independent of spin index $k$, corresponding to (324) when the spin expectation stabilises with respect to the spin index:

$$\frac{d}{dt} q(t) = (\gamma - 1)q(t) + \frac{\mu B(t)}{kT}(1 - \gamma \eta)$$

(324)

which can be integrated directly to give the particular solution $q(t) = \frac{\mu B(t)}{kT(1 - \gamma \eta)} \int_{t_0}^{t} e^{-\alpha(1-\gamma)(t-t')}B(t')dt'$. Thus the general solution to the inhomogeneous equation is:
when the magnetic field is applied at solution to the particular solution.

of \( t \) into (376):

\[
q(t) = e^{-\alpha(t-t_0)} \sum_i q_i(t_0) I_{k-i} \gamma \alpha(t-t_0)
\]

\[+
\frac{\mu}{kT} \frac{1 - \eta^2}{1 + \eta^2} \int_0^t e^{-\alpha(1-\gamma)(t-t')} B(t') d\alpha d't'
\]

(374)

Since the model is assumed to be in thermal equilibrium when the magnetic field is applied at \( t_0 \), the initial values of \( q_i \) can be considered vanishing. This kills the general solution to homogeneous system and reduces the general solution to the particular solution.

Define the **Stochastic Magnetisation Function**:

\[M(t) = \mu \sum_m \sigma_m(t)\]

(375)

whose expectation value is given by:

\[\langle M(t) \rangle = \mu \sum_m q_m(t)\]

(376)

In order to make the calculation easier, we let initial time \( t_0 \) extend back to negative infinity. Substitute (374) into (376):

\[\langle M(t) \rangle = \mu^2 N \frac{1 - \eta^2}{1 + \eta^2} \int_{-\infty}^t e^{-\alpha(1-\gamma)(t-t')} B(t') d\alpha d't'\]

(377)

For the case of a harmonically varying magnetic field \( B(t) = \chi(\omega) B_0 e^{-i\omega t} \), the complex valued **Magnetic Susceptibility** is computed by:

\[\langle M(t) \rangle = \chi(\omega) B_0 e^{-i\omega t}\]

(378)

The susceptibility is then:

\[
\chi(\omega) \equiv \mu^2 N \frac{1 - \eta^2}{1 + \eta^2} \int_0^\infty e^{-[\alpha(1-\gamma) - i\omega] \Delta t} d\alpha d(\Delta t)
\]

(379)

\[
= \frac{\mu^2 N}{kT} \frac{1 - \eta^2}{1 + \eta^2} \frac{\alpha}{\alpha(1-\gamma) - i\omega}
\]

In the low frequency limit \( \omega \to 0 \), we have \( \chi(0) = \frac{\mu^2 N}{kT} \frac{1 + \eta^2}{1 - \eta^2} \).

The one-dimensional stochastic Ising model can be mapped onto a surface growth model and provide a theoretical framework to solving the latter problem.

### 5.2 Two-Dimensional Surface Growth Models

The evolution of the interface between two phases of matter, for example the crystal growth or the bacterial colonies, has been displaying many interesting behaviours and is relevant to the studies of the exactly solved models. The kind of model in consideration is a two-dimensional strip of particles where new particles falls from above vertically, and deposit onto the existing strip in a tetris fashion, while old particles detach from the strip and evaporate. As we can imagine, this kind of surface growth will exhibit large fluctuations in terms of the height of particle strip. The calculation and characterisation of those fluctuations in long time limit, when the surface evolution becomes stationary, will be at the core of our research. Given the highly stochastic nature of the model, we choose to characterise the surface with **Critical Exponents**, which are the scaling dimensions of macroscopic quantities. Two such exponents are particularly important and have been shown by Monte Carlo simulations of the Eden process to be sufficient in describing the surface evolution models [Plischke, Racz (1985)]. They are **Static Critical Exponent** \( \eta \), which determines the scaling of time-independent quantities such as the Width of the Active Zone \( \zeta \), and **Dynamic Critical Exponent** \( z \), which specifies the scaling of the characteristic time scale \( \tau \) that the system requires to reach stationary-state fluctuations. The width of active zone, which is proportional to the magnitude of fluctuations on the surface, scales with the horizontal linear size \( L \) of the strip as \( \zeta \sim L^{1.2} \). The time scale is related to the linear size as \( \tau \sim L^z \). We also make the hypothesis that \( \eta \) and \( z \) to be universal within a certain class of growth models, meaning that the exponents only depend on the intrinsic features of the systems such as dimensionality, symmetries of stationary state and equation of motion. Growth models are categorised into different **Universality Classes** according to their exponents. One of the perks of the universality is that in order to determine the critical exponents in a certain class, we only have to study a simple model in the class instead of a hard one. We will go through a few random deposition models in this section [Liu, Plischke (1988)]. Their analytical results will be compared with the empirical results from numerical simulations in past literatures. The numerical method used is **Monte Carlo simulation**, which relies on repeated random sampling to obtain the results to the deterministic problems.
5.2.1 Equilibrium And Non-equilibrium Single Step Model

Now we examine a generalised version of the Single Step Model of the random deposition, where both deposition and evaporation are allowed, constructed by [Plischke, Racz, Liu (1987)] in relation to the one-dimensional stochastic Ising model to solve for the critical exponents analytically, which belongs to either EW or KPZ universality classes depending on the existence of the interface motion.

The model proposed for the surface evolution is set up in a square lattice with tilted square particles of length \(\sqrt{2}a\) piling on each other. The growth of surface is restricted in the vertical direction of the strip. Time is discretised by \(t_n = n\tau\), and in each time step a new particle is deposited onto the surface with probability \(p_p\) at a "+" site or an old particle evaporates from surface with probability \(p_- = 1 - p_p\) at a "-" site. The site \(x_i = ia\) where surface changes is considered random. The initial condition at \(t = 0\) is a flat surface of particles. The linear size is denoted as \(L\), which comprises of \(L/2\) particle horizontally. A rough sketch of this configuration is displayed in figure 5.2.1(1):

For example, the spin configuration corresponding to figure 5.2.1(1) before the indicated surface change is:

\[
\downarrow\uparrow\uparrow\uparrow\uparrow\uparrow\uparrow\uparrow\uparrow\uparrow\uparrow\uparrow\uparrow\uparrow\uparrow
\]

The spin configuration after surface change is:

\[
\downarrow\uparrow\uparrow\uparrow\uparrow\uparrow\uparrow\uparrow\uparrow\uparrow\uparrow\uparrow\uparrow\uparrow\uparrow\uparrow\uparrow\uparrow\uparrow
\]

In order to obtain the macroscopic properties of the model, we need to know the time evolution of the height of the surface \(h_i(t_n)\) measured from the bottom particle at site \(x_i = ia\) at time \(t_n\). The Average Surface Height at a given time can be calculated as:

\[
\langle h(t_n) \rangle = \frac{1}{L} \sum_{i=1}^{L} \left\langle h_i(t_n) \right\rangle = \frac{1}{L} L (p_p(2a) + p_-(-2a))n = (2p_p - 1) \frac{2a}{\tau} t_n
\] (380)

It can be seen that for the equilibrium case \((p_p = 1/2)\) the average surface height is zero, which means that on the average the surface remains at the same level with the initial condition. While for non-equilibrium case, the surface moves (upwards if \(p_p > p_-\), downwards otherwise).

