Non-Equilibrium Statistical Field Theory

Lecture Notes

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Recommended Books and Resources

Non-equilibrium statistical field theory is a relatively new research field. Its origins date to the 1970s but it has only received significantly more attention since the 1990s. As with all active research fields, different trends are competing and no single resource – including these lecture notes – can possibly present a balanced view on all of its aspects. In fact, these lecture notes are intentionally ignoring an important branch of the subject, namely Landau-Ginzburg type models, because some of them will be covered in the course on *Theoretical Physics of Soft Condensed Matter*.

Because of its youth, the number of textbooks that cover this topic is relatively limited. An excellent textbook is

Uwe Täuber *Critical Dynamics*, Cambridge University Press, 2014,

which covers everything in this course and much more. For the parts of the lectures on Master Equations and on Langevin Equations *the* classic reference textbook is

N.G. van Kampen *Stochastic Processes in Physics and Chemistry*, Elsevier 1992,

which is worthwhile reading for any researcher with interests in statistical physics as it elegantly covers Master Equations, Fokker-Planck Equations, and Langevin Equations in some detail.

Doi-Peliti field theory is also covered in the following lecture notes:

John Cardy *Lecture Notes on Field Theory and Nonequilibrium Statistical Mechanics*, available at https://www-thphys.physics.ox.ac.uk/people/JohnCardy/

Gunnar Pruessner *Lecture Notes on Non-equilibrium Statistical Mechanics*, available at http://wwwf.imperial.ac.uk/~pruess/publications/Gunnar_Pruessner_field_theory_notes.pdf,

of which the former is very condensed, while the latter provides more details on the derivation of Doi-Peliti field theory.

Contents

Introduction

Non-equilibrium statistical physics is a huge research area covering collective behaviour on all scales from quantum phenomena to population dynamics. It is impossible to create a single comprehensive course on the topic and many exciting subfields have to be left aside. The aim in creating these lectures notes is to provide an introduction to two field theories, Doi-Peliti Field Theory and the Response Field Formalism. Statistical Field theories based on the Landau-Ginzburg type models are treated for the equilibrium case in the *Statistical Field Theory* course and for the non-equilibrium case in the *Theoretical Physics of Soft Condensed Matter* course.

The course does not require you to be familiar with any specific physics subject. In particular, the Statistical Physics course in Part II is not a requirement. What is needed is a basic understanding of probability theory, differential equations and complex methods and an interest in stochastic processes of particles.

Chapter 1

Master Equation

Master Equations are one of the fundamental types of models in Statistical Physics. A plethora of other models can be derived starting from Master Equations, including Fokker-Planck Equations, Langevin Equations, van Kampen system size expansions (also known as Ω expansion), and Kramers-Moyal expansions. Most of these models are explained at length in *Stochastic Processes in Physics and Chemistry*, van Kampen 1992. For Fokker-Planck Equations and Kramers-Moyal expansions, I also recommend Risken 1989.

1.1 Stochastic Processes without Memory

At the heart of Master Equations lies the desire to describe stochastic processes that are *continuous in time* and that are built out of *memoryless* subprocesses. Although time-continuity appears to be the easier characteristic, we start by considering what it means to be memoryless first.

To set the scene, let's define a *stochastic process* to be a sequence of random variables $N(t)$. The variable $t \in T$ can be discrete or continuous but must be *totally ordered* allowing us to interpret it as time. Furthermore, we choose $N(t) \in \mathbb{N}_0$ to take non-negative integer values because we want to count things like particles or people, and we write $P(N(t) = n)$ for the probability that there are n in the system at time t. To enable a compact notation, we allow writing $N(t) < 0$ but enforce that its probability is zero. The interpretation of the set T as time means that we can naturally talk about what happens *before* or *after* and about *memory*. For now, let's say $T = \Delta t\mathbb{Z}$, i.e. a time-line with steps of size Δt. We say $N(t)$ is the state of the system at time t.

The random variable $N(t)$ does not have to depend on any other $N(s)$ but it could in principle depend on arbitrarily many. However, a stochastic process is called memoryless

or *Markovian* if for all times $t_1 < t_2 < \cdots < t_n < t_{n+1}$, we find

$$P\Big(N(t_{n+1})\Big|N(t_n),\ldots,N(t_1)\Big) = P\Big(N(t_{n+1})\Big|N(t_n)\Big), \tag{1.1}$$

which means that the probability distribution of the *next* state of the system only depends on the *most recent* known state. However, it does not mean that $N(t_{n+1})$ is uncorrelated to $N(t_{n-1}), N(t_{n-2}), \ldots$ – an important distinction that is worked out in more detail in the example in Sec. 1.3.3 and subsequently in Sec. 3.2.1. As a commonly used word, 'memoryless' can create associations that can lead to confusion in this mathematical context. We therefore will prefer to use the word Markovian henceforth.

Being Markovian appears to be intuitively true for non-living matter and Ii therefore seems reasonable to model chemical reactions like this. Although it might still be true for bacteria, surely it can't be true for dogs, elephants or humans. However, we are interested in collective behaviour and in using these models, we *assume* that collectively, they are memoryless.

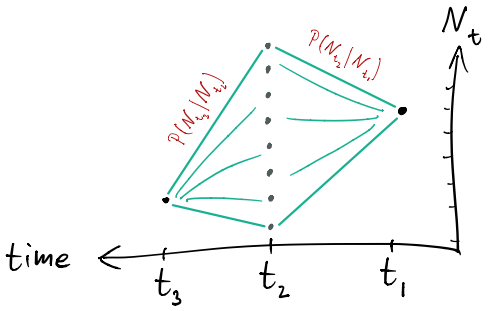


Figure 1.1: The Chapman-Kolmogorov Equation. It describes how transitions of the system between two times can be expressed as a sum over transitions to and from intermediate times.

Being Markovian has far reaching consequences for a process. When expressing how the final state of the system depends on the initial state, we can insert the probabilities to be in other states at intermediate times. Considering the states at times $t_1 < t_2 < t_3$, the joint probability can written in terms of conditional probabilities

$$P\Big(N(t_3),N(t_2),N(t_1)\Big) = P\Big(N(t_3)\Big|N(t_2),N(t_1)\Big)P\Big(N(t_2)\Big|N(t_1)\Big)P\Big(N(t_1)\Big). \tag{1.2}$$

Using the Markovian property, $P\big(N(t_3)|N(t_2),N(t_1)\big) = P\big(N(t_3)|N(t_2)\big)$, we can sum over all values of $N(t_2)$ and divide by $P\big(N(t_1)\big)$ to find the *Chapman-Kolmogorov* Equation

$$P\Big(N(t_3)\Big|N(t_1)\Big) = \sum_{N(t_2)} P\Big(N(t_3)\Big|N(t_2)\Big)P\Big(N(t_2)\Big|N(t_1)\Big). \tag{1.3}$$

Reading this from right to left, it can be interpreted as follows: Given an initial state, the final state is determined by all possible concatenations of transitions from the initial state to an intermediate state and from that intermediate state to the final one.

We can repeat this procedure for n intermediate steps $t_0 < t_1 < \cdots < t_n < t_{n+1}$ and find:

$$P\Big(N(t_{n+1})\Big|N(t_0)\Big) = \sum_{N(t_1),\ldots,N(n)} P\Big(N(t_{n+1})\Big|N(t_n)\Big)P\Big(N(t_n)\Big|N(t_{n-1})\Big)\ldots P\Big(N(t_1)\Big|N(t_0)\Big). \tag{1.4}$$

Again, reading from right to left, it can be interpreted as follows: Given an initial state, the final state is determined by all possible intermediate transitions which form a path from $N(t_0)$ to $N(t_{n+1})$. If you know at this point that in a few lectures time, we want to construct path integrals, then the Chapman-Kolmogorov Equations and its multistep version look already like the nucleus of a path integral.

So far, we have created a stochastic process that is Markovian. In order to arrive at the Master Equation, we have to incorporate continuous time. We could have done this already by simply defining $T = \mathbb{R}$. This demand, would not have changed any of the above results. However, what we really need to think about is, what kind of properties should $P\big(N(t)\big)$ have in continuous time. None of our results require $P\big(N(t)\big)$ to be continuous or differentiable and it could have been a really rough function until now.

1.2 The Continuous-Time Limit

From now on, we use continuous time $T = \mathbb{R}$. While the states of the system remain *discrete*, i.e. non-negative integers, we want that probabilities change *smoothly* over time. In particular, we define probability transition rates $W_t(N'|N)$ as

$$W_t\big(N'\big|N\big) = \frac{\partial P\big(N'(t')\big|N(t)\big)}{\partial t'}\Big|_{t'=t}. \tag{1.5}$$

Note that for W, we drop the dependence of N' and N on t and write it for convenience as index of W. These transition rates are the central objects in each model and describe chemical reactions or interactions between individuals. Further below, we will explore what shape these transitions rates take. But first, we are going to find out what they imply for the Chapman-Kolmogorov Eq. (1.3).

Since the probabilities are smooth, we can use Taylor expansions to describe small changes in time

$$P\Big(N'(t+\Delta t)\Big|N(t)\Big) = \underbrace{P\Big(N'(t)\Big|N(t)\Big)}_{=\delta_{N'(t),N(t)}} + \Delta t\, W_t\big(N'\big|N\big) + \mathcal{O}\big(\Delta t^2\big), \tag{1.6}$$

where the first term in the right hand side is a Kronecker-δ, telling us that the system is with certainty in state $N(t)$ given that we know it is. In particular, the probability $P\big(N(t+\Delta t) = N(t)\big|N(t)\big)$ to stay in state N over an infinitesimal time Δt is 1 minus the probability to leave state N in that time:

$$P\Big(N(t+\Delta t) = N(t)\Big|N(t)\Big) = 1 - \sum_{N'\neq N} P\Big(N'(t+\Delta t)\Big|N(t)\Big) \tag{1.7}$$

$$1 - \Delta t \sum_{N'\neq N} W_t\big(N'\big|N\big) + \mathcal{O}\big(\Delta t^2\big). \tag{1.8}$$

But $P\big(N(t)\big|N(t)\big) = 1$, which implies that the probability transition rate to stay in state N equals

$$\frac{\partial P\big(N'(t') = N(t)\big|N(t)\big)}{\partial t'}\Big|_{t'=t} = W_t\big(N\big|N\big) = -\sum_{N'\neq N} W_t\big(N'\big|N\big), \tag{1.9}$$

which is the negative sum of the rates to leave the state. The second equality implies that the sum over all transition rates is zero

$$\sum_{N'} W_t\big(N'\big|N\big) = 0, \tag{1.10}$$

which we could have actually realized from the start because summing $P\big(N'\big|N\big)$ over N' gives 1. This intermediate result Eq. (1.10) means then that, in order for the total probability to be conserved, all changes in probability must sum to zero.

How do we apply this to the Chapman-Kolmogorov Equation (1.3)? We assume that the final time t_3 and the intermediate time t_2 are very close to each other, $t_3 = t_2 + \Delta t$, and Taylor-expand $P\big(N(t_3)\big|N(t_2)\big)$ for small Δt:

$$P\Big(N(t_3)\Big|N(t_1)\Big) = \sum_{N(t_2)} \big\{\delta_{N(t_2),N(t_3)} + \Delta t\, W_{t_2}\big(N(t_3)\big|N(t_2)\big) + \mathcal{O}(\Delta t^2)\big\} P\Big(N(t_2)\Big|N(t_1)\Big) \tag{1.11}$$

$$\begin{aligned} &= P\Big(N(t_2) = N(t_3)\Big|N(t_1)\Big) + \\ &\quad + \Delta t \sum_{N(t_2)\neq N(t_3)} \Big\{W_{t_2}\big(N(t_3)\big|N(t_2)\big) P\Big(N(t_2)\Big|N(t_1)\Big) - W_{t_2}\big(N(t_2)\big|N(t_3)\big) P\Big(N(t_3)\Big|N(t_1)\Big)\Big\}, \end{aligned}$$

where in the last line, we write the case $N(t_2) = N(t_3)$ in the sum separately and use Eq. (1.9). We can rearrange this equation and finally take the continuous-time limit $\Delta t \to 0$ to discover the *Master Equation*:

$$\frac{\partial P\big(N(t)\big|N(t_0)\big)}{\partial t} = \sum_{N'(t)\neq N(t)} \Big\{W_t\big(N(t)\big|N'(t)\big) P\Big(N'(t)\Big|N(t_0)\Big) - W_t\big(N'(t)\big|N(t)\big) P\Big(N(t)\Big|N(t_0)\Big)\Big\}. \tag{1.12}$$

There is some crucial insight that we can learn here if we unpack the expression on the right hand side. We can split up the sum in Eq. (1.11) into two parts. The first is called *gain* and describes the transition into state N from a different state N'. The second part describes the transition out of state N into another state N', called *loss*. The gain is the first part, the loss is the second in Eq. (1.12).

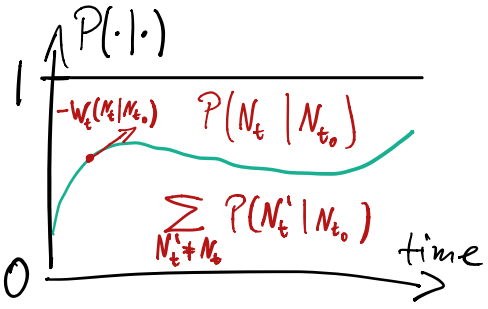


Figure 1.2: Conservation of probability implies that transition rates sum to zero.

The Master Equation (1.12) describes a stochastic process as an infinite system of ordinary differential equations – one equation for each state N. More precisely, it describes the time evolution of a probability distribution with range $\mathbb{N}_0$. From a dynamic systems point of view, it is natural to ask about fixed points and their stability for the system of differential equations. Such fixed points are called *steady states*. They do not necessarily describe a single state and do not imply that the system does not change over time. It only implies that the probability distribution stays constant over time. The state of the system $N(t)$ can still change dynamically, as we will work out in Sec. 1.3.3. However, if the system does not change dynamically at the fixed point, then it describes an *absorbing state* (or states) from which the system cannot escape. A single absorbing state is shown in Sec. 1.3.1, while a system with infinitely many absorbing states appears in Ex. 1.4.

How can the transition rates be found? Well, that depends on the process you are modelling. You can choose any transition rates that satisfy Eq. (1.10). In the following sections, we are going to look at a few examples. In principle, transition rates can be explicitly time-dependent. However, we are only going to look at time-independent rates.

1.3 In Zero Dimensions

1.3.1 Extinction

An extinction process makes particles disappear spontaneously. It does not require interactions between particles. Symbolically, this is written for a particle species A as

$$A \to \emptyset. \tag{1.13}$$

A particle simply waits until it disappears without having a memory of how long it has waited already. The waiting time therefore follows an exponential distribution with some rate ϵ. Because the extinction process kills a single particle at a time, the only valid transitions are from $N > 0$ particles to $N-1$. But what is the transition rate from state N to state $N-1$ if the single particle extinction rate is ϵ?

Each particle undergoes the same identically distributed and independent waiting process. The waiting time for the first of N particles to go extinct is therefore exponentially distributed with rate equal to the sum of the individual rates:

$$W(N-1|N) = N\epsilon. \tag{1.14}$$

Hence, the master equation is

$$\frac{\partial}{\partial t}P\big(N(t)\big|N(t_0)\big) = \underbrace{\epsilon(N(t)+1)P\big(N(t)+1\big|N(t_0)\big)}_{\text{gain}} - \underbrace{\epsilon N(t)P\big(N(t)\big|N(t_0)\big)}_{\text{loss}}, \tag{1.15}$$

where $N(t_0)$ is an initial condition at time t_0.

Setting the left hand side to zero reveals that the only steady state solution is the empty system with $P\big(N(t) = n\big|N(t_0)\big) = \delta_{n,0}$. Therefore, $N = 0$ is an absorbing state.