Using the average surface height, we introduce the Width of the Surface Zone \(\zeta\) to characterise the fluctuations in the co-moving frame:

\[
\zeta^2(L,t) = \frac{1}{L} \sum_{j=1}^{L} \left( h_j(t) - \langle h(t) \rangle \right)^2
\] (381)

which can be interpreted as the variance of the surface height from the average.

We also define the Time-Independent Structure Factor:

\[
S(k,t) = \langle \hat{h}_k(t) \hat{h}_{-k}(t) \rangle
\] (382)

where \(\hat{h}_k(t)\) is simply a Fourier transform of the height deviation from the average \(h_j(t) - \langle h(t) \rangle\):

\[
\hat{h}_k(t) = \frac{1}{\sqrt{L}} \sum_{j=1}^{L} \left( h_j(t) - \langle h(t) \rangle \right) e^{ikj}
\] (383)

We expect the long-time limit of the surface evolution to be stationary, which makes \(\zeta^2(L,t)\) and \(S(k,t)\) become time independent. The Relaxation towards the stationary

\[
\zeta^2(L,t) \to \zeta^2 \quad \text{as} \quad t \to \infty
\]

\[
S(k,t) \to S(k) \quad \text{as} \quad t \to \infty
\]
state, which describes the dynamics of system near stationary state, is defined as:

\[ \Phi(k, t) = \lim_{t \to \infty} \frac{\langle \hat{h}_k(t + t')\hat{h}_k(t) \rangle}{S(k, t)} \]  

(384)

The relaxation describing the dynamics of the system far away from the stationary state, is formulated as:

\[ \Psi(k, t) = \lim_{t \to \infty} \frac{S(k, t') - S(k, t)}{S(k, t'') - S(k, 0)} \]  

(385)

Since there is no restriction to the surface fluctuations in the model proposed, we expect the fluctuations to diverge in large-size limit (\( \lim_{L \to \infty} C^2(L, t) = \infty \)). This limit acts as a critical point of the system, which induces dynamic scaling for the structure factor and the relaxation functions.

Now we are ready to derive the analytical results following the framework of the stochastic Ising model. To do this we make the time steps continuous and start from describing the system with the master equation (14):

\[ \frac{\partial P(\{h\}, t)}{\partial t} = - \sum_{i=1}^{L} T_i(\{h\}_i|\{h\}) P(\{h\}, t) \]

\[ + \sum_{i=1}^{L} T_i(\{h\}|\{h\}_i) P(\{h\}_i, t) \]  

(386)

where \( \{h\} \) denotes a configuration of the system growth and \( \{h\}_i \) denotes the system where a particle has been added to or deleted from site \( i \), provided it is possible at site \( i \). \( T_i(\{h\}_i) \) is the rate of the particle deposition or evaporation at site \( i \):

\[ T_i(\{h\}_i) = \begin{cases} 
  p_+/\tau_0 & \text{if site } i \text{ is in local minimum} \\
  (1 - p_+)/\tau_0 & \text{if site } i \text{ is in local maximum} \\
  0 & \text{otherwise}
\end{cases} \]  

(387)

where \( \tau_0 \) is a time-scale parameter that measures the amount of time it takes for a single fluctuation to occur.

Now we can make the identification between the spin variables and the surface slope variables:

\[ \sigma_i = \frac{h_i - h_{i-1}}{a} = \pm 1 \]  

(388)

where the boundary condition is the same for any closed Ising chain: \( \sigma_L = \sigma_0 \). This condition makes sure the total spin \( \sum_{i=1}^{L} \sigma_i = 0 \).

Master equation (386) can then be rewritten in terms of the spin variables with the probability distribution \( P_I \) of the Ising chain:

\[ \frac{\partial P_I(\{\sigma\}, t)}{\partial t} = - \sum_{i=1}^{L} T_i^{(I)}(\{\sigma\}_i|\{\sigma\}) P_I(\{\sigma\}, t) \]

\[ + \sum_{i=1}^{L} T_i^{(I)}(\{\sigma\}|\{\sigma\}_i) P_I(\{\sigma\}_i, t) \]  

(389)

The rate of the spin flip is given by:

\[ T_i^{(I)}(\{\sigma\}_i|\{\sigma\}) = \frac{1}{4\tau_0} \left[ 1 - \sigma_i\sigma_{i+1} + \alpha(\sigma_{i+1} - \sigma_i) \right] \]  

(390)

This can be easily verified to be true. For instance, at a local minimum corresponding to the particle deposition, \( \sigma_i = -1 \) and \( \sigma_{i+1} = 1 \), \( T_i^{(I)}(\{\sigma\}_i|\{\sigma\}) = p_+/\tau_0 \) exactly matches (387).

The two-point correlation function for the equivalent Ising model, from which the width of surface zone and structure factor can be constructed, is:

\[ \langle \sigma_i\sigma_m \rangle = \sum_{\{\sigma\}} \sigma_i\sigma_m P_I(\{\sigma\}, t) \]  

(391)

Consequently, the boundary condition implies that:

\[ \sum_{i=1}^{L} \sum_{j=1}^{L} \langle \sigma_i\sigma_j \rangle = \left( \sum_{i=1}^{L} \sigma_i \right) \left( \sum_{j=1}^{L} \sigma_j \right) = 0 \]  

(392)

The height deviation from the average is given in terms of the spin variables:

\[ \delta h_j = h_j - \langle h \rangle = h_j - h_0 - \langle (h - h_0) \rangle \]

(388)

\[ = h_j - h_0 - \frac{1}{L} \sum_{i=1}^{L} (h_i - h_0) \]

(393)

So the width of surface zone can be calculated as.
\[ \zeta^2(L, t) = \frac{1}{L} \sum_{j=1}^{L} (\langle \delta h_j \rangle)^2 \]
\[ = \frac{a^2}{L} \sum_{j=1}^{L} \left( \sum_{m=1}^{j} \sum_{m'=1}^{j} \langle \alpha_m \alpha_{m'} \rangle - \frac{2}{L} \sum_{n=1}^{L} \sum_{i=1}^{j} \langle \alpha_m \alpha_i \rangle \right) \]
\[ + \frac{1}{L^2} \sum_{m=1}^{L} \sum_{n=1}^{L} \sum_{i=1}^{m} \sum_{j=1}^{n} \langle \alpha_i \alpha_j \rangle \]

By induction on \( L \) and (392) \[ \frac{a^2}{L^2} \sum_{m=1}^{L} \sum_{n=1}^{L} \sum_{i=1}^{m} \sum_{j=1}^{n} \langle \alpha_i \alpha_j \rangle = \]

(394)

Multiply both sides of the master equation (389) by \( \sum_{\alpha} \alpha \) and we can find the time evolution of the correlation function as a set of differential equations, which can be solved explicitly for the equilibrium case \( (p_+ = \frac{1}{2} \rightarrow \alpha = 0) \), similarly to what we did for the one dimensional Ising chain in previous section (349):

If \( m > j + 1 \):

\[ 2 \alpha \frac{\partial}{\partial t} \langle \alpha_i \alpha_j \rangle = -4 \langle \alpha_i \alpha_j \rangle + \langle \alpha_{i+1} \alpha_j \rangle + \langle \alpha_{j-1} \alpha_j \rangle + \langle \alpha_j \alpha_{j+1} \rangle \]
\[ + \langle \alpha_{i-1} \alpha_j \rangle - \alpha \langle \alpha_{i-1} \alpha_j \rangle - \langle \alpha_j \alpha_{i+1} \rangle \]
\[ + \langle \alpha_{i+1} \alpha_{j-1} \rangle - \langle \alpha_j \alpha_{j-1} \rangle \]

(395)

If \( m = j + 1 \), then it can be further reduced to:

\[ 2 \alpha \frac{\partial}{\partial t} \langle \alpha_i \alpha_{j+1} \rangle = -2 \langle \alpha_i \alpha_{j+1} \rangle + \langle \alpha_{i-1} \alpha_{j+1} \rangle + \langle \alpha_{j} \alpha_{j+2} \rangle \]
\[ - \alpha \langle \alpha_{i-1} \alpha_{j+1} \rangle - \langle \alpha_j \alpha_{j+1} \rangle \]

(396)

\textbf{Equilibrium Case} \( \alpha = 0 \)

For the equilibrium case, all three point correlation functions in those differential equations vanish and we can expect to find an analytical solution. While in the non-equilibrium case the Time-Reversal Symmetry is broken for \( p_+ \neq p_- \) and we need to find other methods to deal with the problem.

We also assume that the initial state as shown in figure 1 is translationally invariant, which means that the correlation function only depends on the distance between two sites : \( \langle \alpha_i \alpha_j \rangle = r_{i-j}(t) \). By this assumption (395) (396) can be reduced to only \( \frac{L}{2} \) equations because of the boundary condition \( r_{j-\frac{L}{2}} = r_{j-\frac{L}{2}+L} = r_{j+\frac{L}{2}} \):

\[ \tau_0 r_1 = r_2 - r_1 \]
\[ \tau_0 r_j = r_{j-1} - 2r_j + r_{j+1}, \quad 2 \leq j \leq \frac{L}{2} \]

(397)

This set of differential equations can be solved by a Discrete Fourier Transform of the correlation functions. We first consider \( j \) takes value from \( \{1, ..., L\} \) (thus \( k \) has \( L-1 \) values) and then seek solutions that meet the symmetry \( \hat{r}_{\frac{L-i}{2}} = \hat{r}_{\frac{L+i}{2}} \).

\[ r_j = \frac{1}{L-1} \sum_{k=1-\frac{L}{2}}^{L-1} \hat{r}_k e^{i q (\frac{L}{2} - j)} \]

(398)

where \( q = \frac{2 \pi k}{L} \), \( k \in \{0, \pm 1, ..., \pm \left( \frac{L}{2} - 1 \right) \} \)

Substitute this Fourier transform into (397) and we obtain a simple first order differential equation of \( \hat{r}_k \):

\[ \frac{\partial}{\partial t} \hat{r}_k = -\frac{\lambda q}{\tau_0} \hat{r}_k, \quad \text{where} \quad \lambda q = 2(1 - \cos q) \]
\[ \rightarrow \hat{r}_k = C_q e^{-\frac{\lambda q}{\tau_0} t} \]

(399)

where \( C_q \) is an integrating constant

Put it back into the Fourier Transform:

\[ r_j = \frac{1}{L-1} \sum_{k=1-\frac{L}{2}}^{L-1} C_q e^{-\frac{\lambda q}{\tau_0} t} e^{i q (\frac{L}{2} - j)} \]

(400)

In order to fix the constant we make another Fourier Transform to map \( C_q \) to \( r_j(0) \). The initial condition in figure 5.2.1(1) indicates that \( r_j(0) = 1 \) for \( j \) even, and \( r_j(0) = 1 \) for \( j \) odd.

\[ C_q = \sum_{j'=-\frac{L}{2}}^{\frac{L}{2}-1} r_{j'}(0) e^{i q j'} = -\frac{1}{\cos \left( \frac{\lambda q}{2} \right)} \]

(401)

Hence the solution to (397) is:

\[ r_j = \frac{1}{L-1} \sum_{k=1-\frac{L}{2}}^{L-1} \left( -\frac{1}{\cos \left( \frac{\lambda q}{2} \right)} \right) e^{-\frac{\lambda q}{\tau_0} t} e^{i q (\frac{L}{2} - j)} \]

(402)

Substitute it into (394) we obtain the expression for the width of the surface zone:

\[ \zeta^2(L, t) = a^2 \left( \frac{L+1}{12} - \frac{1}{L} \sum_{q \neq 0} \frac{1}{\lambda q} e^{-\frac{\lambda q}{\tau_0} t} \right) \]

(403)
In order to evaluate the structure factor $S(k,t)$, let us Fourier transform the following equation:

$$a^2 r_m(t) = a^2 \langle \sigma_i \sigma_{i+m} \rangle \quad (388)$$

where $g_m(t) = \left( (h_i - \langle h \rangle)(h_{i+m} - \langle h \rangle) \right)$.

Now that we have a look at the scaling of $\zeta(L,t)$ and $S(k,t)$ at large time. Since in both (403) and (405) $t$ only occurs as a negative on the exponential, the only non-vanishing terms in the summation would be those with small $k$. In mathematical terms, we are looking for the limit at $L \to \infty$.

The results found by [Plischke, Racz, Liu (1987)] are:

$$\zeta(L, t) \approx L^{1/2} f(t/L^2)$$

$$S(k, t) \approx k^{-2} f'(k^2 t, kL) \quad (406)$$

Now it is time to introduce the famous KPZ Equations, which is a simple nonlinear Langevin equation with a noise term, proposed by [Kardar, Parisi, Zhang (1986)] in attempt to describe the time evolution of the surface growth height. For a two-dimensional surface growth, it is formulated as:

$$\frac{\partial h}{\partial t} = v \frac{\partial^2 h}{\partial x^2} + \frac{\lambda}{2} \left( \frac{\partial h}{\partial x} \right)^2 + F(x, t) \quad (413)$$

The term $\partial^2 h/\partial x^2$ represents the relaxation of the surface due to tension while $v$ is viscosity. $(\partial h/\partial x)^2$ is the simplest nonlinear term indicating the motion of the interface in the non-equilibrium case and $\lambda$ is proportional
to the velocity of the interface. $F(x, t)$ as defined previously is a Gaussian white noise. By making a substitution by $u(x, t) = \partial h/\partial x$, where $u$ is interpreted as the slope of the surface, we obtain the Burgers Equation, which was proposed by [Burgers (1974)] originally for modelling the turbulence:

$$\frac{\partial u}{\partial t} = v \frac{\partial^2 u}{\partial x^2} + \lambda u \left( \frac{\partial u}{\partial x} \right)^2 + \frac{\partial F(x, t)}{\partial x} \quad (414)$$

We may argue that our non-equilibrium single step model is equivalent to the Burgers equation because we can find two correspondences between two models. The particle deposition and evaporation in single step model is essentially a surface tension driven relaxation process indicated by $\partial^2 h/\partial x^2$. And the motion of interface in non-equilibrium case is suggested by $(\partial h/\partial x)^2$. If two models are equivalent, then they belong to the same universality class. The question now turns to solving Burgers equation for the critical exponents. Luckily, a lot of studies have been conducted on the Burgers equation, for example by renormalisation group method [Medina et al (1989)] and by Bethe ansatz [Gwa, Spohn (1992)], where three fixed points have been found. Those results are verified and supported by kinetic Monte Carlo simulations [Pischke, Racz, Liu (1987)].