The described extinction process sounds a lot like a decay process. Are they linked? Yes, they are essentially the same process. However, decay is often associated with the decay rate equation, which can be derived from the Master Equation as a mean field approximation by multiplying Eq. (1.15) with $N(t)$ and then summing over $N(t)$:

$$\frac{\partial}{\partial t}\mathbb{E}[N(t)|N(t_0)] = -\epsilon\mathbb{E}[N(t)|N(t_0)]. \tag{1.16}$$

Exercise 1.1 Take the Master Equation for an extinction process,

$$\frac{\partial}{\partial t}P\big(N(t)\big|N(t_0)\big) = \epsilon\Big((N(t)+1)P\big(N(t)+1\big|N(t_0)\big) - N(t)P\big(N(t)\big|N(t_0)\big)\Big),$$

and derive a differential equation for the nth moment of $N(t)$.

Exercise 1.2 Solve the master equation for an extinction process,

$$\frac{\partial}{\partial t}P\big(N(t)\big|N(0)\big) = \epsilon\Big((N(t)+1)P\big(N(t)+1\big|N(0)\big) - N(t)P\big(N(t)\big|N(0)\big)\Big),$$

for all $N(t) \in \mathbb{N}_0$ with $N(0) = m$ and calculate $\mathbb{E}[N(t)|N(0) = m]$. What is the distribution of the extinction time T_e of the entire population, i.e. the time when the last particle goes extinct? Having found n particles at time t, what is the maximum likelihood estimator for ϵ?

1.3.2 Spontaneous Creation

In the previous system, the particle number can only decrease over time which implies that dynamics, i.e. the non-equilibrium aspect, is short-lived. A process that can counter the particle loss is the spontaneous creation, which is symbolically drawn for a particle species A as

$$\emptyset \to A. \tag{1.17}$$

It places new particles in the system without being influenced by how many are already there and without knowing when the last particle was put in. Hence, it is completely described by a rate γ for an exponential distribution:

$$W(N+1|N) = \gamma. \tag{1.18}$$

As the process creates only one particle at a time, the only allowed transitions add a single particle. Compared to extinction, Eq. (1.14), it does not depend on how many particles are in the system because there are not several simultaneous processes happening.

Therefore, the master equation equals

$$\frac{\partial}{\partial t}P\big(N(t)\big|N(t_0)\big) = \underbrace{\gamma P\big(N(t)-1\big|N(t_0)\big)}_{\text{gain}} - \underbrace{\gamma P\big(N(t)\big|N(t_0)\big)}_{\text{loss}}, \tag{1.19}$$

where $N(t_0)$ is an initial condition at time t_0. Does this process have a steady state? Setting the time derivative equal to zero, implies that $P\big(N(t)\big|N(t_0)\big) = P\big(N(t)-1\big|N(t_0)\big)$ for $N > 0$, which cannot be solved while maintaining normalization. Hence, no steady state exists in this system. In fact, the particle number can never decrease and there is no upper bound to the particle number in the system.

1.3.3 Dynamic steady state

So far, we have seen two example process, extinction and spontaneous creation. The former had a steady state, albeit a boring one, while the latter did not have a steady state at all. The 'problem' was that both processes could only change the particle number in one direction. Now we want to turn to a process that has an interesting steady state. We therefore need to consider a process that can both increase and decrease the particle number. The easiest way to achieve this is by simply combining extinction and spontaneous creation into one process.

But how can we combine them? We assume that extinction and spontaneous creation are independent in the sense that their probability transmission rates $W(N'|N)$ are added. This way, condition (1.10) remains fulfilled automatically. The transmission rates are

$$W(N-1|N) = \epsilon N \qquad \text{and} \qquad W(N+1|N) = \gamma. \tag{1.20}$$

Hence, the master equation reads

$$\frac{\partial}{\partial t}P\big(N(t)\big|N(t_0)\big) = \underbrace{\epsilon(N(t)+1)P\big(N(t)+1\big|N(t_0)\big)}_{\text{gain}} - \underbrace{\epsilon N(t)P\big(N(t)\big|N(t_0)\big)}_{\text{loss}} \tag{1.21}$$

$$+ \underbrace{\gamma P\big(N(t)-1\big|N(t_0)\big)}_{\text{gain}} - \underbrace{\gamma P\big(N(t)\big|N(t_0)\big)}_{\text{loss}}. \tag{1.22}$$

The first line of the right hand side contains the extinction and its second line contains the spontaneous creation. What is the steady state distribution $\lim_{t\to\infty} P\big(N(t)\big|N(t_0)\big) = P\big(N\big|N(t_0)\big)$ of this system? If we first consider the case $N = 0$, we find an inductive

relation

$$P\big(1\big|N(t_0)\big) = \frac{\gamma}{\epsilon} P\big(0\big|N(t_0)\big) \tag{1.23a}$$

$$P\big(2\big|N(t_0)\big) = \frac{1}{2}\left(\frac{\gamma}{\epsilon}\right)^2 P\big(0\big|N(t_0)\big) \tag{1.23b}$$

$$P\big(3\big|N(t_0)\big) = \frac{1}{6}\left(\frac{\gamma}{\epsilon}\right)^3 P\big(0\big|N(t_0)\big) \tag{1.23c}$$

$$\vdots \qquad \vdots$$

$$P\big(N\big|N(t_0)\big) = \frac{1}{N!}\left(\frac{\gamma}{\epsilon}\right)^N P\big(0\big|N(t_0)\big). \tag{1.23d}$$

Normalization implies $P\big(0\big|N(t_0)\big) = e^{-\gamma/\epsilon}$. Hence in steady state, the particle number is Poisson distributed with parameter γ/ϵ, no matter what the initial conditions $N(t_0)$ were. The pure extinction process from Sec. 1.3.1 and the pure spontaneous creation process from Sec. 1.3.2 can be regarded as limiting cases: considering its mean particle number $\mathbb{E}[N|N(t_0)] = \gamma/\epsilon$, the absorbing state $N = 0$ is found for $\gamma \to 0$ while a divergence is found in the case $\epsilon \to 0$.

Even though the steady state particle number distribution is time-independent, this does not mean that the system becomes static. In fact, if the system is in state N, then the next extinction or spontaneous creation occurs after a time τ which is exponentially distributed with rate $N\epsilon + \gamma$. Thus, the Poisson distribution $P\big(N\big|N(t_0)\big)$ can be seen as a *prior* distribution of the waiting time τ between events that change the particle number in the system. Its conditional probability density function is

$$f(\tau|N) = (N\epsilon + \gamma)e^{-(N\epsilon+\gamma)\tau} \tag{1.24}$$

and hence its marginal probability density function equals

$$f(\tau) = \sum_{N=0}^{\infty} f(\tau|N) P\big(N\big|N(t_0)\big) = \gamma e^{\frac{\gamma}{\epsilon}(e^{-\epsilon\tau}-1)-\gamma\tau}\left(1 + e^{-\epsilon\tau}\right) \tag{1.25}$$

and cumulative distribution function $F(\tau)$

$$F(\tau) = 1 - e^{\frac{\gamma}{\epsilon}(e^{-\epsilon\tau}-1)-\gamma\tau}. \tag{1.26}$$

As the Poisson distribution is naturally associated with the exponential distribution, it is worth emphasizing that τ is *not* exponentially distributed.

The fact that the particle number can only change by ± 1 at any specific time implies that there are time correlations. However, relating $N(t_1)$ to $N(t_2)$ is a difficult task. The difficulty lies in the time-continuity: there is no definite number of how many spontaneous creations or extinctions happened between t_1 and t_2. The system could have taken any of the infinite allowed paths in the configuration space $[t_1, t_2] \times \mathbb{N}_0$. It is one of the strengths of Doi-Peliti field theory to deal with such problems elegantly and efficiently. Particularly the example of extinction and spontaneous creation will be continued and solved in Sec. 3.2.1.

1.3.4 Coagulation

The previous examples included simple decreases and increases of the particle number through extinction and spontaneous creation. However in those examples, particles did not really *interact*. It is interactions that not only enrich a system's dynamics but also show that directly solving the master equation becomes a daunting prospect. Luckily, it thus provides an excellent motivation for Doi-Peliti field theory in Chap. 3.

Coagulation is the interaction of two particles that has only one particle as end product. It can be imagined as two particles colliding and acting as one from then on. We draw it as

$$\begin{matrix} A \\ A \end{matrix} \!\!\searrow\!\!\longrightarrow A \qquad \text{or} \qquad 2A \to A. \tag{1.27}$$

If the system contains N particles, there are $\binom{N}{2}$ choices of particle pairs that can coagulate. The probability transition rates are therefore

$$W(N-1|N) = \lambda \binom{N}{2}, \tag{1.28}$$

where λ serves as a base rate for the interaction. Setting $\binom{0}{2} = \binom{1}{2} = 0$ enforces that coagulation cannot happen if there is no or only one particle in the system. Hence in a system with only coagulation, there are two possible absorbing states: the empty system and the system with a single particle.

However, as we have seen with extinction and spontaneous creation, the more complex behaviour appears when we combine several processes. The master equation of a system with all three processes together equals

$$\frac{\partial}{\partial t} P\big(N(t)\big|N(t_0)\big) = \underbrace{\epsilon(N(t)+1)P\big(N(t)+1\big|N(t_0)\big)}_{\text{gain}} - \underbrace{\epsilon N(t) P\big(N(t)\big|N(t_0)\big)}_{\text{loss}} \tag{1.29a}$$

$$+ \underbrace{\gamma P\big(N(t)-1\big|N(t_0)\big)}_{\text{gain}} - \underbrace{\gamma P\big(N(t)\big|N(t_0)\big)}_{\text{loss}} \tag{1.29b}$$

$$+ \underbrace{\lambda \binom{N(t)+1}{2} P\big(N(t)+1\big|N(t_0)\big)}_{\text{gain}} - \underbrace{\lambda \binom{N(t)}{2} P\big(N(t)\big|N(t_0)\big)}_{\text{loss}}. \tag{1.29c}$$

Is there a steady state? Compared to the system with only extinction and spontaneous creation, including coagulation only increases the reduction of particles. Therefore, it is reasonable to expect a steady state. Using the same approach as in Eq. (1.23), we find

the inductive relation

$$P\big(1\big|N(t_0)\big) = \frac{\gamma}{\epsilon} P\big(0\big|N(t_0)\big) \tag{1.30a}$$

$$P\big(2\big|N(t_0)\big) = \frac{\gamma^2}{(2\epsilon+\lambda)\epsilon} P\big(0\big|N(t_0)\big)\big) \tag{1.30b}$$

$$P\big(3\big|N(t_0)\big) = \frac{\gamma^3}{(3\epsilon+3\lambda)(2\epsilon+\lambda)\epsilon} P\big(0\big|N(t_0)\big) \tag{1.30c}$$

$$P\big(4\big|N(t_0)\big) = \frac{\gamma^4}{(4\epsilon+6\lambda)(3\epsilon+3\lambda)(2\epsilon+\lambda)\epsilon} P\big(0\big|N(t_0)\big) \tag{1.30d}$$

$$\vdots \qquad \vdots$$

$$P\big(N\big|N(t_0)\big) = \left(\prod_{k=1}^{N} \frac{\gamma}{\big(k\epsilon + \binom{k}{2}\lambda\big)}\right) P\big(0\big|N(t_0)\big). \tag{1.30e}$$

However, normalizing $P\big(N\big|N(t_0)\big)$ is tricky and it is not obvious how to extract means or higher moments of this distribution.

Considering that processes can be terribly complex and difficult to solve exactly, what are possible approximation schemes? We are going to compare three approaches: the van-Kampen System size expansion, the Kramers-Moyal Expansion and Doi-Peliti field theory.

But before we continue with solution schemes, we continue to explore what Master equations can model. This way, we not only collect different models but also different problems that can arise before we see how different approaches tackle those different problems.

1.3.5 Multiple Particle Species

So far, we have only considered one particle species, which is an unnecessary restriction on our models. It is easily overcome by allowing the random variables $N(t)$ to be random vectors. While we could set up independent particle systems by considering separate master equations, multiple-particle system become only interesting in their own right if we allow them to interact.

Transmutation

The simplest interaction is the *transmutation*. It is the reaction in which one particle of one species can transform into another particle of another species:

$$A \to B. \tag{1.31}$$

We denote the particle number of the first species by M, the particle number of the second species by N and assume that particles wait exponentially distributed waiting times with rate τ before transmuting. Hence the probability transition rate is

$$W(M-1, N+1|M, N) = M\tau. \tag{1.32}$$

We can write down the Master Equation of the pure transmutation:

$$\begin{aligned}\frac{\partial}{\partial t}P\big(M(t), N(t)\big|M(t_0), N(t_0)\big) = &\underbrace{\tau(M(t)+1)P\big(M(t)+1, N(t)-1\big|M(t_0), N(t_0)\big)}_{\text{gain}} \\ &\underbrace{-\tau M(t)P\big(M(t), N(t)\big|M(t_0), N(t_0)\big)}_{\text{loss}},\end{aligned} \tag{1.33}$$

and solve it, but we would quickly realize that this process is simply a superposition of i.i.d. exponential distributions. Once all the particles transmuted, nothing happens anymore. However, it becomes more interesting once other processes are combined with transmutation.

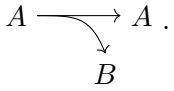
Exercise 1.3 Consider the master equation for pure transmutation from species A to species B, with particle numbers $M(t)$ and $N(t)$ respectively:

$$\begin{aligned}\frac{\partial}{\partial t}P\big(M(t), N(t)\big|M_0, 0\big) = \tau\Big(&(M(t)+1)P\big(M(t)+1, N(t)-1\big|M_0, 0\big) \\ &- M(t)P\big(M(t), N(t)\big|M_0, 0\big)\Big).\end{aligned}$$

Assume that the system is initialized with $M_0 = M(0)$ particles of species A at time $t_0 = 0$ and no particles of species B, i.e. $N(0) = 0$. Calculate $P\big(M(t), N(t)\big|M_0, 0\big)$. What is the steady state? Determine the expected time to reach it.

Spawning

While transmutation keeps the overall particle number constant, we can also allow particles to produce other particles without having an effect on itself. This is called *spawning* and in its simplest setting, species A produces species B:



(1.34)

Its probability transition rate is very similar to the one of the transmutation process, see Eq. (1.32):

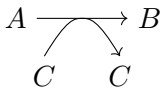
$$W(M, N+1|M, N) = M\tau. \tag{1.35}$$

From the previous processes, we can deduce how this system behaves: Once initialized with a certain number of A particles, the B particles will start to appear just like in the spontaneous creation process, Sec. 1.3.2. So, is spawning just a complicated way of writing spontaneous creation? No, because we can allow species A to follow a stochastic process. Thus, species B will have a varying creation rate. However, we have to be careful not to confuse deterministically varying creation rates, which are simply functions of time, with stochastically varying creation rates, as will be shown in Ex. 1.4 below.

Exercise 1.4 A system contains species A and B. A particle of species A goes extinct with rate ϵ and spawns to species B with rate τ. Write the master equation of the system and find its absorbing state given that it was initialized with M_0 particles of species A and no particles of species B. Compare the result to the steady state of a system with only spontaneous creation of species B, where the creation rate $\gamma(t)$ is determined by the extinction process of species A: $\gamma(t) = \tau M(t) P\big(M(t)\big|M_0\big)$.

Catalyst

Once we have the ability to use Master Equation to model the stochastic interaction of multiple particle species, chemistry provides a plethora of example processes. One example from chemistry is that of a catalyst. It is a particle which promotes reactions. For example the transmutation of particle species A to species B might be very slow on its own, but if a catalyst of species C takes part in the reaction, it might be sped up significantly.



(1.36)

Its probability transition rates involves the particles numbers L, M, N of all three species A, B and C, respectively:

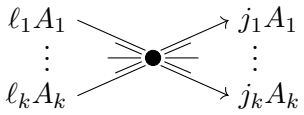
$$W(L-1, M+1, N|L, M, N) = LN\eta, \tag{1.37}$$

where η is the base rate. We see that the transition rate increases linearly in the catalyst particle number. If the catalyst does not follow any other stochastic process, then it simply serves as an effective transmutation rate. But does this remain true if the catalyst particle number fluctuates? Ex. 1.5 below explores this question.

Exercise 1.5 Assume that species C undergoes extinction with rate ϵ and spontaneous creation with rate γ and that C is a catalyst for the transmutation of species A into species B. Determine the Master Equation for the process and reduce it to a Master Equation for species A and B only. Assume that particles of species C are in steady state and that the system is otherwise empty for $t < 0$. At time $t = 0$, L_0 particles of species A are put into the system. Determine how long it takes until all A particles have turned into B particles.

1.3.6 General Reactions

Having seen many concrete examples in the previous sections, we can confidently make the leap to a generalization. Any interaction of particles consists of reactants and products, which can only appear in portions of non-negative integers. Let's assume that the entire system contains k particle species that can appear as reactants and products and that species i appears ℓ_i times as a reactant and j_i times as a product:



(1.38)

As the only defining feature of a particle is its species, particles of the same species have to be treated as being indistinguishable. Hence, the probability transition rates must contain a count of the number of ways to choose all the reactants necessary for the interaction:

$$W\big(N_1 - \ell_1 + j_1, \ldots, N_k - \ell_k + j_k \big| N_1, \ldots, N_k\big) = r\binom{N_1}{\ell_1} \cdots \binom{N_k}{\ell_k}, \tag{1.39}$$

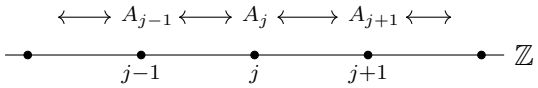
where r is a, possibly time-dependent, base rate of the interaction. Despite having reached this general expression that allows us to capture almost any process describable by Master Equations, we have not explored the full extent of interpretation yet. What has been missing in particular is the modelling of a space on which particles move.

1.4 Processes in Space

Up until now, we have not thought about in what kind of space these stochastic processes take place. Particles have only reacted but they have not move. In fact, we can think of all the previous examples as processes in zero dimensions. While mathematically it makes sense to think of zero dimensions as a point, chemically it makes more sense to think of it as fast mixing of reactants. Any particle density difference is alleviated so quickly compared to the time scale of reactions that it is fair to assume that the particle number is equal everywhere. Sometimes, this is referred to *homogeneity assumption* and any reaction equation that does not include any movement is, sometimes tacitly, modelling a homogenous particle system.

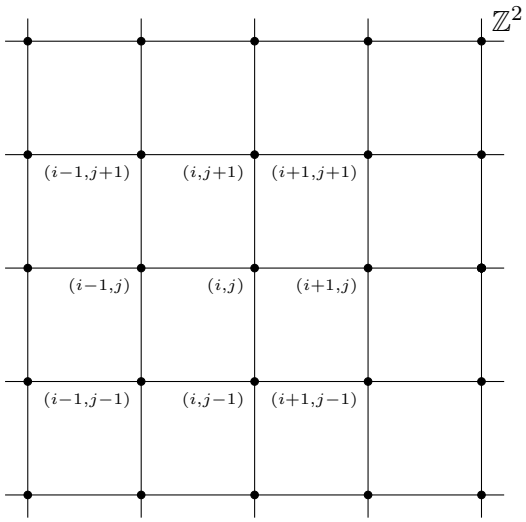
How can we include movement of a particle? By imagining that at every position, the system has a different particle species, which we label by its coordinate. The movement of a particle from position x to position y is thus modelled by the transmutations that link particle species A_x to particle species A_y. However, we can only regard A_x as the same particle species as A_y if they behave otherwise identically. As transmutations are discrete events, the space too has to be discrete at this stage.

Although, we can force particles to move only in one direction, typically particles can move back and forth, which is implemented by including transmutations in both directions. The first example, and one of the easiest to draw is that of a discrete line with coordinates $j \in \mathbb{Z}$:



(1.40)

But remember, there is no metric on this space yet. In order to think of movement, we need to assign a distance measure of which the simplest is the one setting a distance h between any neighboring sites. Similarly, the system can be placed in a two dimensional square lattice by introducing particle species $A_{(i,j)}$ for position $(i, j) \in \mathbb{Z}^2$ with transmutations following either horizontal or vertical connections:



(1.41)

The approach of square lattices can be continued to any hyper lattice $\mathbb{Z}^d$ in d dimensions, but in principle we can create any discrete space by creating particle species for every site. Furthermore, we can put more than one species on every site in order to model several types of particles, with possibly different movements, on the same space and allow them to interact through any of the processes described in zero dimensions.

What types of movements can be modelled on these spaces? The most natural movement in the context of chemistry is diffusion, but we can also include directed motion or nonlocal motion. In addition, movement can be induced by interactions of particles and conversely, moving particles can become immobile due to interactions.

1.4.1 Diffusion

Diffusion is the stochastic process of a particle moving to all nearest neighbors with equal probability at equal rates. Denoting the space by X and assuming that nearest

neighbors x and y have distance $|x-y|=1$, a Master Equation for a diffusive movement process can be written as

$$\frac{\partial}{\partial t}P\big(N\big|N_0\big) = \frac{D}{h^2}\sum_{x\in X}\sum_{\substack{y\in X\\ |x-y|=h}}\Big((N_x+1)P\big(N+1_x-1_y\big|N_0\big) - N_xP\big(N\big|N_0\big)\Big), \quad (1.42)$$

where $N\in\mathbb{N}_0^X$ is the particle number vector with entries N_x and $1_x\in\mathbb{N}_0^X$ is the vector that is zero except at entry x, where it contains a 1. We have omitted all the time dependencies to make the equation more readable and denote the initial condition by $N_0\in\mathbb{N}_0^X$. The hopping rate to nearest neighbors is set to equal D/h^2, where h is the distance between neighbors and D is the diffusion constant. Because of the symmetry of the movement, the expected position does not change in time.

Eq. (1.42) models diffusion on a microscopic level with discrete positions and discrete particle numbers. How does it relate to the better known diffusion equation? We relate them by calculating the expected particle number for a specific site z:

$$\mathbb{E}[N_z|N_0] = \sum_N N_zP\big(N\big|N_0\big). \quad (1.43)$$

If we multiply the Master Equation by N_z and sum it over all N, we find

$$\frac{\partial}{\partial t}\mathbb{E}[N_z|N_0] = \sum_N N_z\frac{D}{h^2}\sum_{x\in X}\sum_{\substack{y\in X\\ |x-y|=h}}\Big((N_x+1)P\big(N+1_x-1_y\big|N_0\big) - N_xP\big(N\big|N_0\big)\Big) \quad (1.44)$$

$$= \frac{D}{h^2}\sum_{\substack{y\in X\\ |z-y|=h}}\Big(\mathbb{E}[(N_y|N_0] - \mathbb{E}[N_z|N_0]\Big) \quad (1.45)$$

$$= D\sum_e \frac{\mathbb{E}[N_{z+e}|N_0] - 2\mathbb{E}[N_z|N_0] + \mathbb{E}[N_{z-e}|N_0]}{h^2} \quad (1.46)$$

$$= D\Delta_z\mathbb{E}[N_z|N_0], \quad (1.47)$$

where from the first to the second line, it is useful to distinguish the three cases $z\neq x\wedge z\neq y$, $z=x$ and $z=y$, and where in the third line, the sum over nearest neighbors y is replaced by a sum over the orthogonal directions e, assuming there are two neighbors for each direction. The Δ_z is the last line is the discrete Laplacian which becomes the standard Laplacian in the continuum limit $h\to 0$.

Thus, we found the standard diffusion equation as the continuum limit of the equation for the expected particle number, i.e. it is a mean field description. It also means that we loose some stochastic information about the microscopic diffusion process when working with the standard diffusion equation. But couldn't we derive a corresponding partial

differential equation for other statistical quantities, say other moments? In some cases, the answer is yes as we can see for correlations. Assuming that $z_1 \neq z_2$, we find

$$\begin{aligned}\frac{\partial}{\partial t}\mathbb{E}[N_{z_1}N_{z_2}|N_0] &= \sum_N N_{z_1}N_{z_2}\frac{D}{h^2}\sum_{x\in X}\sum_{\substack{y\in Y\\|y-x|=h}}\Big((N_x+1)P\big(N+1_x-1_y\big|N_0\big)-N_xP\big(N\big|N_0\big)\Big)\\ &= \frac{D}{h^2}\sum_{\substack{y\in Y\\|y-z_1|=h}}\Big(\mathbb{E}[N_yN_{z_2}|N_0]-\mathbb{E}[N_{z_1}N_{z_2}|N_0]\Big)+\frac{D}{h^2}\sum_{\substack{y\in Y\\|y-z_2|=h}}\Big(\mathbb{E}[N_yN_{z_1}|N_0]-\mathbb{E}[N_{z_1}N_{z_2}|N_0]\Big)\\ &= D(\Delta_{z_1}+\Delta_{z_2})\mathbb{E}[N_{z_1}N_{z_2}|N_0], \qquad (1.48)\end{aligned}$$

for which a continuum limit $h \to 0$ can be taken. However, applying this approach to $\mathbb{E}[N_z^2|N_0]$ does not admit a continuum limit. In particular, we have to be aware that for a differentiable function $f(z_1, z_2)$ in general $\Delta_{z_1}\lim_{z_2\to z_1} f(z_1, z_2) \neq \lim_{z_2\to z_1}\Delta_{z_1} f(z_1, z_2)$.

What is the point of these derivations? We see that the Master Equation allows extracting secondary equations for specific statistical properties which might be easier solved. However, the resulting equations come at the cost of losing a more precise descriptions of the stochasticity of the process.

1.4.2 Ballistic Movement

The word ballistic is often associated with deterministic unidirectional movement in which the displacement increases linear with time. A stochastic process such as the ones we considered here cannot imitate the deterministic aspect, but it can imitate the time-dependence in expectation. The movement is associated with a direction vector e such that for any position x the next position $x+e$ is also on the lattice. In the following Master Equation the hopping rate is denoted by ν:

$$\frac{\partial}{\partial t}P\big(N\big|N_0\big) = \nu\sum_{x\in X}\Big((N_x+1)P\big(N+1_x-1_{x+e}\big|N_0\big)-N_xP\big(N\big|N_0\big)\Big). \qquad (1.49)$$

In comparison with diffusion, the time-dependence of the mean square displacement is often cited as quadratic increase for ballistic, linear increase for diffusive behavior.

Exercise 1.6 Let a particle move ballistically on $\mathbb{Z}$ with hopping rate ν, starting at position $j = 0$ at time $t = 0$. The lattice spacing is h. Determine the particle's expected speed, variance of the speed, the mean square displacement and probability to be at position $j \neq 0$ at time $t > 0$. Does the particle have a maximum speed?

1.4.3 Induced Movement

Both diffusion and ballistic movement continue independently of any other particles around. They just carry on as time goes by not caring about what happens around them. However, we can include interactions with other particles to disturb them. We can include a reaction that induces a change in direction of ballistic motion, or a change of the diffusion constant or a switch between the two types of motion, which is called run-and-tumble and performed by certain bacteria.

On the other hand, we can also consider otherwise immobile particles that jump one step whenever a reaction occurs. Denoting by N_x the particle number of the jumping particle and M_x the particle number of the inducer, the probability transition rate equals

$$W\big(N_{x+e}+1, N_x-1, M_x\big|N_{x+e}, N_x, M_x\big) = \mu M_x N_x, \tag{1.50}$$

where μ is the base rate for this interaction.

1.4.4 Induced Immbolization

While in the previous section, movement was induced by a reaction, we can also reverse the set up by including reactions of moving particles that turn them into stationary ones. A useful picture might be that of epitaxy where diffusive particles become immobile if there come next to another immobile one and react with it. Let's denote by M_x the diffusive particle's number at position x and by N_x the crystalized ones. Hence, its probability transition rate is

$$W\big(M_x-1, N_x+1, N_y\big|M_x, N_x, N_y\big) = \kappa M_x N_y \qquad \text{with } |x-y|=1, \tag{1.51}$$

where κ is the crystallization rate.

1.5 Outlook

Master Equations are more a starting point for scientific investigation than an end result. They are easily used to create microscopic models but solving them is often really hard, which has led to the development of several tools and instruments that allow simplifying, extracting and approximating properties of the model. They include Fokker-Planck Equations, Langevin Equations, van Kampen system size expansion, Kramers Moyal expansion, Doi-Peliti field theory and the Response Field Formalism, of which only Doi-Peliti field theory is equivalent to the full Master Equation in the sense that it does not enforce a simplification but provides a different approach to solving it. In some cases, depending on the exact Master Equation, the other tools can be an equivalent representation as well.

Exercises

Ex. 1.1 Take the Master Equation for an extinction process,

$$\frac{\partial}{\partial t}P\big(N(t)\big|N(t_0)\big) = \epsilon\Big((N(t)+1)P\big(N(t)+1\big|N(t_0)\big) - N(t)P\big(N(t)\big|N(t_0)\big)\Big),$$

and derive a differential equation for the nth moment of $N(t)$.

Ex. 1.2 Solve the master equation for an extinction process,

$$\frac{\partial}{\partial t}P\big(N(t)\big|N(0)\big) = \epsilon\Big((N+1)P\big(N(t)+1\big|N(0)\big) - NP\big(N(t)\big|N(0)\big)\Big),$$

for all $N(t) \in \mathbb{N}_0$ with $N(0) = m$ and calculate $\mathbb{E}[N(t)|N(0) = m]$. What is the distribution of the extinction time T_e of the entire population, i.e. the time when the last particle goes extinct? Having found n particles at time t, what is the maximum likelihood estimator for ϵ?

Ex. 1.3 Consider the master equation for pure transmutation from species A to species B, with particle numbers $M(t)$ and $N(t)$ respectively:

$$\begin{aligned}\frac{\partial}{\partial t}P\big(M(t),N(t)\big|M_0,0\big) = \tau\Big((M(t)+1)P\big(M(t)+1,N(t)-1\big|M_0,0\big)\\ - M(t)P\big(M(t),N(t)\big|M_0,0\big)\Big).\end{aligned}$$

Assume that the system is initialized with $M_0 = M(0)$ particles of species A at time $t_0 = 0$ and no particles of species B, i.e. $N(0) = 0$. Calculate $P\big(M(t),N(t)\big|M_0,0\big)$. What is the steady state? Determine the expected time to reach it.

Ex. 1.4 A system contains species A and B. A particle of species A goes extinct with rate ϵ and spawns to species B with rate τ. Write the master equation of the system and find its absorbing state given that it was initialized with M_0 particles of species A and no particles of species B. Compare the result to the absorbing state of a system with only spontaneous creation of species B, where the creation rate $\gamma(t)$ is determined by the extinction process of species A: $\gamma(t) = \tau M(t)P\big(M(t)\big|M_0\big)$.

Ex. 1.5 Assume that species C undergoes extinction with rate ϵ and spontaneous creation with rate γ and that C is a catalyst for the transmutation of species A into species B. Determine the Master Equation for the process and reduce it to a Master Equation for species A and B only. Assume that particles of species C are in steady state and that the system is otherwise empty for $t < 0$. At time $t = 0$, L_0 particles of species A are put into the system. Determine how long it takes until all A particles have turned into B particles.

Ex. 1.6 Let a particle move ballistically on $\mathbb{Z}$ with hopping rate ν, starting at position $j = 0$ at time $t = 0$. The lattice spacing is h. Determine the particle's expected speed, variance of the speed, the mean square displacement and probability to be at position $j \neq 0$ at time $t > 0$. Does the particle have a maximum speed?