- **Gaussian Universality Class**

  With the last fixed point $(v^* = 0, \lambda^* = 0)$, KPZ equation reduces to:

  $$\frac{\partial h}{\partial t} = F(x, t) \quad (415)$$

  This is a random deposition without surface tension and interface motion. The surface height on each site is independent of each other and only subject to a Gaussian white noise. The corresponding category is called Gaussian Universality Class. Unfortunately, the fixed point here cannot be reached within the parameter restraint of the single step model.

- **EW Universality Class**

  $(v^* \neq 0, \lambda^* = 0)$ are found to correspond to the critical exponents $(\eta = 0, z = 2)$. In this case the KPZ equation reduces to the Edwards-Wilkinson Model developed by [Edwards, Wilkinson (1982)] in their study of surface fluctuations in settled granular material:

  $$\frac{\partial h}{\partial t} = v \frac{\partial^2 h}{\partial x^2} + F(x, t) \quad (416)$$

  This model defines the EW Universality Class which includes all models with the given exponents. Obviously the equilibrium single step model belongs to this class.

In this surface growth model, as depicted in figure 5.2.1(2), square particles deposit on the surface with surface relaxation (diffusion), meaning that if the surface is locally flat, then the particle remains where it deposition; if only one of the nearest neighbour site is lower than deposition site, then the particle slides onto that nearest local minimum; if both neighbouring sites are lower than deposition site, then the particle slides randomly onto either of its neighbouring site. This rule makes particles smooth the surface automatically. Surface relaxation introduces correlations between columns, which makes its scaling forms non-trivial.

- **KPZ Universality Class**

  ![Figure 5.2.1(2) : Particle deposition in EW model](image-url)
Figure 5.2.1(3) : Particle deposition in ballistic model

\( v^* \neq 0, \lambda^* \neq 0 \), which makes sure a non-vanishing interface motion term in the KPZ equation (413), are found with the critical exponents \( \eta = 0, z = \frac{3}{2} \), which defines KPZ universality Class. The non-equilibrium single step model with surface drift naturally belongs to this category. Examples of physical phenomena modelled by the KPZ class include crystal growth on a thin film [Takeuchi, Sano (2010)] and burning front [Maunuksela et al (1997)]. The growth model typically associated with this class is Ballistic Deposition Model [Meakin et al (1986)]. In this model as illustrated in figure 5.2.1(3), if neighbouring sites are both lower than the deposition site, then particle simply falls on top and does not slide; otherwise it can stick to the first occupied neighbouring site along its trajectory. This way of deposition creates a lot of voids inside of the interface and its corresponding surface is imaginably rougher than EW model.

Note that the surface growth models, which only comprises of a finite number of sites, are discrete versions of the continuous equations of motion of the universality classes (413) (415) (416). Those continuous equations can be derived and analysed by various means. The most intuitive one that comes into mind is coarse-graining the discrete height columns into continuous ones.

5.2.2 Derivation of Edwards-Wilkinson Equation by Lattice Transition Rules

Here we present a way of deriving the EW model by the transition rules of the lattice growth models, which is also the first time a statistically equivalent stochastic continuous equation of motion has been derived directly from the non-analytical lattice transition rules [Vvedensky (2003)]. This is done by coarse-graining the discrete Langevin equations for the height fluctuations of the lattice models, which are obtained from the Kramers-Moyal expansion (see equation (28)) of the master equation, and applying the relaxation rules.

Now consider a one-dimensional lattice in a surface growth model on which particles are deposited with an average rate of \( \tau_0^{-1} \) per site, with only nearest-neighbour interaction. Then by Kramers-Moyal expanding the master equation, the time evolution of the height \( h_i \) at site \( i \) can be described as [Baggio et al (2001)]:

\[
\frac{dh_i}{d\tau} = K_{i}^{(1)} + F_i
\]

where \( K_{i}^{(1)} \) is the first moment of the transition rate:

\[
K_{i}^{(1)} = \sum_{\{h'\}} (h'_i - h_i) T(\{h'\}|\{h\})
\]

It can also be represented by variables \( w_i^j \), which incorporates the local relaxation rules:

\[
K_{i}^{(1)} = \frac{1}{\tau_0} \left[ w_i^{(1)} + w_{i+1}^{(2)} + w_{i-1}^{(3)} \right]
\]

where \( \tau_0^{-1} \) is the average rate of the particle deposition per site. \( F_i \) are the Gaussian white noises with zero mean and correlation function:

\[
\langle F_i(\tau)F_i(\tau') \rangle = K_i^{(1)} \delta_{ij} \delta(\tau - \tau')
\]

It makes intuitive sense that \( K_i^{(1)} \), as the first moment of the transition rate, indicates the strength of the noise correlation. The higher the transition rate is, the stronger the noise appears to be.

Remember that a particle slides onto its neighbouring site only if the height of the deposition site is higher than its neighbours. If it is higher than both neighbours, then the particle choose randomly which one to relax onto. Now we can code the relaxation rules of the EW model into the expression of \( K_i^{(1)} \) via \( w_i^j \) [Vvedensky (1993)]:

\[
w_i^{(1)} = \theta_i^+ \theta_i^-
\]
\[
w_i^{(2)} = \theta_i^+ (1 - \theta_i^-) + \frac{1}{2} (1 - \theta_i^+) (1 - \theta_i^-)
\]
\[
w_i^{(3)} = \theta_i^- (1 - \theta_i^+) + \frac{1}{2} (1 - \theta_i^-) (1 - \theta_i^+)
\]
where \( \theta_i^\pm = \theta(h_i+1 - h_i) \) is the unit step function:

\[
\theta(x) = \begin{cases} 1 & \text{if } x \geq 0 \\ 0 & \text{if } x < 0 \end{cases} \tag{422}
\]

In equation (421) \( w_i^{(j)} \) can be interpreted as the condition for a particle incident on site \( i \) to stay there \( (j = 1) \), to relax onto site \( i-1 \) \( (j = 2) \) or site \( i+1 \) \( (j = 3) \).

The easily checked identity:

\[
w_i^{(1)} + w_i^{(2)} + w_i^{(3)} = 1 \tag{423}
\]

guarantees that the particle deposition is always onto the incident site or its two neighbouring sites.