Chapter 2

Second Quantization of Master Equation

Although the title of this chapter sounds very dramatic not least due to its obscurity, the essence of this chapter is the transformation of the system of linear ordinary differentials equations (ODEs) that make up the Master Equation into a *single* partial differential equation (PDE). *Second Quantization* refers to the compact representation of the resulting PDE, which allows efficient handling. A less threatening but also less exciting title of this chapter would have been: "Casting the Master Equation in terms of the Probability Generating Function".

But we don't stop there. Once we derived the PDE for the probability generating function, we start transforming it into the path integral, which unfortunately comes with a few technical points. However, we are rewarded at the end of this chapter by finding the full path integral – although we will not know what to do with it yet.

2.1 Casting the Master Equation in terms of the Probability Generating Function

Given the probability distribution $P(N|N_0)$, which is short for $P\big(N(t)\big|N(t_0)\big)$, of a stochastic process, the corresponding probability generating function is

$$\mathcal{M}(z,t) = \sum_{N=0}^{\infty} P\big(N\big|N_0\big) z^N. \tag{2.1}$$

If there is only one particle species in the system, z is a scalar variable. However, if there are k particle species in the system, then the generating function equals

$$\mathcal{M}(z_1,\dots,z_k,t) = \sum_{N_1,\dots,N_k=0}^{\infty} P\big(N_1,\dots,N_k\big|N_{10},\dots,N_{k0}\big) z_1^{N_1}\cdots z_k^{N_k}, \tag{2.2}$$

which we continue to write as Eq. (2.1) for short – even if there are infinitely many species involved.

From the Master Equation (1.12) we derive a differential equation for the probability generating function by taking the time derivative of $\mathcal{M}(z,t)$ and replacing the occurring time derivatives of $P\big(N\big|N_0\big)$ by their expressions in the Master Equation:

$$\begin{aligned}\frac{\partial}{\partial t}\mathcal{M}(z,t) &= \sum_{N=0}^{\infty}\frac{\partial}{\partial t}P\big(N\big|N_0\big)z^N \\ &= \sum_{N=0}^{\infty}\sum_{N'\neq N}\Big\{W(N|N')P\big(N'\big|N_0\big) - W(N'|N)P\big(N\big|N_0\big)\Big\}z^N.\end{aligned} \tag{2.3}$$

Although we have now written the entire system of ODEs of the Master Equation into one equation for an analytic function in z, we haven't really gained anything so far.

Let's look at an explicit example to see if we can find a more useful expression. The Master Equation for the extinction process was

$$\frac{\partial}{\partial t}P\big(N\big|N_0\big) = \epsilon\Big((N+1)P\big(N+1\big|N_0\big) - NP\big(N\big|N_0\big)\Big), \tag{1.15}$$

omitting the explicit t-dependence of $N(t)$. Hence, Eq. (2.3) can be written as

$$\frac{\partial}{\partial t}\mathcal{M}(z,t) = \epsilon\left(\sum_{N=0}^{\infty}(N+1)P\big(N+1\big|N_0\big)z^N - \sum_{N=0}^{\infty}NP\big(N\big|N_0\big)z^N\right) \tag{2.4}$$

$$= \epsilon\left(\sum_{N=0}^{\infty}\frac{\mathrm{d}}{\mathrm{d}z}P\big(N+1\big|N_0\big)z^{N+1} - \sum_{N=0}^{\infty}z\frac{\mathrm{d}}{\mathrm{d}z}P\big(N\big|N_0\big)z^N\right) \tag{2.5}$$

$$= \epsilon(1-z)\frac{\mathrm{d}}{\mathrm{d}z}\mathcal{M}(z,t). \tag{2.6}$$

Now, we have actually found a different expression of the systems dynamics: instead of describing it as an infinite system of coupled linear ODEs, it is described as a single linear PDE. Whether this is more useful depends on what tools have to solve them. Although the general rule of thumb is that ODEs are easier to solve than PDEs, infinitely many coupled ODEs might be very difficult to solve compared to a single PDE.

In the example of the extinction process, the PDE involves two variables t and z. However, we also consider stochastic processes with multiple particle species, which implies that the PDE will involve more z variables. For example, the Master Equation for the

transmutation process from species A to species B, with particle numbers M and N respectively, is

$$\frac{\partial}{\partial t}P\big(M,N\big|M_0,N_0\big)=\tau\Big((M+1)P\big(M+1,N-1\big|M_0,N_0\big)-MP\big(M,N\big|M_0,N_0\big)\Big). \tag{1.33}$$

We use auxiliary variables z_A and z_B for species A and B to express the PDE for the probability generating function as

$$\begin{aligned}\frac{\partial}{\partial t}\mathcal{M}(z,t)=&\tau\sum_{M,N=0}^{\infty}\Big((M+1)P\big(M+1,N-1\big|M_0,N_0\big)-MP\big(M,N\big|M_0,N_0\big)\Big)z_A^M z_B^N\\ =&\tau\Bigg(\sum_{M,N=0}^{\infty}z_B\frac{\mathrm{d}}{\mathrm{d}z_A}P\big(M+1,N-1\big|M_0,N_0\big)z_A^{M+1}z_B^{N-1}+\\ &\qquad-\sum_{M,N=0}^{\infty}z_A\frac{\mathrm{d}}{\mathrm{d}z_A}P\big(M,N\big|M_0,N_0\big)z_A^M z_B^N\Bigg)\\ =&\tau(z_B-z_A)\frac{\mathrm{d}}{\mathrm{d}z_A}\mathcal{M}(z,t).\end{aligned} \tag{2.7}$$

We can repeat the transformation of the Master Equation into a PDE of the probability generating function for all the processes we discussed in Chap. 1, see Ex. 2.1.

Exercise 2.1 The Master Equations for the (a) spontaneous creation process with rate γ, (b) coagulation process with rate λ and (c) diffusion with rate D/h^2 are:

$$(a)\qquad \frac{\partial}{\partial t}P\big(N\big|N_0\big)=\gamma P\big(N-1\big|N_0\big)-\gamma P\big(N\big|N_0\big)$$

$$(b)\qquad \frac{\partial}{\partial t}P\big(N\big|N_0\big)=\lambda\binom{N+1}{2}P\big(N+1\big|N_0\big)-\lambda\binom{N}{2}P\big(N\big|N_0\big)$$

$$(c)\qquad \frac{\partial}{\partial t}P\big(N\big|N_0\big)=\frac{D}{h^2}\sum_{x\in X}\sum_{\substack{y\in X\\|x-y|=h}}\Big((N_x+1)P\big(N+1_x-1_y\big|N_0\big)-N_xP\big(N\big|N_0\big)\Big),$$

Derive the corresponding PDEs for the moment generating function $\mathcal{M}(z,t)$.

Having arrived at PDE descriptions for stochastic processes, can we derive interesting properties without solving the full PDE? Sometimes yes: in Sec. 1.3.3, we explored the dynamic steady state of a single-particle-species system undergoing extinction and spontaneous creation. We found the steady state by iteratively solving of every algebraic equation that is part of the Master Equation in which the time derivative is set to zero.

Could we have found the solution more directly by solving the corresponding equation for $\mathcal{M}(z,t)$?

$$\frac{\partial}{\partial t}\mathcal{M}(z,t) = 0 = \Big(\epsilon(1-z)\frac{\mathrm{d}}{\mathrm{d}z} + \gamma(z-1)\Big)\mathcal{M}(z,t) \tag{2.8a}$$

$$\iff \quad \frac{\mathrm{d}}{\mathrm{d}z}\mathcal{M}(z,t) = \frac{\gamma}{\epsilon}\mathcal{M}(z,t) \tag{2.8b}$$

$$\implies \quad \mathcal{M}(z,t) = e^{\frac{\gamma}{\epsilon}(z-1)} \tag{2.8c}$$

$$\implies \quad P(N|N_0) = \frac{1}{N!}\left(\frac{\gamma}{\epsilon}\right)^N e^{-\frac{\gamma}{\epsilon}}, \tag{1.23d}$$

where we used the normalization of probability distribution, expressed as $\mathcal{M}(1,t) = 1$, as boundary condition. We recover the previous result of the Poisson distribution with coefficient γ/ϵ.

Using the PDE viewpoint of the Master Equation gives us an additional way of understanding stochastic processes. However, we have to be careful because some PDEs will have several solutions of which some are not analytical in z.[1] In such cases, we have to choose the solution that is analytic in z on $z \in [0,1]$ and which fits the definition of probability generating function, Eq. (2.1).

Unfortunately, the PDEs we find for stochastic processes don't fit into many standard solution schemes and we have to come up with our own way of solving them – at least approximately: the path integral. But before we build up to the derivation of the path integral, we want to consider one more trick that simplifies the Master Equation, the derived PDE and later on the path integral form. The trick is called the *Doi-shift*.

2.2 The Doi-Shift

The Doi-shift[2] is the shift of the *multiplication operator* z in the PDE:

$$\text{Doi-shift in multiplication operator} \qquad \widetilde{z} = z - 1. \tag{2.9}$$

Why are we not simply saying that we shift the *variable* z? Because the shift is applied neither to the differentiation operator $\mathrm{d}/\mathrm{d}z$ nor to the function $\mathcal{M}(z,t)$. On the surface, this does not make any sense and likely introduces more confusion than it could possible bring benefit. There are three arguments to refute this justified skepticism:

1. An explicit example is the PDE for a single particle species undergoing extinction, spontaneous creation and coagulation. Using the Frobenius method, we find that it has two steady state solutions: one is a series in z^k, the other in $z^{k+1-2\epsilon/\lambda}$ with $k \in \mathbb{N}_0$. However, the probability generating $\mathcal{M}(z,t)$ function can only contain integer powers of z.

2. The Doi-shift is named after Masao Doi who introduced it, in the language of Second Quantization, as the shift of the creation operator by 1: $a^\dagger = \widetilde{a} + 1$ in Doi 1976.

- In the remainder of this section, we are going to show that this shift is indeed beneficial in many cases and we will continue to discuss its benefits on the level of Doi-Peliti field theory in Sec. 3.2.6.
- Operators are defined in the way they act on functions. Let's look at a pathological example: The multiplication operator z applied to the function z produces the function z^2. The Doi-shifted multiplication operator $\widetilde{z}$ applied to the function z produces the function $z^2 - z$. There is nothing to worry about except that the notation might become horrendously confusing.
- The confusing notation is mitigated by using the language of Second Quantization, which will be introduced below in Sec. 2.3.

One of the benefits of the Doi-shift is that it makes many of the PDEs easier and allows extracting more useful properties of the system without solving the PDE completely. In fact, we are unable to solve most of the PDEs of the interesting stochastic processes completely, but we still want to determine some of its properties. What are useful properties of a stochastic process? If we were only allowed to determine one property, it is reasonable to ask for the mean particle number rather than any specific probability, because it says something about the typical behaviour of the process. In fact, the 2nd, 3rd and 4th moments also seem more useful because they give us the variance, skewness and kurtosis of the distribution.

How do we shift the focus of our model from probabilities to moments? It is the Doi-shift that helps us do that. However, there is a caveat. The Doi-shift will allow extracting *factorial moments* directly rather than the usual moments. Let's recall their defintions:

$$k\text{-th moment} \qquad \mathbb{E}\left[N^k(t)\middle|N(t_0)\right] = \sum_{N=0}^{\infty} N^k P\big(N(t)\big|N(t_0)\big) \tag{2.10}$$

$$k\text{-th facotrial moment} \qquad \mathbb{E}\left[\big(N(t)\big)_k\middle|N(t_0)\right] = \sum_{N=k}^{\infty} \frac{N!}{(N-k)!} P\big(N(t)\big|N(t_0)\big) \tag{2.11}$$

How on earth can factorial moments possibly be useful? They just seem to be unnecessarily complicated objects. Let's consider the Master Equation of the pure extinction process again

$$\frac{\partial}{\partial t} P\big(N(t)\big|N(t_0)\big) = \epsilon(N(t)+1)P\big(N(t)+1\big|N(t_0)\big) - \epsilon N(t) P\big(N(t)\big|N(t_0)\big), \tag{1.15}$$

where $N(t_0)$ is an initial condition at time t_0. If you solved Ex. 1.1, you saw that equations for the nth moments are complicated. But what do we find if we derive

equations for the factorial moments?

$$\frac{\partial}{\partial t}\mathbb{E}[N(t)|N(t_0)] = -\epsilon\mathbb{E}[N(t)|N(t_0)] \tag{2.12a}$$

$$\frac{\partial}{\partial t}\mathbb{E}[(N(t))_2|N(t_0)] = -2\epsilon\mathbb{E}[(N(t))_2|N(t_0)] \tag{2.12b}$$

$$\frac{\partial}{\partial t}\mathbb{E}[(N(t))_3|N(t_0)] = -3\epsilon\mathbb{E}[(N(t))_3|N(t_0)] \tag{2.12c}$$

$$\vdots \qquad\qquad \vdots$$

$$\frac{\partial}{\partial t}\mathbb{E}[(N(t))_n|N(t_0)] = -n\epsilon\mathbb{E}[(N(t))_n|N(t_0)] \tag{2.12d}$$

When working with factorial moments, the Master Equation system decouples! Although this is exciting, you should rightly be skeptical: surely switching to factorial moments cannot decouple Master equations for *all* stochastic processes. That's right, but it does remarkably simplify a lot of the standard processes.

Exercise 2.2 Consider the Master Equation for the spontaneous creation process with rate γ:

$$\frac{\partial}{\partial t}P\big(N(t)\big|N(t_0)\big) = \gamma P\big(N(t)-1\big|N(t_0)\big) - \gamma P\big(N(t)\big|N(t_0)\big).$$

Derive equations for the nth moment and the nth factorial moment.

Having seen the simplification of the Master Equation for the extinction process due to using factorial moments, we might be more inclined to use them going forward. But how do we implement them in the PDE? We will see how this is done indirectly at the level of the path integral in Sec. 2.3.7.

2.3 Second Quantization

Second Quantization[3] is a language that allows working efficiently with functions and operators in a vector space with scalar product and in a way that makes their interpretation with the regards to the modelled system more immediate.

A good way of thinking about the difference between Second Quantization and the usual way of writing functions and operators can be found by using the analogy to the difference between roman and arabic number systems. In principle, you can work in both, but for some specific tasks one might be more efficient than the other.

Second Quantization is its own research field. A great introduction is Berezin 1966. In the context of stochastic processes modelled by Master Equations, Second Quantization

3. In the context of Quantum Field Theory, this type of approach is called canonical quantization.

has nothing to do with quantum mechanics or quantum-many-body systems. The quantization part of the name simply stems from the fact that it was first used in connection with quantum systems.

In the context of Master Equations and their corresponding PDEs, Second Quantization is the representation of functions and operators as follows:

usual representation		representation in Second Quantization	
function	z^N	$\|N\rangle$	N-particle state
multiplication operator	z	$a^\dagger$	creation operator
differentiation operator	$\frac{\mathrm{d}}{\mathrm{d}z}$	a	annihilation operator
Doi-shifted multiplication operator	$\widetilde{z}$	$\widetilde{a}$	Doi-shifted creation operator
probability generating function	$\mathcal{M}(z,t)$	$\|\mathcal{M}(t)\rangle$	system state

From these conventions, several rules follow which describe how operators act on states and how they commute:

$$a|N\rangle = N|N-1\rangle \tag{2.13a}$$

$$a^\dagger|N\rangle = |N+1\rangle \tag{2.13b}$$

$$aa^\dagger - a^\dagger a =: [a, a^\dagger] = 1 \tag{2.13c}$$

Not only do we introduce new symbols to write the PDE but also new names which requires additional justification:

- The N-particle state is the new name for the function z^N. If $\mathcal{M}(z,t) = z^N$, then we had $P(N(t) = N|N_0) = 1$ and $P(N(t) \neq N|N_0) = 0$, which means the system contains N particles with probability 1.
- Creation operator is the new name for the multiplication operator z. If the system contains N particles, then $z \cdot z^N = z^{N+1}$ represents the creation of an additional particle.
- Annihilation operator is the new name for the differentiation operator. If the system contains N particles, then $M(z,t) = z^N$, and $\frac{\mathrm{d}}{\mathrm{d}z} z^N = N z^{N-1}$ represents the destruction of one of the particles. However, an additional factor N prevents us from saying that the system is in state $N-1$ because the system state, being equal to the probability generating function, must follow the normalization condition $\mathcal{M}(1,t) = 1$. $N z^{N-1}$ does not fulfill that condition. This caveat we have to keep in mind.

If you are familiar with the use of this kind of representations in Quantum Mechanics, you will notice small but important differences. The names of the operators seem to be the same, but their action on states is different *and* the interpretation of states is different

too. This is because in Quantum Mechanical systems, functions and operators have a different definition. They are fitted for an efficient representation of the Schrödinger Equation and not of the PDE of the Master Equation.

So far, we have only looked at states and operators for a single particle species. Accommodating more species is straightforward:

usual representation		representation in Second Quantization	
function	$z_j^{N_j}$	$\|N_j\rangle$	N_j-particle state
multiplication operator	z_j	$a_j^\dagger$	creation operator
differentiation operator	$\frac{\mathrm{d}}{\mathrm{d}z_j}$	a_j	annihilation operator
Doi-shifted multiplication operator	$\widetilde{z}_j$	$\widetilde{a}_j$	Doi-shifted creation operator
general functions	$z_j^{N_j} z_k^{N_k}$	$\|N_j, N_k\rangle$	N_j, N_k-particle state

There is an entire algebraic theory around the relation of the multiple-species state $|N_j, N_k\rangle$ to the single-species states $|N_j\rangle$ and $|N_k\rangle$, which involves operations such as symmetrizations and tensor products and other complicated notions. This background knowledge would be important if we were interested in modelling fermions, i.e. particle species which can have at most one particle at a specific position. However, we allow several particles of the same species to be at the same position. Such particles are called bosons and they don't pose great algebraic challenges. We only need to use $|N\rangle$ in a flexible way like a vector: if there are many particles, then $|N\rangle = |N_1, \dots\rangle$ represents the entire array of particle numbers, thus keeping our notation nicely compact. Then, we write the addition/subtraction of one particle of species j as $|N \pm 1_j\rangle$, such as in $a_j^\dagger|N\rangle = |N + 1_j\rangle$ or $a_k|N\rangle = N_k|N - 1_k\rangle$.

What have we achieved so far? We claimed that we might be able to solve the Master Equation by transforming it into a PDE in Sec. 2.1, then we shifted the goal post and argued that solving the PDE completely is not everything in life, but extracting factorial moments might be good enough, and finally we seemingly changed topic and introduced a new notation.[4] You might think that we're beating around the bush and you're right. The reason is that solving the PDE by introducing path integrals comes with several technicalities which when written out explicitly don't look aesthetically pleasing at all – to put it mildly. Nonetheless, let's get on with solving the PDEs. They have the general form

$$\frac{\partial}{\partial t}|\mathcal{M}(t)\rangle = \mathcal{L}[a^\dagger, a]|\mathcal{M}(t)\rangle, \tag{2.14}$$

4. What we did seems to be the opposite of how Henri Poincaré described mathematics in his book Science et Méthode: "Mathematics is the art of giving the same name to different things." (Poincaré 1908). Introducing Second Quantization appears to be more aligned with the associated quote "Poetry is the art of giving different names to the same thing."

where $\mathcal{L}[a^\dagger, a]$ is the operator for the specific stochastic process. It can include different species with their corresponding operators $a_j^\dagger, \ldots$ and $a_j, \ldots$, but we prefer the compact notation in Eq. (2.14).

Formally, we solve Eq. (2.14) as

$$|\mathcal{M}(t)\rangle = e^{\mathcal{L}[a^\dagger,a](t-t_0)}|\mathcal{M}(t_0)\rangle \tag{2.15}$$

for some initial condition $|\mathcal{M}(t_0)\rangle$. But we already said that a complete solutions might be impossible and that we would be content with moments. How do we extract them? By using *dual*-states.

2.3.1 Dual states – the bra in bracket

The word dual appears in connection with linear algebra in notions such as dual vector or dual space and we will use dual states as word for dual vector. We prefer to use the word state instead of vector because we describe systems with particle states $|N\rangle$. In fact, we originally called the state $|N\rangle$ a function and wrote it as z^N. Now we are saying we also could call it a vector – so we've collected already three names for the same object. But if $|N\rangle = z^N$ is a vector, to what vector space does it belong? As we restrict $\mathcal{M}(z,t) = |\mathcal{M}\rangle$ to analytic functions, the vector space must be the space of analytic functions. We choose it to be a *real* vector space (instead of complex, or any other field) because we are interested in probabilities and particle numbers. Complex probabilities or a complex number of particles would just be too esoteric for us.

In this context, the **dual space** is the space of all linear functionals from the space of real analytic functions (e.g. z^N or $\mathcal{M}(z,t)$) to the real numbers (e.g. 0.14 or 32.7). Said differently, the dual space is the space of all linear maps from the space of particle states (e.g. $|N\rangle$ or $|\mathcal{M}(t)\rangle$) to the real numbers. The Riesz lemma (or sometimes it's called the Fréchet-Riesz theorem) tells us that for each basis of states $|N\rangle$ there is a basis of dual states $\langle M|$ such that

$$\langle M|N\rangle = \delta_{M,N}, \tag{2.16}$$

where $\delta_{M,N}$ is the Kronecker-δ.[5] The notation of dual states as $\langle M|$ is a convention that hints at the fact that dual states can be described in terms of an inner product of the vector space. Furthermore, $\langle M|N\rangle$ forms something that looks like a bracket, which motivates the use of the terminology *bra*-vector for $\langle M|$, and *ket*-vector for $|N\rangle$. Don't ask me what happened to the c in the middle of the word bracket.[6] If we use the notation of $|N\rangle$ as function z^N, then what is that inner product and what is the dual

5. For the precise statement and proof see Reed and Simon 1980.

6. The shape of the second quantized vectors (angular brackets) and the names 'bra-vector' and 'ket-vector' were introduced by Paul Dirac originally for use in quantum mechanics, see Dirac 1939.

state $\langle M|$? The inner product is an integral such that

$$\langle \bullet | N \rangle = \int \bullet \, z^N \mathrm{d}z, \tag{2.17}$$

from which follows that the dual state equals

$$\langle M | \bullet \rangle = \int \frac{(-1)^M}{M!} \delta^{(M)}(z) \bullet \, \mathrm{d}z, \tag{2.18}$$

where $\delta^{(M)}(z)$ is the Mth derivative of the δ-function, defined as:

$$\int \delta^{(M)}(z) f(z) \mathrm{d}z = (-1)^M \frac{\mathrm{d}^M}{\mathrm{d}z^M} f(z) \Big|_{z=0}. \tag{2.19}$$

Thus, we find that $\langle M|$ is a linear functional. We can see from Eqs. (2.17), (2.18) and (2.19) that staying in the original notation for functions z^N becomes notationally very lengthy once we work with dual vectors. The language of Second Quantization, as used in Eq. (2.16), does convey the same content more succinctly and, to be honest, before introducing dual states, the notational advantage of Second Quantization over the usual notation wasn't that great.

We motivated the introduction of dual states by claiming they would be used to extract information about the stochastic process from $|\mathcal{M}(t)\rangle$:

$$\langle M | \mathcal{M}(t) \rangle = \sum_{N=0}^{\infty} P\big(N(t) = N \big| N(t_0)\big) \langle M | N \rangle = P\big(N(t) = M \big| N(t_0)\big), \tag{2.20}$$

which took the M-th derivative of $\mathcal{M}(z,t)$ and evaluated it at $z = 0$. But wait a second, we have already an operator to take derivatives, the annihilation operator a. Can we link dual states to annihilation and creation operators? Yes!, and we have two ways of finding out how: the Second Quantization language and the usual function perspective. In the language of Second Quantization, we find

$$\langle M | a | N \rangle = N \delta_{M,N-1} \quad \Longrightarrow \quad \langle M | a = (M+1) \langle M+1 | \tag{2.21a}$$

$$\langle M | a^\dagger | N \rangle = \delta_{M,N+1} \quad \Longrightarrow \quad \langle M | a^\dagger = \langle M-1 |, \tag{2.21b}$$

where it seems that creation and annihilation operators reverse their interpretation, which seems to align well with the word duality.

Exercise 2.3 Find out what the action of the differentiation operator $\mathrm{d}/\mathrm{d}z$ and multiplication operator z is on the dual vector $\frac{(-1)^M}{M!} \int \delta^{(M)}(z) \bullet \mathrm{d}z$ without using Second Quantization.

In Eq. (2.20) we extracted the probability distribution from $|\mathcal{M}(t)\rangle$, but earlier, we argued that extracting moments is more useful when we can't solve the PDE completely. If we take z-derivatives of the probability generating functions $\mathcal{M}(z,t)$ and evaluate them at $z=1$, we find

$$\frac{\mathrm{d}^k}{\mathrm{d}z^k}\mathcal{M}(z,t)\Big|_{z=1} = \mathbb{E}\left[\big(N(t)\big)_k \big| N(t_0)\right], \tag{2.22}$$

which is the kth factorial moment! How can we express the dual vector $(-1)^k \int \delta^{(k)}(z-1)\bullet \mathrm{d}z$ in terms of $\langle M|$? We can simplify this problem by using the annihilation operator k times, a^k and then use Eq. (2.21a). Thus, we only need to find out how to express $\int \delta(z-1)\bullet \mathrm{d}z$ in terms of $\langle M|$.

As we are working with analytic functions, say f, and $\delta(z-1)$ evaluates a function at $z=1$, we can express $f(1)$ in terms of its derivatives at $z=0$, denoted by $f^{(n)}(0)$, as a complete Taylor series:

$$f(1) = \sum_{n=0}^{\infty} \frac{f^{(n)}(0)}{n!}. \tag{2.23}$$

But we know how to express $f^{(n)}(0)$ using the dual vectors:

$$f(1) = \int \delta(z-1) f(z)\mathrm{d}z = \sum_{n=0}^{\infty} \frac{(-1)^n}{n!} \int \delta^{(n)}(z) f(z)\mathrm{d}z, \tag{2.24}$$

which implies that $\delta(z-1)$ can be written as

$$\int \delta(z-1)\bullet \mathrm{d}z = \sum_{M=0}^{\infty} \langle M|\bullet\rangle = \langle 0|e^a|\bullet\rangle =: \langle \dot{\varsigma}|\bullet\rangle. \tag{2.25}$$

The dual state $\langle \dot{\varsigma}|$ is sometimes (dramatically) called *the abyss*, but it simply evaluates any analytic function at $z=1$.

The above result Eq. (2.24) shows that for all intents and purposes the δ function is analytic. How can this be? We can regard the δ function as the limit of a sequence of Gaussians, which are analytic. The limit of the Gaussians tending towards the δ function and the limit of a complete Taylor expansion can be exchanged because we are applying them to analytic functions f. In particular, we can evaluate an analytic function at a different point ξ using dual states $\langle 0|e^{\xi a}$.

Thus, the kth factorial moment can be expressed in the language of Second Quantization as

$$\langle \dot{\varsigma}|a^k|\mathcal{M}(t)\rangle = \mathbb{E}\big[\big(N(t)\big)_k \big| N(t_0)\big] \tag{2.26}$$

Similarly, the kth moment can be expressed as

$$\big\langle \dot{\varsigma}\big|\big(a^\dagger a\big)^k\big|\mathcal{M}(t)\big\rangle = \mathbb{E}\big[N^k(t)\big|N(t_0)\big]. \tag{2.27}$$

Exercise 2.4 Show that the kth moment can be written in the language of Second Quantization as

$$\langle \text{☼} | \big(a^\dagger a\big)^k | \mathcal{M}(t) \rangle = \mathbb{E}\big[N^k(t) \big| N(t_0)\big]. \tag{2.28}$$

2.3.2 Identities operators

We now know how to express the moments once we have the probability generating function $|\mathcal{M}(t)\rangle$. However, the list of things we need to find out is still long: how do we find $|\mathcal{M}(t)\rangle$ and how do we calculate objects like $\langle \text{☼} | a^k | \bullet \rangle$ explicitly? In particular it still seems like we have to solve the Master Equation or its associated PDE completely, before we can do any of the above.

Above, we found a formal solution of the PDE for $|\mathcal{M}(t)\rangle$

$$|\mathcal{M}(t)\rangle = e^{\mathcal{L}[a^\dagger, a](t-t_0)} |\mathcal{M}(t_0)\rangle, \tag{2.15}$$

which still contains operators $a^\dagger$ and a. How can we get rid of them? By using a property of the exponential function

$$e^t = \lim_{n\to\infty} \left(1 + \frac{t}{n}\right)^n. \tag{2.29}$$

Hence, we discretize time in steps of Δt and insert identities $\mathbb{I}$:

$$|\mathcal{M}(t)\rangle = \lim_{\Delta t \to 0} \mathbb{I}\big(1 + \Delta t \mathcal{L}[a^\dagger, a]\big)\mathbb{I}\big(1 + \Delta t \mathcal{L}[a^\dagger, a]\big) \dots \big(1 + \Delta t \mathcal{L}[a^\dagger, a]\big)\mathbb{I} |\mathcal{M}(t_0)\rangle, \tag{2.30}$$

where there are $(t - t_0)/\Delta t = n$ terms of $\big(1 + \Delta t \mathcal{L}[a^\dagger, a]\big)\mathbb{I}$. Inserting identities seems superfluous, but we will see that identities can be expressed in different ways, of which one way will help us get rid of the operators.

In finite dimensional vector spaces, identities are straightforward. We typically write vectors as columns and the identity as a matrix. How can we extend this to infinite dimensional spaces such as the space of analytic functions? We don't want to write infinitely long and infinitely wide matrices. If the vector space is equipped with an inner product, then an identity can be expressed using an orthonormal basis of the vector space. Let's say we have orthonormal basis vectors $e_1, \dots, e_n$ and inner product $\langle \cdot, \cdot \rangle$, then any vector v is identically reproduced if its first projected onto the basis vector and then multiplied by the basis vector:

$$v = \sum_{k=1}^{n} e_k \langle e_k, v \rangle. \tag{2.31}$$

So the identity operator is $\sum_k e_k \langle e_k, \cdot \rangle$. This really corresponds to the identity matrix in euclidean space, where $\langle e_k, v \rangle = e_k^T v$ can be expressed with the transpose e_k^T. Then the identity matrix is $\sum_k e_k e_k^T$. In particular $\langle e_k, \cdot \rangle$ acts as a dual vector to e_k.

Exercise 2.5 Consider the two dimensional vector space $\mathbb{R}^2$ with the euclidean inner product $\langle \cdot, \cdot \rangle$. Use the orthonormal basis

$$e_1 = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix} \qquad e_2 = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -1 \end{pmatrix}$$

to show that $\sum_k e_k \langle e_k, \cdot \rangle$ is the identity matrix.