The step function in (422) is discontinuous and that is why we said earlier that the EW relaxation rules are non-analytical. The non-analyticity causes a major difficulty for coarse-graining the discrete Langevin equations (417). This problem is solved by expressing step function in a limit of an analytical quantity, which in this case is chosen to be the maximum function (checkable by Taylor expansion):

\[
\max(x, y) = \lim_{\epsilon \to 0^+} \left[ \epsilon \ln(e^{x/\epsilon} + e^{y/\epsilon}) \right] \tag{424}
\]

The corresponding representation of \( \theta(x) \) is chosen to be:

\[
\theta(x) = \max(x + 1, 0) - \max(x, 0) \\
= \lim_{\epsilon \to 0^+} \left\{ \epsilon \ln \left[ \frac{e^{(x+1)/\epsilon} + 1}{e^{x/\epsilon} + 1} \right] \right\} \text{ for } x \in \mathbb{Z} \tag{425}
\]

Taylor expanding the right hand side of (425) in terms of \( x \) and we have:

\[
\theta_\epsilon(x) = A + \frac{Bx}{2} - \frac{B^2x^2}{8\epsilon} - \ldots \tag{426}
\]

where

\[
A = \epsilon \ln \left[ \frac{1}{2}(1 + e^{1/\epsilon}) \right] = 1 - \epsilon \ln 2 + \ldots \tag{427}
\]

\[
B = \frac{e^{1/\epsilon} - 1}{e^{1/\epsilon} + 1}
\]

with the property that:

\[
\lim_{\epsilon \to 0^+} A = \lim_{\epsilon \to 0^+} B = 1 \tag{428}
\]

Now we can substitute the analytical approximation of the step function (426) into \( w_i^{(j)} \) variables and find an expression for \( K_i^{(1)} \):

\[
K_i^{(1)} = \frac{1}{\tau_0} \left\{ 1 + B\Delta^2 h_i + \frac{1}{4} B(1 - A)\Delta^4 h_i - \ldots \right\} \tag{429}
\]

where the Difference Operators (which can also be seen as the Discrete Derivatives of \( h_i \) with respect to site index \( i \), if \( i \) is imagined to be continuous) are defined as:

\[
\Delta^\pm h_i = \mp h_i \pm h_i \pm 1, \quad \Delta^2 h_i = \Delta^+ (\Delta^- h_i) = \Delta^- (\Delta^+ h_i) \quad \text{and} \quad \Delta^4 h_i = \Delta^2 (\Delta^2 h_i).
\]

Let us introduce the coarse-grained space and time variables \( x \) and \( t \):

\[
x = i\epsilon a_h, \quad t = \epsilon^2 \tau \tag{430}
\]

where \( a_h \) is the horizontal lattice spacing and \( z \) is a constant to be determined. \( \epsilon \) indicates the degree of coarse graining with \( \epsilon \to 0 \) corresponding to the continuous limit. The coarse-grained height function is thus:

\[
u(x, t) = \epsilon^a a_v \left( h_i - \frac{\tau}{\tau_0} \right) \tag{431}
\]

where \( a_v \) is the vertical lattice spacing and \( a_v \tau/\tau_0 \) is the average growth rate. \( \alpha \) is a constant to be determined.

Differentiate (431) in terms of \( t \) and we have:

\[
dh_i \frac{dt}{\tau} = \frac{1}{\tau_0} + \frac{\epsilon^{2-\alpha} \partial u}{a_v \partial t} \tag{432}
\]

Now we write the difference operators \( \Delta h_i \) as differential quotients \( dh_i/di \), which can be approximated by the continuous derivative \( \partial u/\partial x \) by differentiating (431) in terms of \( x \):

\[
\frac{\partial u}{\partial x} = \frac{\epsilon^a a_v}{\epsilon a_h} \frac{dh_i}{di} \quad \rightarrow \quad \frac{\partial^2 u}{\partial x^2} = \frac{\epsilon^a a_v}{(\epsilon a_h)^2} \frac{d^2 h_i}{di^2} \tag{433}
\]

\[
\Delta h_i = \frac{d^2 h_i}{di^2} = \frac{\epsilon^{2-\alpha} a_h^2}{a_v} \frac{\partial^2 u}{\partial x^2}
\]

Substitute (433) into \( K_i^{(1)} \) and we have (note that the dependence of \( K_i^{(1)} \) on \( i \) has been erased by the continuous approximation \( \partial u/\partial x \)):

\[
K^{(1)}(u) = \frac{1}{\tau_0} + \frac{\epsilon^{2-\alpha} a_h^2 B}{\tau_0 a_v} \left[ \frac{\partial^2 u}{\partial x^2} + \frac{1}{12} \epsilon^2 (4 - 3A) a_h^2 \frac{\partial^4 u}{\partial x^4} - \ldots \right] \tag{434}
\]
Equation (430) can be rewritten in terms of the delta functions:

$$\delta_{ij} = \epsilon a_h \delta(x - x'), \quad \delta(\tau - \tau') = \epsilon^2 \delta(t - t')$$

(435)

Substitute (434) and (435) into the correlation function of the noise term (420):

$$\langle F_i(\tau) F_i(\tau') \rangle = \epsilon^{1+\alpha} a_h \kappa(1) \delta(x - x') \delta(t - t')$$

(436)

Truncate to leading order of $\epsilon$

Thus the coarse grained noise $\xi$ is defined as:

$$\xi(x, t) = a_v \epsilon^{-(1+\alpha)/2} F_i(\tau)$$

(437)

with zero mean and correlation function:

$$\langle \xi(x, t) \xi(x', t') \rangle = \frac{a_v^2 a_h}{\tau_0} \delta(x - x') \delta(t - t')$$

(438)

5.2.3 From Ballistic Deposition to KPZ Equation

Through Limiting Procedure

Ballistic deposition model is generally believed to be the discrete version of the continuous model described by the KPZ equation (413). Some physical arguments can be developed to justify the addition of the non-linear term $(\partial h/\partial x)^2$ to the EW equation (416) but no mathematically rigorous derivation has been put forward until [Nagatani (1998)] proposed a formal derivation via limiting procedure, inspired by the ultra-discretisation method in which the Korteweg-de Vries equation is transformed into a cellular automaton [Tokihiro et al (1996)]. We have already seen the limiting procedure before when we use maximum function to represent unit step function (425). Now let us see how it works for deriving the non-linear term in the KPZ equation.