In the space of analytic functions, i.e. the space of particle states, we have an orthonormal basis $|N\rangle$, see Eq. (2.16). Thus, the identity can be expressed as

$$\sum_{N=0}^{\infty} |N\rangle\langle N|. \tag{2.32}$$

However, we saw above that we can express the identity differently using different orthonormal bases. What would be the advantage of that? Let's assume that we are applying an operator on the left of the identity. In finite dimensional spaces, operators are just matrices. Now, if the basis in which the identity is expressed is an eigenbasis of the operator then we find a simpler expression. Let's say A is the operator and $Ae_k = \lambda_k e_k$, then

$$A\mathbb{I} = \sum_{k=1}^{n} \lambda_k e_k \langle e_k, \cdot \rangle. \tag{2.33}$$

If furthermore, we apply an operator B from the right side and the e_k are left eigenvectors of B with eigenvalues μ_k, then

$$A\mathbb{I}B = \sum_{k=1}^{n} \lambda_k \mu_k e_k \langle e_k, \cdot \rangle. \tag{2.34}$$

This is a really useful result, because it shows that we can get rid of operators and work with their eigenvalues instead if we attach identities left or right of them which must be cast in terms of their eigenvectors. In our original problem in Eq. (2.30), we added identities left and right of the operator $(1 + \Delta t \mathcal{L}[a^\dagger, a])$. The 1 is just a scalar and when regarded as an operator, it has any vector as eigenvector. Similarly Δt is just a scalar and will not pose any difficulties. However, inside $\mathcal{L}$, we have the ladder operators $a^\dagger$ and a. What are their eigenvectors?

Let's start with a. It represents the derivative $\mathrm{d}/\mathrm{d}z$ and its (right) eigenvector is the function $e^{\phi z}$ with eigenvalue $\phi \in \mathbb{C}$, which is written as $e^{\phi a^\dagger}|0\rangle =: |\phi\rangle$ in the language of Second Quantization.

What about $a^\dagger$? What are its eigenvectors? It turns out that it does not have a right eigenvector!

Exercise 2.6 Prove that $a^\dagger$ does not have a right eigenvector in the space of analytic functions.

Can we find left eigenvectors for a and $a^\dagger$? Left eigenvectors of matrices are a straightforward extension of right eigenvectors. But with operators this becomes more difficult to understand. What could possibly be the left eigenvector of $\mathrm{d}/\mathrm{d}z$? How can we apply anything from the left in a meaningful way? It is again the concept of dual vectors and the elegant notation of Second Quantization that saves us here. We previously worked out what $\langle M|a$ and $\langle M|a^\dagger$ means in Eq. (2.21). We thus can conclude that $\langle 0|e^{\phi^\dagger a}$ is a left eigenvector of $a^\dagger$ with eigenvalue $\phi^\dagger \in \mathbb{C}$. By analogy (or better duality), we can also conclude that a does not have a left eigenvector because $a^\dagger$ did not have a right eigenvector.

At this stage, the eigenvalues ϕ and $\phi^\dagger$ are arbitrary complex numbers. However, we still have to create a representation of the identity out of the eigenvectors, which will link ϕ to $\phi^\dagger$ such that $\phi^\dagger$ is the complex conjugated of ϕ.

Given the identity operator in terms of $|N\rangle\langle N|$ in Eq. (2.32), how can we rewrite it in terms of $|\phi\rangle\langle\phi^\dagger|$? We find

$$|\phi\rangle\langle\phi^\dagger| = e^{\phi a^\dagger}|0\rangle\langle 0|e^{\phi^\dagger a} \tag{2.35}$$

$$= \sum_{M,N=0}^{\infty} \frac{\phi^N \phi^{\dagger M}}{N!}|N\rangle\langle M|. \tag{2.36}$$

If you are confused why $N!$ appears but not $M!$, compare Eq. (2.13b) and Eq. (2.21a). The solution to our problem is therefore an integral over $\phi^N\phi^{\dagger M}$ such that its result is $\delta_{M,N}N!$. More explicitly, we are looking for a function $g(\phi)$ such that

$$\int \phi^N \phi^{\dagger M} g(\phi)\mathrm{dRe}\phi\mathrm{dIm}\phi = \int_0^\infty \int_0^{2\pi} \rho^{N+M} e^{i\theta(N-M)} g(\rho e^{i\theta})\rho\,\mathrm{d}\theta\mathrm{d}\rho = \delta_{M,N}N!, \tag{2.37}$$

where we used polar coordinates ρ and θ in the complex plane. We can find a Kronecker-δ if we choose g to be a function of ρ only and then consider the θ integral:

$$\int_0^{2\pi} e^{i\theta(N-M)}\mathrm{d}\theta = 2\pi\delta_{M,N} \tag{2.38}$$

Thus, we need to find $g(\rho)$ such that

$$\frac{N!}{2\pi} = \int_0^\infty \rho^{2N+1} g(\rho)\,\mathrm{d}\rho. \tag{2.39}$$

Having the Γ-function in mind, we use a transformation of variables $\rho^2 = x$ and set $g(\rho) = e^{-\rho^2}/\pi$ to find

$$\int_0^\infty \rho^{2N+1} g(\rho)\,\mathrm{d}\rho = \frac{1}{2\pi}\int_0^\infty x^N e^{-x}\mathrm{d}x = \frac{N!}{2\pi}. \tag{2.40}$$

Thus, the identity operator can be written in term of the eigenstates of a and $a^\dagger$ as

$$\mathbb{I} = \sum_{N=0}^{\infty} |N\rangle\langle N| = \int e^{-\phi^\dagger\phi}|\phi\rangle\langle\phi^\dagger|\frac{\mathrm{dRe}\phi\mathrm{dIm}\phi}{\pi} \tag{2.41}$$

Exercise 2.7 Operators that act in a linear space can be written using a basis and its dual basis. Write the annihilation and creation operators a and $a^\dagger$ in the form

$$a = \sum_{j,k=0}^{\infty} A_{j,k}|j\rangle\langle k| \qquad \text{and} \qquad a^\dagger = \sum_{j,k=0}^{\infty} A^\dagger_{j,k}|j\rangle\langle k|,$$

i.e. find the values of $A_{j,k}$ and $A^\dagger_{j,k}$. Find the analogous form of the combined operator $a^\dagger a$.

2.3.3 Time evolution

We have successfully found a promising version of the identity! Now we use it to describe the time evolution of the probability generating function $\mathcal{M}(z,t)$ in its Second Quantized form $|\mathcal{M}(t)\rangle$, the system state. As a reminder of where we wanted to use the identity, we copy the discretized time evolution here again:

$$|\mathcal{M}(t)\rangle = \lim_{\Delta t\to 0} \mathbb{I}\big(1+\Delta t\mathcal{L}[a^\dagger,a]\big)\mathbb{I}\big(1+\Delta t\mathcal{L}[a^\dagger,a]\big)\ldots\big(1+\Delta t\mathcal{L}[a^\dagger,a]\big)\mathbb{I}|\mathcal{M}(t_0)\rangle. \quad (2.30)$$

As our identity operator has right eigenvectors of a and left eigenvectors of $a^\dagger$, we enforce that the operator $\mathcal{L}[a^\dagger,a]$ has in every term $a^\dagger$ positioned on the left and a positioned on the right. This is called *normal ordering*[7] and can always be achieved by using the commutation rules of a with $a^\dagger$, see Eq. (2.13c).

The term $(1+\Delta t\mathcal{L}[a^\dagger,a])$ is surrounded by two identity operators. In particular, on its left, there is $\langle\phi^\dagger|$ and on its right is $|\phi\rangle$. Hence, we need to evaluate $\langle\phi^\dagger|1+\Delta t\mathcal{L}[a^\dagger,a]|\phi\rangle$. However, when considering $\langle\phi^\dagger|1+\Delta t\mathcal{L}[a^\dagger,a]|\phi\rangle$ we have to be careful, because $\langle\phi^\dagger|$ and $|\phi\rangle$ came from different identity operators and hence from different integrals, see Eq. (2.41). Therefore the values $\phi^\dagger$ on the left and ϕ on the right are not complex

7. Normal ordering was introduced under the name 'well-ordering' by Paul Dirac in his 1933 paper, where he also introduced the basics of path integrals, see Dirac 1933.

conjugates of each other! We have to keep track of which $\phi^\dagger$ is the complex conjugate of which ϕ in Eq. (2.30). This is a nightmare! We circumvent this notational meltdown by labeling ϕ and $\phi^\dagger$ according to how close they are to the initial system state vector $|\mathcal{M}(t_0)\rangle$. The identity directly left of it will be labeled $\mathbb{I}_{t_0}$ and its integral variables are labeled ϕ_{t_0} and $\phi^\dagger_{t_0}$. The next identity operator on its left, after the first $(1+\Delta t\mathcal{L}[a^\dagger, a])$, will be labelled $\mathbb{I}_{t_0+\Delta t}$ and its variables are $\phi_{t_0+\Delta t}$ and $\phi^\dagger_{t_0+\Delta t}$. We thus continue until the last identity operator after the final $(1 + \Delta t\mathcal{L}[a^\dagger, a])$ is labelled $\mathbb{I}_t$ and its values ϕ_t and $\phi^\dagger_t$.

Now we can evaluate $\langle\phi^\dagger_{t'+\Delta t}|1 + \Delta t\mathcal{L}[a^\dagger, a]|\phi_{t'}\rangle$ for some $t' \in \{t_0, t_0 + \Delta t, \ldots, t - \Delta t\}$. We use linearity and start with the easy part $\langle\phi^\dagger_{t'+\Delta t}|1|\phi_{t'}\rangle$:

$$\langle\phi^\dagger_{t'+\Delta t}|1|\phi_{t'}\rangle = \langle\phi^\dagger_{t'+\Delta t}|\phi_{t'}\rangle = \sum_{k=0}^{\infty}\sum_{\ell=0}^{\infty}\frac{\phi^{\dagger k}_{t'+\Delta t}\phi^\ell_{t'}}{\ell!}\underbrace{\langle k|\ell\rangle}_{=\delta_{k,\ell}} = e^{\phi^\dagger_{t'+\Delta t}\phi_{t'}} \tag{2.42}$$

Next, we consider that a term in $\mathcal{L}[a^\dagger, a]$ will be of the form $a^{\dagger k}a^\ell$ for some $k, \ell \in \mathbb{N}_0$. Thus, we need to evaluate $\langle\phi^\dagger_{t'+\Delta t}|a^{\dagger k}a^\ell|\phi_{t'}\rangle$:

$$\langle\phi^\dagger_{t'+\Delta t}|a^{\dagger k}a^\ell|\phi_{t'}\rangle = \phi^{\dagger k}_{t'+\Delta t}\phi^\ell_{t'}e^{\phi^\dagger_{t'+\Delta t}\phi_{t'}}, \tag{2.43}$$

where we used that these bra- and ket-vectors are eigenvectors of a and $a^\dagger$ and we used Eq. (2.42). Although there are lots of super- and subscripts floating around, in essence $a^{\dagger k}$ is replaced by $\phi^{\dagger k}_{t'+\Delta t}$ and a^ℓ is replaced by $\phi^\ell_{t'}$ times a factor $e^{\phi^\dagger_{t'+\Delta t}\phi_{t'}}$. Thus, we can summarize the two previous calculations by

$$\langle\phi^\dagger_{t'+\Delta t}|1 + \Delta t\mathcal{L}[a^\dagger, a]|\phi_{t'}\rangle = \Big(1 + \Delta t\mathcal{L}\big[\phi^\dagger_{t'+\Delta t}\phi_{t'}\big]\Big)e^{\phi^\dagger_{t'+\Delta t}\phi_{t'}}. \tag{2.44}$$

So far so good. Next, we would have to recombine all the terms for every t' and take the continuum limit $\Delta t \to 0$ in Eq. (2.30). Denoting $n = (t - t_0)/\Delta t$, we find

$$\lim_{\Delta t\to 0}\mathbb{I}\big(1 + \Delta t\mathcal{L}[a^\dagger, a]\big)\mathbb{I}\big(1 + \Delta t\mathcal{L}[a^\dagger, a]\big)\ldots\big(1 + \Delta t\mathcal{L}[a^\dagger, a]\big)\mathbb{I} = \tag{2.45}$$

$$= \lim_{\Delta t\to 0}\mathbb{I}_t\prod_{j=0}^{n-1}\big(1 + \Delta t\mathcal{L}[a^\dagger, a]\big)\mathbb{I}_{t_0+j\Delta t} \tag{2.46}$$

$$= \lim_{\Delta t\to 0}\int|\phi_t\rangle\langle\phi^\dagger_{t_0}|\prod_{j=0}^{n-1}\left\{e^{\phi^\dagger_{t_0+(j+1)\Delta t}\phi_{t_0+j\Delta t}}\Big(1 + \Delta t\mathcal{L}\big[\phi^\dagger_{t_0+(j+1)\Delta t}, \phi_{t_0+\Delta t}\big]\Big)\right\}\cdot$$
$$\cdot\prod_{k=0}^{n}\left\{e^{-\phi^\dagger_{t_0+k\Delta t}\phi_{t_0+k\Delta t}}\frac{\mathrm{dRe}\phi_{t_0+k\Delta t}\mathrm{dIm}\phi_{t_0+k\Delta t}}{\pi}\right\}, \tag{2.47}$$

where it might come as a surprise that in one of the products the index j goes only to $n - 1$, while in the other product the index k goes to n. The reason is that there are $n + 1$ identities but only n terms of $(1 + \Delta t\mathcal{L}[a^\dagger, a])$ in the expression (2.45).

In order to finally take the continuum limit $\Delta t \to 0$, we consider the terms of the form $(1 + \Delta t \mathcal{L}[\phi^\dagger_{t_0+(j+1)\Delta t}, \phi_{t_0+\Delta t}])$ again. They appear in a product as follows

$$\prod_{j=0}^{n-1}\Big(1 + \Delta t \mathcal{L}\big[\phi^\dagger_{t_0+(j+1)\Delta t},\phi_{t_0+\Delta t}\big]\Big) = \prod_{j=0}^{n-1}\Big\{\exp\Big(\Delta t \mathcal{L}\big[\phi^\dagger_{t_0+(j+1)\Delta t}, \phi_{t_0+\Delta t}\big]\Big) + \mathcal{O}(\Delta t^2)\Big\} \tag{2.48}$$

$$= \exp\left(\Delta t \sum_{j=0}^{n-1} \mathcal{L}\big[\phi^\dagger_{t_0+(j+1)\Delta t}, \phi_{t_0+\Delta t}\big]\right) + \mathcal{O}(\Delta t^2), \tag{2.49}$$

which then in the continuum limit becomes the exponential of an integral:

$$\lim_{\Delta t\to 0} \exp\left(\Delta t \sum_{j=0}^{n-1} \mathcal{L}\big[\phi^\dagger_{t_0+(j+1)\Delta t}, \phi_{t_0+\Delta t}\big]\right) + \mathcal{O}(\Delta t^2) = \exp\left(\int_{t_0}^{t} \mathcal{L}[\phi^\dagger(t'), \phi(t')]\mathrm{d}t'\right), \tag{2.50}$$

where we turned the discrete set of values $\phi_{t'}$ and $\phi^\dagger_{t'}$ into functions $\phi(t')$ and $\phi^\dagger(t')$.

Similarly, we take the n terms of the form $e^{\phi^\dagger_{t_0+(j+1)\Delta t}\phi_{t_0+j\Delta t}}$ and combine them with the term of the form $e^{-\phi^\dagger_{t_0+k\Delta t}\phi_{t_0+k\Delta t}}$ for all k except $k = 0$. We will treat $e^{-\phi^\dagger_{t_0}\phi_{t_0}}$ separately later on. Hence, we find

$$\lim_{\Delta t\to 0} \prod_{j=0}^{n-1} e^{\phi^\dagger_{t_0+(j+1)\Delta t}\phi_{t_0+j\Delta t}} e^{-\phi^\dagger_{t_0+(j+1)\Delta t}\phi_{t_0+(j+1)\Delta t}} = \tag{2.51}$$

$$= \lim_{\Delta t\to 0} \exp\left(-\sum_{j=0}^{n-1} \phi^\dagger_{t_0+(j+1)\Delta t}\Big(\phi_{t_0+(j+1)\Delta t} - \phi_{t_0+j\Delta t}\Big)\right) \tag{2.52}$$

$$= \exp\left(-\int_{t_0}^{t} \phi^\dagger(t')\frac{\mathrm{d}}{\mathrm{d}t'}\phi(t')\mathrm{d}t'\right). \tag{2.53}$$

Finally, in order to make out notation more compact, we define

$$\mathcal{D}[\phi^\dagger, \phi] := \lim_{\Delta t\to 0} \prod_{k=0}^{n} \frac{\mathrm{dRe}\phi_{t_0+k\Delta t}\mathrm{dIm}\phi_{t_0+k\Delta t}}{\pi} \tag{2.54}$$

We combine those individual continuum limit results from Eqs. (2.50), (2.53) and (2.54)

in the following summary

$$\lim_{\Delta t\to 0} \mathbb{I}\big(1+\Delta t\mathcal{L}[a^\dagger,a]\big)\mathbb{I}\big(1+\Delta t\mathcal{L}[a^\dagger,a]\big)\dots\big(1+\Delta t\mathcal{L}[a^\dagger,a]\big)\mathbb{I} = \tag{2.45}$$

$$= \int |\phi(t)\rangle\langle\phi^\dagger(t_0)| \exp\left(-\int_{t_0}^{t} \phi^\dagger(t')\frac{\mathrm{d}}{\mathrm{d}t'}\phi(t') - \mathcal{L}[\phi^\dagger(t'),\phi(t')]\,\mathrm{d}t' - \phi^\dagger(t_0)\phi(t_0)\right)\mathcal{D}[\phi^\dagger,\phi]. \tag{2.55}$$

What we have found is a representation of the operator $e^{\mathcal{L}[a^\dagger,a](t-t_0)}$ in Eq. (2.15) in terms of eigenstates $|\phi\rangle$ and $\langle\phi^\dagger|$ of the operators a and $a^\dagger$. In the continuum limit $\Delta t \to 0$, the eigenvalues ϕ and $\phi^\dagger$ turned into functions $\phi(t)$ and $\phi^\dagger(t)$, which we will call *fields* (hence the name field theory). In discrete time, we integrated a finite number of variables ϕ and $\phi^\dagger$ (one for each time step), but in the continuum limit, we are integrating over fields using the measure $\mathcal{D}[\phi^\dagger,\phi]$. We therefore call the right-hand-side of Eq. (2.55) our initial form of the path integral. In the following sections, we are going to mould it further into a nicer shape.

Given the origin of $\phi^\dagger$ and ϕ as eigenvalues of the creation and annihilation operators, we call $\phi^\dagger(t)$ and $\phi(t)$ the creation field and annihilation field, respectively. In line with the Doi-shift of the multiplication operator $\widetilde{z}\cdot = z\cdot -1\cdot$ and its Second Quantized version for the creation operator $\widetilde{a} = a^\dagger - 1$, we will also use the Doi-shift for fields $\widetilde{\phi} = \phi^\dagger - 1$.

2.3.4 Initialization – Kicking it all off

We applied the operator $e^{\mathcal{L}[a^\dagger,a](t-t_0)}$ to the initial system state $|\mathcal{M}(t_0)\rangle$. What are typical choices for such an initial state? Here, we present three examples

$$\text{single particle} \qquad |\mathcal{M}(t_0)\rangle = |1\rangle = a^\dagger|0\rangle \tag{2.56}$$

$$\text{Poisson distributed particles} \qquad |\mathcal{M}(t_0)\rangle = e^{-\lambda}\sum_{k=0}^{\infty}\frac{\lambda^k a^{\dagger k}}{k!}|0\rangle \tag{2.57}$$

$$j \text{ particles} \qquad |\mathcal{M}(t_0)\rangle = a^{\dagger j}|0\rangle. \tag{2.58}$$

The initial system states $|\mathcal{M}(t_0)\rangle$ is paired with $\langle\phi^\dagger(t_0)|$ from the time evolution operator in Eq. (2.55). We find

$$\text{single particle} \qquad \langle\phi^\dagger(t_0)|\mathcal{M}(t_0)\rangle = \langle\phi^\dagger(t_0)|a^\dagger|0\rangle = \phi^\dagger(t_0) \tag{2.59}$$

$$\text{Poisson distr. particles} \qquad \langle\phi^\dagger(t_0)|\mathcal{M}(t_0)\rangle = e^{-\lambda}\sum_{k=0}^{\infty}\langle\phi^\dagger(t_0)|\frac{\lambda^k a^{\dagger k}}{k!}|0\rangle = e^{-\lambda+\lambda\phi^\dagger(t)} \tag{2.60}$$

$$j \text{ particles} \qquad \langle\phi^\dagger(t_0)|\mathcal{M}(t_0)\rangle = \phi^{\dagger j}(t_0). \tag{2.61}$$

Thus, we have found an expression of the probability generating function at some time t after initializing the system at time t_0 in a specified way:

single particle

$$|\mathcal{M}(t)\rangle = \int |\phi(t)\rangle\phi^\dagger(t_0) e^{\left(-\int_{t_0}^{t} \phi^\dagger(t)\frac{\mathrm{d}}{\mathrm{d}t'}\phi(t) - \mathcal{L}[\phi^\dagger(t),\phi(t)]\,\mathrm{d}t' - \phi^\dagger(t_0)\phi(t_0)\right)} \mathcal{D}[\phi^\dagger,\phi] \tag{2.62}$$

Poisson distr. particles

$$|\mathcal{M}(t)\rangle = \int |\phi(t)\rangle e^{\left(-\int_{t_0}^{t} \phi^\dagger(t)\frac{\mathrm{d}}{\mathrm{d}t'}\phi(t) - \mathcal{L}[\phi^\dagger(t),\phi(t)]\,\mathrm{d}t' - \phi^\dagger(t_0)\phi(t_0) - \lambda + \lambda\phi^\dagger(t_0)\right)} \mathcal{D}[\phi^\dagger,\phi] \tag{2.63}$$

j particles

$$|\mathcal{M}(t)\rangle = \int |\phi(t)\rangle\phi^{\dagger j}(t_0) e^{\left(-\int_{t_0}^{t} \phi^\dagger(t)\frac{\mathrm{d}}{\mathrm{d}t'}\phi(t) - \mathcal{L}[\phi^\dagger(t),\phi(t)]\,\mathrm{d}t' - \phi^\dagger(t_0)\phi(t_0)\right)} \mathcal{D}[\phi^\dagger,\phi] \tag{2.64}$$

2.3.5 Interference at intermediate times – Poking the system

The somewhat natural extension of the problem of initializing the system is the problem of having to interfere with the system at intermediate times. How would that work?

On the level of Second Quantization, we assume the system was initialized at time t_0 with state $|\mathcal{M}(t_0)\rangle$. To make it explicit, we use the example of j particle from above, Eq. (2.64), which means that $|\mathcal{M}(t_0)\rangle = a^{\dagger j}|0\rangle$. It then evolves until time $t_1 > t_0$ and becomes state $|\mathcal{M}(t_1)\rangle = e^{\mathcal{L}[a^\dagger,a](t_1-t_0)}|\mathcal{M}(t_0)\rangle$, see Eq. (2.15). At time t_1, we want to influence the system, which we do by some operator, which is a linear combination of terms of the form $a^{\dagger k}a^\ell$ for some $k,\ell \in \mathbb{N}_0$. We will look at examples of useful interference later on. For now, we are interested in how to do it in principle. Finally, we are interested in the system's state $|\mathcal{M}(t_2)\rangle$ at a later time $t_2 > t_1 > t_0$:

$$|\mathcal{M}(t_2)\rangle = e^{\mathcal{L}[a^\dagger,a](t_2-t_1)} a^{\dagger k} a^\ell \underbrace{e^{\mathcal{L}[a^\dagger,a](t_1-t_0)} \overbrace{|\mathcal{M}(t_0)\rangle}^{=a^{\dagger j}|0\rangle}}_{=|\mathcal{M}(t_1)\rangle} \tag{2.65}$$

$$= \int |\phi(t_2)\rangle\langle\phi^\dagger(t_1)| e^{\left(-\int_{t_1}^{t_2} \phi^\dagger(t)\frac{\mathrm{d}}{\mathrm{d}t'}\phi(t) - \mathcal{L}[\phi^\dagger(t),\phi(t)]\,\mathrm{d}t' - \phi^\dagger(t_1)\phi(t_1)\right)} \cdot$$

$$a^{\dagger k}a^\ell|\phi(t_1)\rangle\phi^{\dagger j} e^{\left(-\int_{t_0}^{t_1} \phi^\dagger(t)\frac{\mathrm{d}}{\mathrm{d}t'}\phi(t) - \mathcal{L}[\phi^\dagger(t),\phi(t)]\,\mathrm{d}t' - \phi^\dagger(t_0)\phi(t_0)\right)} \mathcal{D}[\phi^\dagger,\phi] \tag{2.66}$$

$$= \int |\phi(t_2)\rangle\phi^{\dagger k}(t_1)\phi^\ell(t_1)\phi^{\dagger j}(t_0) e^{\left(-\int_{t_0}^{t_2} \phi^\dagger(t)\frac{\mathrm{d}}{\mathrm{d}t'}\phi(t) - \mathcal{L}[\phi^\dagger(t),\phi(t)]\,\mathrm{d}t' - \phi^\dagger(t_0)\phi(t_0)\right)} \mathcal{D}[\phi^\dagger,\phi], \tag{2.67}$$

where we used Eq. (2.43), resulting in the term $\langle\phi^\dagger(t_1)|a^{\dagger k}a^\ell|\phi(t_1)\rangle = \phi^{\dagger k}(t_1)\phi^\ell(t_1)e^{\phi^\dagger(t_1)\phi(t_1)}$, of which the exponential function cancels with the corresponding part in the time evolution operator. The two integrals in the two exponential functions simply merged into a single integral.

In summary we conclude: whenever we want to interfere with the time evolution of the system with an operator $a^{\dagger k}a^\ell$ at time t_1, we just transform that operator into $\phi^{\dagger k(t_1)}\phi^\ell(t_1)$ and integrate it into the path integral just like an initialization of the system.

What are useful examples of interferences in the time evolution? The easiest example is the injection of k particles into the system. If we insert $a^{\dagger k}$ at time t_1, then we find that

$$a^{\dagger k}|\mathcal{M}(t_1)\rangle = a^{\dagger k}\sum_{j=0}^{\infty} P\big(N(t_1)=j\big|N(t_0)\big)|j\rangle = \sum_{j=0}^{\infty} P\big(N(t_1)=j\big|N(t_0)\big)|j+k\rangle, \quad (2.68)$$

which implies that if the system was in state $N=j$ with probability $P\big(N(t_1)=j\big|N(t_0)\big)$, it is now in state $N=j+k$ with that same probability. In particular, the probability of the system to be in any state $N<k$ is zero immediately after the injection of k particles. Thus to inject k particles at time t_1, we simply insert $\phi^{\dagger k}(t_1)$ in the path integral.

Next, let's assume that the system evolved up to time t_1 to an unknown state with potentially many particles. We want to set the system back to zero particles and let it evolve again. The operator to do this is

$$|0\rangle\langle\text{☼}| = \sum_{j=0}^{\infty}|0\rangle\langle j|. \quad (2.69)$$

It is sandwiched between the time evolution operators before and after t_1, see Eq. (2.65). In particular, we need to evaluate

$$\sum_{j=0}^{\infty}\langle\phi^\dagger(t_1)|0\rangle\langle j|\phi(t_1)\rangle = \sum_{j=0}^{\infty}\frac{\phi^j(t_1)}{j!} = e^{\phi(t_1)}. \quad (2.70)$$

However, we need to keep in mind that there is the factor $e^{-\phi^\dagger(t_1)\phi(t_1)}$ in Eq. (2.66), which cancelled previously, but which does not cancel here. Hence, starting with the viewpoint of a time evolution from t_0 to t_2, the interruption of the time evolution by setting the system to zero particles at time t_1 is implemented by inserting the term $e^{-(\phi^\dagger(t_1)-1)\phi(t_1)} = e^{-\widetilde{\phi}(t_1)\phi(t_1)}$ into the path integral.

Increasing the number of particles at an intermediate time seemed fairly straight forward. What about decreasing the number of particles? It turns out, this is surprisingly complicated. Particle numbers can be decreased using the operator a, but this causes two difficulties. First, a applied to a state multiplies an additional factor to the state. Second, the state of zero particles $|0\rangle$ can have a non-zero probability, which would be lost because $a|0\rangle = 0$. Instead, we need to extract the probability for state $N=j+1$

and attach it to state $N = j$, which can be achieved by the operator d (for deduction/delete/decrease)

$$d = \sum_{j=0}^{\infty} |j\rangle\langle j+1| + |0\rangle\langle 0| = \sum_{j=0}^{\infty} a^{\dagger j}|0\rangle\langle 1|\frac{a^j}{(j+1)!} + |0\rangle\langle 0|, \tag{2.71}$$

where the additional term $|0\rangle\langle 0|$ enforces that the probability for an empty system in which the particle number cannot be reduced any further is not lost.

Inserting d between the time evolution operator from t_0 to t_1 and the time evolution operator from t_1 to t_2 in Eq. (2.65), requires us to evaluate

$$\langle\phi^\dagger(t_1)|d|\phi(t_1)\rangle = \sum_{j=0}^{\infty} \phi^{\dagger j}(t_1)\frac{\phi^{j+1}(t_1)}{(j+1)!} + 1 = \frac{1}{\phi^\dagger(t_1)}\Big(e^{\phi^\dagger(t_1)\phi(t_1)} - 1\Big) + 1. \tag{2.72}$$

Careful!, this is not the end of this problem. In deriving how to insert operators, we found that the term $e^{-\phi^\dagger(t_1)\phi(t_1)}$ cancelled, see Eq. (2.66). However, it does not cancel in the case of operator d. Hence, in order to reduce the particle number by one at time t_1 requires to insert the term $\big(1 - e^{-\phi^\dagger(t_1)\phi(t_1)} + \phi^\dagger(t_1)e^{-\phi^\dagger(t_1)\phi(t_1)}\big)/\phi^\dagger(t_1)$ into the path integral.

2.3.6 Extension of time evolution from $t_0 = -\infty$

In the previous section, we saw that once the system evolves in time, we can still influence it at intermediate times. This means, that the initiatiation of the system can actually be seen as an interruption of the system that actually started at time $t_0 = -\infty$. At $t_0 = -\infty$ we can initialize the system as we wish and we know for sure that it will have reached a steady state once we initialize the system at a finite time. In fact, if there is a unique steady state, then it doesn't matter how we initialize the system at $t_0 = -\infty$ and we can simply use the empty system $|0\rangle$ as initialization.

Furthermore, the factor $e^{-\phi^\dagger(-\infty)\phi(\infty)}$ will not play a role from now on and we choose to absorb it into the measure $\mathcal{D}[\phi^\dagger, \phi]$. So what we are left with is an initialization $\mathcal{I}_0(t_0)$ at a finite time t_0, and potentially a few interruptions $\mathcal{I}_1(t_1), \mathcal{I}_2(t_2), \dots$ at later times $t_0 < t_1 < t_2 < \cdots < t$:

$$|\mathcal{M}(t)\rangle = \int |\phi(t)\rangle \dots \mathcal{I}_2(t_2)\mathcal{I}_1(t_1)\mathcal{I}_0(t_0)e^{-\int_{-\infty}^{t} \phi^\dagger(t)\frac{\mathrm{d}}{\mathrm{d}t'}\phi(t) - \mathcal{L}[\phi^\dagger(t),\phi(t)]\,\mathrm{d}t'}\mathcal{D}[\phi^\dagger, \phi]. \tag{2.73}$$

This completes the path integral representation of the complete moment generating function / system state. So far we have only put in information, either through initializations and interruptions $\mathcal{I}$ of the time evolution or by providing a description of how the time evolution works, which is encoded in $\mathcal{L}[\phi^\dagger, \phi]$.