Remember that the incident particle in the Ballistic growth model either fall directly onto the incident site, or stick to one of its nearest neighbours, in which case the height of incident site will be the same as the neighbouring height. So $h_i(\tau + 1)$ can be represented by the maximum function as:

$$h_i(\tau + 1) = \max[h_{i-1}(\tau), h_i(\tau) + 1, h_{i+1}(\tau)]$$

(441)

The difference between two nearest neighbours is:

$$h_i(\tau + 1) - h_{i-1}(\tau + 1) = \max[h_{i-1}(\tau), h_i(\tau) + 1, h_{i+1}(\tau)] - \max[h_{i-2}(\tau), h_{i-1}(\tau) + 1, h_i(\tau)]$$

(442)

Now we invoke the limiting procedure which expresses the maximum function as a limit of an analytical function, similar to (424):

$$\max[x, y, z] = \lim_{\epsilon \to 0^+} \epsilon \ln(e^{x/\epsilon} + e^{y/\epsilon} + e^{z/\epsilon})$$

(433)

(442) can be rewritten as:

$$h_i(\tau + 1) - h_{i-1}(\tau + 1) = \lim_{\epsilon \to 0^+} \epsilon \ln \left[ \frac{e^{h_{i-1}(\tau)}/\epsilon + e^{h_i(\tau) + 1}/\epsilon + e^{h_{i+1}(\tau)/\epsilon}}{e^{h_{i-2}(\tau)/\epsilon} + e^{h_{i-1}(\tau) + 1}/\epsilon + e^{h_i(\tau)/\epsilon}} \right]$$

(444)

Define $c_i(\tau) = e^{(h_i(\tau) - h_{i-1}(\tau))/\epsilon}$ and $\delta = e^{-1/\epsilon}$ for notational simplicity and (444) can be turned into a Difference-Difference Equation, which comprises a coupled ordinary differential equation (in $t$) and a recurrence relation (in $i$):

$$c_i(\tau + 1) = \frac{\delta c_{i-1}(\tau) + c_{i-1}(\tau) c_i(\tau) + \delta c_{i-1}(\tau) c_i(\tau) c_{i+1}(\tau)}{\delta + c_{i-1}(\tau) + \delta c_{i-1}(\tau) c_i(\tau)}$$

(445)
(445) can be further analysed by a long-wavelength expansion with respect to the horizontal lattice spacing $a_h$.

Write the coarse-grained space and time variables $x$ and $t$ as follows:

$$x = a_h, \quad t = \delta a_h^2 \tau \quad (446)$$

Define $v$ by $\ln c_i(\tau) = a_h v_{ia_h}(\delta a_h^2 \tau) = a_h v_x(t)$ and we can expand $c_i(\tau), c_{i-1}(\tau), c_{i+1}(\tau)$ and $c_i(\tau + 1)$ in terms of $a_h$ to third order:

$$c_i(\tau) = e^{a_h v_x(t)} = 1 + a_h v + a_h^2 v^2 + a_h^3 v^3 + ... \quad (447)$$

$$c_{i-1}(\tau) = 1 + a_h v_{(i-1) a_h} + \frac{a_h^2 v_{(i-1) a_h}^2}{2} + \frac{a_h^3 v_{(i-1) a_h}^3}{6} + ...$$

$$= 1 + a_h v + \frac{a_h^2 (v^2 - \partial_x v)}{2} + a_h^3 \left( \frac{v^3}{6} - v \partial_x v + \frac{1}{2} \partial_x^2 v \right) + ... \quad (448)$$

where $v_{(i-1) a_h} = v_{ia_h} - a_h$ can be expanded around $v_{ia_h}$ by Taylor series:

$$v_{ia_h} - a_h = v_{ia_h} - a_h \partial_x v_{ia_h} + \frac{1}{2} a_h^2 \partial_x^2 v_{ia_h} \quad (449)$$

And similarly for $c_{i+1}(t)$ and $c_i(t+1)$ by Taylor expanding both $c$ and $v$ in terms of $a_h$ and we have:

$$c_{i+1}(\tau) = 1 + a_h v + a_h^2 \left( \frac{v^2}{2} + \partial_x v \right) + a_h^3 \left( \frac{v^3}{6} - v \partial_x v + \frac{1}{2} \partial_x^2 v \right) + ... \quad (450)$$

$$c_i(\tau + 1) = 1 + a_h v + a_h^2 \left( \frac{v^2}{2} + \partial_x v \right) + a_h^3 \left( \frac{v^3}{6} + \delta \partial_t v \right) + ... \quad (451)$$

Substitute (447) (448) (450) (451) into (445). The first and second orders of $a_h$ cancel and we obtain the Burgers equation (414) in its deterministic form (without noise term):

$$\partial_t v = \frac{2}{1 + 2 \delta} v \partial_x v + \frac{1}{1 + 2 \delta} \partial_x^2 v \quad (452)$$

If we identify $v$ as the slope of surface $\partial_x h$, then (452) turns into a deterministic KPZ equation (413):

$$\partial_t \partial_x h = \frac{2}{1 + 2 \delta} (\partial_x h) \partial_x^2 h + \frac{1}{1 + 2 \delta} \partial_x^2 \partial_x h$$

Integrate by parts with respect to $x$

$$\partial_t \int \partial_x h \, dx = \frac{2}{1 + 2 \delta} \int (\partial_x h) \partial_x^2 h \, dx + \frac{1}{1 + 2 \delta} \int \partial_x^2 \partial_x h \, dx$$

$$\partial_x h = \frac{1}{1 + 2 \delta} (\partial_x h)^2 + \frac{1}{1 + 2 \delta} \partial_x^2 h \quad (453)$$

We recover the non-linear term in the equation of motion just as expected.

The limiting procedure can also be applied to a modified version of the ballistic model as shown next, where the falling particles stick to the upper edges of nearest neighbours, as called "next-nearest-neighbour" rule.

Figure 5.2.3 : Particle deposition in modified ballistic model

The height of the particle sites, represented by the maximum function, is given by:

$$h_i(\tau + 1) = \max \{ h_{i-1}(\tau) + 1, h_i(\tau) + 1, h_{i+1}(\tau) + 1 \} \quad (454)$$

The difference-difference equation obtained by going through the limiting procedure is:

$$c_i(\tau + 1) = \frac{\delta c_{i-1}(\tau) + c_{i-1}(\tau) c_i(\tau) + c_{i-1}(\tau) c_i(\tau) c_{i+1}(\tau)}{1 + c_{i-1}(\tau) + c_{i-1}(\tau) c_i(\tau)} \quad (455)$$
By applying the perturbation method to (455), we have the modified KPZ equation:

$$\partial_{t} h = \frac{1}{3} \left( \partial_{x}h \right)^{2} h + \partial_{x}^{2} h$$ (456)

which differs from the KPZ equation of the unmodified ballistic model (453) only by a factor.

### 5.2.4 Hopf-Cole Solutions to the KPZ Equation with Sharp Wedge Initial Conditions

In their original paper published in 1986, Kardar, Parisi and Zhang not only proposed the ground breaking KPZ equation for the evolution of growing interfaces (413), but also noted that it can be turned into a linear equation by the so called **Hopf-Cole Transform**:

$$Z(x, t) = \exp \left[ \frac{\lambda}{2v} h(x, t) \right]$$ (457)

And $Z$ satisfies:

$$\partial_{t} Z(x, t) = v \partial_{x}^{2} Z(x, t) + \frac{\lambda}{2v} F(x, t) Z(x, t)$$ (458)

This linear equation can then be solved by the Feynman-Kac formula (85). Let $\{b_{t}\}$ be the auxiliary Brownian motion and the noise term can be represented as $F(b(t), t)$. The solution is then:

$$Z(x, t) = \mathbb{E}_{0} \left[ \exp \left\{ \alpha \int_{0}^{2vt} ds F(b(s), s) \right\} \exp \left\{ \frac{\lambda}{2v} h(b(2vt), t) \right\} \right]$$ (459)

with $\alpha = (2v)^{3/2}/\lambda$.

The sharp wedge initial conditions, $h(x, 0) = -|x|/\delta$ in the limit $\delta \to 0$, have been extensively studied, which translates under Hopf-Cole to:

$$Z(x, 0) = \delta(x)$$ (460)

The action integral in (459) is not well defined for typical realisations of Brownian motion and of white noise, but a few approximation schemes of $Z(x, t)$ can go around this issue and make it possible for the solution to the KPZ equation to be defined by (457) [Sasamoto, Spohn (2010)]. We discuss those schemes separately.

**Approximations of Cole-Hopf Solution:**

- **1. Multiple Itô Integrals**

  We expand the exponential in (459) and average over Brownian motion, which gives the $n$-th coefficient:

  $$\alpha^{n} \int_{0 \leq t_{1} \leq \ldots \leq t_{n} \leq 2vt} dt_{1} \ldots dt_{n}$$

  $$\times \int_{\mathbb{R}^{n}} dx_{1} \ldots dx_{n} \prod_{j=1}^{n} F(x_{j}, t_{j}) p_{0}(x_{1}, t_{1}; \ldots; x_{n}, t_{n}; x, 2vt)$$

  (461)

  with $p_{0}$ being the probability density for the Brownian motion to start at $t = 0$, to be at $x_{j}$ at time $t_{j}$ and to be at $x$ at time $2vt$. Then we integrate in terms of $x$ by Itô’s lemma (70) and obtain a multiple Itô integral in the forward discretisation:

  $$\langle Z(x, t)^{2} \rangle = \sum_{n=0}^{\infty} \alpha^{2n} \int_{0 \leq t_{1} \leq \ldots \leq t_{n} \leq 2vt} dt_{1} \ldots dt_{n}$$

  $$\times \int_{\mathbb{R}^{n}} dx_{1} \ldots dx_{n} p_{0}(x_{1}, t_{1}; \ldots; x_{n}, t_{n}; x, 2vt)^{2} < \infty$$

  (462)

  Since the integral is bounded, $Z(x, t)$ is a well-defined random variable.

- **2. Coloured Noise**

  In this scheme we introduce the **Mollifier** $\phi_{k}(x) = k \phi(kx)$, which is usually used to smooth the sharp features of the functions, with $\phi \geq 0$, $\phi(x) = \phi(-x)$ and $\int dx \phi(x) = 1$. The noise can then spatially mollified to $F_{k}(x, t) = \int dx' \phi_{k}(x - x') F(x', t)$. The Hopf-Cole transformation remains valid and the action is now properly defined. The average of mollified $Z(x, t)$ is given by:

  $$\langle Z_{k}(x, t) \rangle = \left\langle \mathbb{E}_{0} \left[ \exp \left\{ \alpha \int_{0}^{2vt} ds F_{k}(b(s), s) \right\} \delta(b(2vt) - x) \right] \right\rangle$$

  $$= p_{0}(x, 2vt) \exp \left[ \frac{1}{2} \alpha^{2} \phi_{k} * \phi_{k}(0) t \right]$$

  (463)

  where $*$ denotes convolution and $p_{0}(x, t) = (2\pi t)^{-1/2} \exp[-x^{2}/2t]$ is the transition probability of standard Brownian motion. As $k \to \infty$, we have $F_{k} \to F$, but $\langle Z_{k}(x, t) \rangle$ diverges since $\langle Z_{k}(x, t) \rangle \propto \exp[(1/2) \alpha^{2} \phi * \phi(0) t]$. In terms of the KPZ equation this means that the average velocity of the interface $\nu_{k} = (1/2) \alpha^{2} \phi_{k} * \phi_{k}(0)$ diverges linearly in $k$. It can be proved, however, that in the frame moving with constant velocity $\nu_{k}$ in the $x$-direction the approximation $Z_{k}(x, t)$ has a well-defined limit:

  $$\lim_{k \to \infty} p_{0}(x, t) Z_{k}(x, t) / \langle Z_{k}(x, t) \rangle = Z(x, t)$$

  (464)
3. Directed Polymer

In the lattice directed polymer setup, we make a discrete approximation to (459) by replacing the Brownian motion \( b(t) \) by a random walk \( w \) on the lattice \( \mathbb{Z}^2 \), where \( w \) starts at \((0, 0)\) and moves with probability \(1/2\) either up or right. At each lattice site there is an independent unit Gaussian potential \( F(i, j) \). This approximation \( Z_N(x, t) \) is also called the partition function of directed polymer:

\[
Z_N(x, t) = \sum_{w:(0,0)} 2^{-tN} e^{-\beta E(w)} \tag{465}
\]

The energy of the walk \( w \) is defined by:

\[
E(w) = \sum_{(i,j)\in w} F(i, j) \tag{466}
\]

It was proved in [Alberts et al (2010)] that in the limit \( N \to \infty \) with \( \beta^4 N = \alpha \) fixed, the discrete approximation \( Z_N(x, t) \) converges to \( Z(x, t) \) and has a well-defined limit:

\[
\lim_{N \to \infty} Z_N(x, t) = Z(x, t) \tag{467}
\]

Exact Solutions to the KPZ Equation:

The exact solutions to the KPZ equation has been discovered in parallel by [Amir et al (2011)] and [Sasamoto, Spohn (2010)], specified in terms of their exact probability distributions and long time limits governed by the KPZ class scaling and statistics. We will introduce the former one, which provides a complete and rigorous proof with credible justification. Before going for the details, we specialise the parameters in the KPZ equation to be \( v = 1/2 \) and \( \lambda = -1 \). Thus the KPZ equation becomes:

\[
\frac{\partial h}{\partial t} = \frac{1}{2} \frac{\partial^2 h}{\partial x^2} - \frac{\lambda}{2} \left( \frac{\partial h}{\partial x} \right)^2 + F(x, t) \tag{468}
\]

This particularisation does not change the general solution \( h_{v, \lambda} \) to the KPZ equation, which can be recovered by changing variables and rescaling as follows:

\[
h_{v, \lambda} = -\frac{\lambda^2}{(2v)^3} h^{\frac{1}{2}}_{-1, -1} \left( \frac{\lambda^2}{(2v)^3} x, -\frac{\lambda^4}{(2v)^5} t \right) \tag{469}
\]

1. Exact Probability Distributions of the Solutions to the KPZ Equation with Sharp Wedge Initial Conditions [Amir et al (2011)]:

For any \( t > 0 \) and \( x \in \mathbb{R} \), the Hopf-Cole solution to the KPZ equation with sharp wedge initial conditions has the following probability distribution:

\[
P\left( h(x, t) - \frac{x^2}{2t} - \frac{t}{24} \geq -s \right) = F_1(s) \tag{470}
\]

where \( F_1(s) \) does not depend on \( x \) and is given by:

\[
F_1(s) = \int_C \frac{d\mu}{\mu} e^{-\mu \det(I - K_{\sigma, \mu})_{L^2(\kappa_1^{-1}s, \infty)}} \tag{471}
\]

where \( \kappa_1 = 2^{-1/3} t^{1/3} \), \( C \) is a contour positively oriented and going from \( +\infty + i\epsilon \) to \( +\infty - i\epsilon \), and \( K_{\sigma} \) is an operator given by its integral kernel:

\[
K_{\sigma}(x, y) = \int_{-\infty}^{\infty} \frac{\mu}{\mu - e^{-\kappa_1 m}} \sigma_{\sigma, \mu}(m) \text{Ai}(x + m) \text{Ai}(y + m) dm \tag{472}
\]

where \( \text{Ai}(x) \) stands for the Airy Function and is defined as:

\[
\text{Ai}(x) = \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{ipx} e^{p^3/3} dp \tag{473}
\]

A corollary of this formula is that as \( t \to \infty \), the statistics of the KPZ equation converge to the Tracy-Widom \( F_{\text{GUE}} \) Distribution under \( t^{1/3} \) scaling, which indicates that the KPZ equation indeed belongs to the KPZ universality class. As \( t \to 0 \), the statistics scale like \( t^{1/4} \) and converge to the Edwards-Wilkinson class.


The Hopf-Cole solution to the KPZ equation with narrow wedge initial data has the following long-time and short-time asymptotics:

\[
\begin{align*}
F_1(2^{-1/3} t^{1/3} s) &\xrightarrow{t \to \infty} F_{\text{GUE}}(s) \\
F_1(2^{-1/2} \pi^{1/4} t^{1/4} (s - \log \sqrt{2\pi t})) &\xrightarrow{t \to 0} G(s)
\end{align*} \tag{474}
\]

The Tracy-Widom GUE Distribution was first discovered in [Tracy, Widom (1994)] and expressed in terms of a Fredholm determinant as well as the solution to the type II Painlevé equation:

\[
F_{\text{GUE}}(s) = \det(I - K_{\lambda_1})_{L^2(s, \infty)} = \exp \left[ - \int_s^{\infty} (x - s) q(x)^2 dx \right] \tag{475}
\]
where \( q(x) \) solves the **Type II Painlevé Equation**:

\[
q''(x) = (x + 2q(x)^2)q(x)
\]

and \( K_{Ai} \) is the **Airy Kernel**, a special kind of integral kernel \( K_\sigma \) where \( \sigma = 1_{t\geq 0} \), defined as:

\[
K_{Ai}(x, y) = \int_{-\infty}^{\infty} 1_{m \geq 0} Ai(x + m)Ai(y + m) dm
\]

\( G(s) \) is the Gaussian distribution:

\[
G(s) = \int_{-\infty}^{s} \frac{1}{\sqrt{2\pi}} e^{-r^2/2} dr
\]

It is also possible to obtain the Hopf-Cole solution with a different type of initial conditions, namely half Brownian initial conditions.

- **2. Exact Probability Distributions of the Solutions to the KPZ Equation with Half Brownian Initial Conditions [Corwin, Quastel (2013)]**:

For any \( t > 0 \) and \( x \in \mathbb{R} \), the Hopf-Cole solution to the KPZ equation with half Brownian initial conditions, given by \( Z(x, 0) = \exp(B(x))1_{x \geq 0} \), has the following probability distribution:

\[
P\left( h(x, t) - \frac{x^2}{2t} - \frac{t}{24} \geq - s \right) = \int_{C} \frac{d\mu}{\mu} e^{-\mu} \det(I - K_{1, x, \mu}^{\Gamma})_{L^2(\sigma^{-1} \times, \infty)}
\]

where \( \kappa_t = 2^{-1/3} t^{1/3} \). \( C \) is a contour positively oriented and going from \( +\infty + i\epsilon \) to \( +\infty - i\epsilon \) and \( K_{1, x, \mu}^{\Gamma} \) is an operator given by its integral kernel:

\[
K_{1, x, \mu}^{\Gamma} = \int_{-\infty}^{\infty} \frac{\mu}{\mu - e^{-\kappa_t m}} Ai^{\Gamma}(x + m, \kappa_t^{-1}, -2^{-2/3}\kappa_t^{-1} x) \times Ai^{\Gamma}(y + m, \kappa_t^{-1}, -2^{-2/3}\kappa_t^{-1} x) dm
\]

The \( \Gamma \) deformed Airy functions are defined as follows:

\[
Ai^{\Gamma}(a, b, c) = \int_{C_{\Gamma}} \exp \left[ \frac{1}{3} z^3 - az \right] \Gamma(-bz + c) dz
\]

\[
Ai^{\Gamma}(a, b, c) = \int_{C_{\Gamma}} \exp \left[ \frac{1}{3} z^3 - az \right] \frac{1}{\Gamma(bz + c)} dz
\]

The contour \( C^{\Gamma} \) comes from \( \infty e^{\pi i/3} \) towards the origin but goes to the left of the pole at \( z = c/b \) and then leaves in the direction \( \infty e^{-\pi i/3} \). The contour \( C^{\Gamma} \) comes from \( \infty e^{\pi i/3} \) towards the origin and then leaves in the direction \( \infty e^{-\pi i/3} \).

### 6 Future Direction

Our enquiry of integrable models in this thesis is merely the beginning of a long journey, along which many interesting perspectives have been brought up for future research in these interactive and interdisciplinary areas.

The analysis for one-dimensional Ising chain in section 3 can be extended to two dimensions using a mathematical tool called dimer statistics [Onsager (1944)], which up to now is only integrable without the presence of magnetic field [McCoy, Wu (2014)].

Following ZRP models characterised by one and two parameters, we can continue to examine the Bethe ansatz solution to the integrable ZRP model with three parameters, which has been proposed by [Povolotsky (2013)].

We can also go up from 2D to 3D surface growth models and investigate their scaling forms by other analytical and numerical methods. For example the single step models can be mapped onto a six-vertex model with equal vertex energies [Meakin et al (1986)].

A classical result that the TASEP converges to the solution of the Burgers equation was proved using subadditive ergodic theorem by [Rost (1981)]. This convergence can be seen as a connection between the discrete transport models in section 4 and the continuous surface models in section 5.

Despite our attempt to introduce some of the techniques to solve KPZ equation, the current research on the topic remains popular and ever growing. A summary of rigorous mathematical treatment of KPZ equation can be found in [Corwin (2011)], including more advanced topics such as the weakly simple exclusion process approximation of the KPZ equation.

It is worthwhile to note that a generalisation of KPZ equation has been proposed by [Hairer, Quastel (2015)]. They found that for a wide range of growth models satisfying the following equation of motion:

\[
\partial_t h = \partial^2_x h + \epsilon P(\partial_x h) + \delta F
\]

where \( P \) is an even polynomial of \( \partial_x h \), it converges to KPZ equation (413) by appropriate rescaling and choice of parameters, and thus those growth models all belong to KPZ class sharing the same critical exponents.

Besides surface growth models, stochastic integrable models are also applicable in other interesting real life sce-
narios such as traffic flow [Schreckenberg et al (1995)] and bus route model [O’Loan et al (1998)], where intensive numerical simulations can be conducted.

7 Bibliography

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