However, we have not derived yet how we can extract information from this path integral representation of $|\mathcal{M}(t)\rangle$. We tackle this problem in the next section.

2.3.7 Measurement – Interrogating the system

In Eqs. (2.26) and (2.27) we found out how to extract factorial moments and the usual moments from $|\mathcal{M}(t)\rangle$, which we recall here for convenience:

$$\langle \text{✡}|a^k|\mathcal{M}(t)\rangle = \mathbb{E}\big[\big(N(t)\big)_k \big| N(t_0)\big] \tag{2.26}$$

$$\big\langle \text{✡}\big|\big(a^\dagger a\big)^k\big|\mathcal{M}(t)\big\rangle = \mathbb{E}\big[N^k(t)\big|N(t_0)\big]. \tag{2.27}$$

Using the path integral in Eq. (2.73), and the fact that $|\phi(t)\rangle$ and $\langle \text{✡}|$ are eigenvectors of a and $a^\dagger$ respectively, we find

$$\langle \text{✡}|a^k|\phi(t)\rangle = \phi^k(t)e^{\phi(t)} \tag{2.74}$$

$$\langle \text{✡}|\big(a^\dagger a\big)^k|\phi(t)\rangle = \sum_{\ell=0}^{k} \left\{ {k \atop \ell} \right\} \phi^\ell(t)e^{\phi(t)}, \tag{2.75}$$

where $\left\{ {k \atop \ell} \right\}$ is the Stirling number of the second kind. It appears because in order to use the eigenvector relation for $(a^\dagger a)^k$, we need to remember first that $a^\dagger$ and a don't commute. For example $(a^\dagger a)^2 = a^\dagger a\, a^\dagger a = a^{\dagger 2}a^2 + a^\dagger a$. Hence $\langle \text{✡}|(a^\dagger a)^2|\phi(t)\rangle = \big(\phi^2(t) + \phi(t)\big)e^{\phi(t)}$. The Stirling number of the second kind produces the right coefficient for the normal ordering of $(a^\dagger a)^k$. The explicit formula for them is

$$\left\{ {k \atop \ell} \right\} = \frac{1}{\ell!}\sum_{j=0}^{\ell}(-1)^j \binom{\ell}{j}(\ell - j)^k, \tag{2.76}$$

assuming $0^0 = 1$ for the case $k = 0$.

In general, extracting moments or other observables will be a linear combination of terms of the form $\phi^k(t)e^{\phi(t)}$ inside the path integral Eq. (2.73). We combine $e^{\phi(t)}$ with the exponential in the path integral as follows:

$$\phi(t) - \int_{-\infty}^{t} \phi^\dagger(t)\frac{\mathrm{d}}{\mathrm{d}t'}\phi(t) - \mathcal{L}[\phi^\dagger(t), \phi(t)]\,\mathrm{d}t' = -\phi(-\infty) - \int_{-\infty}^{t} \widetilde{\phi}(t)\frac{\mathrm{d}}{\mathrm{d}t'}\phi(t) - \mathcal{L}[\phi^\dagger(t), \phi(t)]\,\mathrm{d}t', \tag{2.77}$$

Thus, we have a factor $e^{-\phi(-\infty)}$ in the path integral, which will not play a role in what follows. We therefore absorb it into the measure $\mathcal{D}[\phi^\dagger, \phi]$ as well. In summary, extracting information from the path integral representation of $|\mathcal{M}(t)\rangle$ is a linear combination of terms such as

$$\langle \phi^k(t)\ldots\mathcal{I}_2(t_2)\mathcal{I}_1(t_1)\rangle := \int \phi^k(t)\ldots\mathcal{I}_2(t_2)\mathcal{I}_1(t_1)\mathcal{I}_0(t_0)e^{-\int_{-\infty}^{t}\widetilde{\phi}(t)\frac{\mathrm{d}}{\mathrm{d}t'}\phi(t) - \mathcal{L}[\phi^\dagger(t),\phi(t)]\,\mathrm{d}t'}\mathcal{D}[\phi^\dagger, \phi], \tag{2.78}$$

where we have introduced the shorthand notation $\langle \phi^k(t) \dots \mathcal{I}_2(t_2)\mathcal{I}_1(t_1)\rangle$. For example: after initializing the system with two particles at time t_1, and after adding three additional particles at time t_2, the fourth factorial moment of the particle number at time t_3 is $\langle \phi^4(t_3)\phi^{\dagger 3}(t_2)\phi^{\dagger 2}(t_1)\rangle$, while the 2nd moment is $\langle \phi^2(t)\phi^{\dagger 3}(t_2)\phi^{\dagger 2}(t_1)\rangle + \langle \phi(t)\phi^{\dagger 3}(t_2)\phi^{\dagger 2}(t_1)\rangle$.

Often, objects like $\langle \phi^k(t) \dots \mathcal{I}_2(t_2)\mathcal{I}_1(t_1)\rangle$ are called n-point correlation functions and we could justify this name by saying that we 'correlate' an initialization and interruptions with the kth factorial moment. However, the word correlations would normally also apply to linking moments at different times to each other. For example, we might want to calculate the correlation of the particle number at time t_1 to the particle number at time $t_2 > t_1$. In essence, we want to be able to measure at different times.

2.3.8 Correlations – Interrogating the system again

Let's assume we have initiated the system and interrupted it as much as we like up to time t_0, represented by $\mathcal{I}(t_0)$. We also made a measurement by observing the system (e.g. its kth moment) at time t_1, represented by $\mathcal{O}(t_1)$. But, we don't want to stop there. We want to observe the system again at a later time t_2 with observable $\mathcal{O}(t_2)$. How can we do that?

Whenever we are unsure how to implement something into the path integral, it's a good idea to first try it in the Second Quantization picture. We use $\mathcal{I}$ and $\mathcal{O}$ as placeholders for whatever needs be inserted to realize an initialization, interruption or observation for both the path integral and the Second Quantization. Observing properties of the system at intermediate times is done in the same way as any other interruption of the time evolution:

$$\langle \dot{\varsigma} | \mathcal{O}(t_2) e^{\mathcal{L}[a^\dagger, a](t_2 - t_1)} \mathcal{O}(t_1) e^{\mathcal{L}[a^\dagger, a](t_1 - t_0)} \mathcal{I}(t_0) | \mathcal{M}(t_0)\rangle, \tag{2.79}$$

where we observe the system at time t_1, which will be done using an operator and then we let the system continue to evolve in time with $e^{\mathcal{L}(t_2 - t_1)}$. Thus, our result for interruptions in Eq. (2.65) still holds. We simply choose different operators that allow us to observe the system rather than manipulate it. When we insert observables, we need to make sure that we actually don't change the state of the system. For example, if we want to extract the expected particle number, we use operator a:

$$a|\mathcal{M}(t_1)\rangle = a \sum_{N=0}^{\infty} P\big(N(t_1) = N | N(t_0)\big)|N\rangle = \sum_{N=0}^{\infty} N P\big(N(t_1) = N | N(t_0)\big)|N-1\rangle. \tag{2.80}$$

However, a alone not only produces the needed factor N but also changes the state $|N\rangle$ to $|N-1\rangle$. We thus unintentionally changed the system state with our measurement!

Luckily, we can repair the damage, by multiplying by $a^\dagger$ afterwards:

$$a^\dagger a|\mathcal{M}(t_1)\rangle = a^\dagger a \sum_{N=0}^{\infty} P\big(N(t_1)=N|N(t_0)\big)|N\rangle = \sum_{N=0}^{\infty} NP\big(N(t_1)=N|N(t_0)\big)|N\rangle. \tag{2.81}$$

In general, whenever we measure at intermediate times, we need to make sure to repair the damage we have done by measuring.

If we want to correlate the expected particle number at time t_1 with the expected particle number at time t_2, then we need to use

$$\mathbb{E}[N(t_2)N(t_1)|N(t_0)] = \langle \text{☼}|a^\dagger a e^{\mathcal{L}[a^\dagger,a](t_2-t_1)} a^\dagger a e^{\mathcal{L}[a^\dagger,a](t_1-t_0)}|\mathcal{M}(t_0)\rangle, \tag{2.82}$$

which in the field theory translates to

$$\mathbb{E}[N(t_2)N(t_1)|N(t_0)] = \langle \phi(t_2)\phi^\dagger(t_1)\phi(t_1)\mathcal{I}(t_0)\rangle. \tag{2.83}$$

In particular, there is no $\phi^\dagger(t_2)$ because $\langle \text{☼}|a^\dagger = \langle \text{☼}|$.

Exercise 2.8

a) Find the operator for measuring the 2nd, 3rd and 4th moment and 2nd, 3rd, and 4th factorial moment at an intermediate time t_0 in terms of $a^\dagger$ and a. What is their normal ordered form?

b) Find the path integral expression for $\mathbb{E}[N^2(t_2)N^2(t_1)|N(t_0)]$.

2.3.9 Extension of time evolution to $t = +\infty$

In the previous section, we saw that we can observe properties of the system at several times. Therefore, we could regard our final observation as an intermediate observation and let the system continue to evolve afterwards until time $t = +\infty$. As future events cannot influence past events, this does not change any observables. However, it does change the look of the path integral, Eq. (2.78). The exponential in the path integral will contain an integral that goes from $t_0 = -\infty$ to $t = +\infty$. More explicitly, for Observations at times t_4 and t_3 and interruptions and initializations at times t_2 and t_1, we find

$$\langle \mathcal{O}(t_4)\mathcal{O}(t_3)\mathcal{I}_2(t_2)\mathcal{I}_1(t_1)\rangle = \int \mathcal{O}(t_4)\mathcal{O}(t_3)\mathcal{I}_2(t_2)\mathcal{I}_1(t_1) e^{-\int_{-\infty}^{\infty} \widetilde{\phi}(t)\frac{\mathrm{d}}{\mathrm{d}t'}\phi(t) - \mathcal{L}[\phi^\dagger(t),\phi(t)]\,\mathrm{d}t'} \mathcal{D}[\phi^\dagger,\phi], \tag{2.84}$$

which we will regard as the standard form of the path integral from now on. However, by standard form, I don't mean that we must have two observables and two initializations/interruptions. That part is as example and in general we could write

$$\langle \bullet \rangle = \int \bullet \, e^{-\int_{-\infty}^{\infty} \widetilde{\phi}(t) \frac{\mathrm{d}}{\mathrm{d}t'} \phi(t) - \mathcal{L}[\phi^\dagger(t), \phi(t)] \, \mathrm{d}t'} \mathcal{D}[\phi^\dagger, \phi]. \tag{2.85}$$

In an attempt to make notation more consistent, we are going to use the Doi-shift $\widetilde{\phi} = \phi^\dagger - 1$ on the fields in the path integral, absorbing this shift in $\mathcal{L}$ and $\mathcal{D}$. In particular we will call the integral inside the exponential the *action* of the stochastic process / of the system and denote it by curly $\mathcal{A}$s:

$$\mathcal{A}[\widetilde{\phi}, \phi] := -\int_{-\infty}^{\infty} \widetilde{\phi}(t) \frac{\mathrm{d}}{\mathrm{d}t} \phi(t) - \mathcal{L}[\widetilde{\phi}(t), \phi(t)] \, \mathrm{d}t, \tag{2.86}$$

which allows us to write the path integral much shorter:

$$\langle \bullet \rangle = \int \bullet \, e^{\mathcal{A}[\widetilde{\phi}, \phi]} \mathcal{D}[\widetilde{\phi}, \phi]. \tag{2.87}$$

Because the probability distributions $P(N(t)|N(t_0))$ are normalized at any time, we found that $\langle \text{☼} | \mathcal{M}(t) \rangle = 1$, which implies now that $\langle 1 \rangle = 1$ in the field theory.

2.3.10 The shortcut

In the previous sections, we have derived the path integral and how initializations, interruptions and measurements can be included into it. Although it is useful to understand the details of the derivation, it is unnecessary to go through them every time. Here, we summarize the steps to get to the path integral, the action and how to implement initializations, interruptions and measurements:

1. Write the Master Equation of the particle system
2. Use the probability generating function $\mathcal{M}(z, t)$ to rewrite the Master equation as a linear partial differential equation:

$$\frac{\partial}{\partial t} \mathcal{M}(z, t) = \mathcal{L}\left[z, \frac{\partial}{\partial z}\right] \mathcal{M}(z, t) \tag{2.88}$$

3. In $\mathcal{L}$, replace z by $a^\dagger$ and $\frac{\partial}{\partial z}$ by a for convenience and normal-order it, i.e. bring in every term the $a^\dagger$s to the left and as to the right using the commutation rule $aa^\dagger - a^\dagger a = 1$.

4. Create the action of the field theory as

$$\mathcal{A}\left[\widetilde{\phi},\phi\right] = -\int_{-\infty}^{\infty} \widetilde{\phi}(t)\frac{\mathrm{d}}{\mathrm{d}t}\phi(t) - \mathcal{L}\left[\widetilde{\phi}(t)+1,\phi(t)\right]\mathrm{d}t \tag{2.89}$$

5. Hence your path integral is

$$\langle\bullet\rangle = \int \bullet\, e^{\mathcal{A}[\widetilde{\phi},\phi]}\mathcal{D}[\widetilde{\phi},\phi] \tag{2.87}$$

6. Replace $\bullet$ by $\phi^k(t_1)\phi^\ell(t_0)$ for the kth factorial moment of the particle distribution at time t_1 given that the system was initialized with ℓ particles at time t_0.

7. For adding m particles at intermediate time $t_{0.33}$, insert $\phi^{\dagger m}(t_{0.33})$.

8. For measuring the nth factorial moment at an intermediate time $t_{0.67}$, insert $\phi^{\dagger n}(t_{0.67})\phi^n(t_{0.67})$.

2.3.11 Outlook

This ends the derivation of the path integral for Doi-Peliti field theory. If you have the feeling that we only have written terms and equations in ever changing forms but haven't actually solved anything, you're right. So far we have worked on transforming Master Equations into a form from which we can start doing field theory, which is the topic of the next chapter.

Exercises

Ex. 2.1 The Master Equations for the (a) spontaneous creation process with rate γ, (b) coagulation process with rate λ and (c) diffusion with rate D/h^2 are:

$$(a)\qquad \frac{\partial}{\partial t}P\big(N\big|N_0\big) = \gamma P\big(N-1\big|N_0\big) - \gamma P\big(N\big|N_0\big)$$

$$(b)\qquad \frac{\partial}{\partial t}P\big(N\big|N_0\big) = \lambda\binom{N+1}{2}P\big(N+1\big|N_0\big) - \lambda\binom{N}{2}P\big(N\big|N_0\big)$$

$$(c)\qquad \frac{\partial}{\partial t}P\big(N\big|N_0\big) = \frac{D}{h^2}\sum_{x\in X}\sum_{\substack{y\in X\\ |x-y|=h}}\Big((N_x+1)P\big(N+1_x-1_y\big|N_0\big) - N_x P\big(N\big|N_0\big)\Big),$$

Derive the corresponding PDEs for the moment generating function $\mathcal{M}(z,t)$.

Ex. 2.2 Consider the Master Equation for the spontaneous creation process with rate γ:

$$\frac{\partial}{\partial t}P\big(N(t)\big|N(t_0)\big) = \gamma P\big(N(t)-1\big|N(t_0)\big) - \gamma P\big(N(t)\big|N(t_0)\big).$$

Derive equations for the nth moment and the nth factorial moment.

Ex. 2.3 Find out what the action of the differentiation operator $\mathrm{d}/\mathrm{d}z$ and multiplication operator z is on the dual vector $\frac{(-1)^M}{M!}\int \delta^{(M)}(z) \bullet \mathrm{d}z$ without using Second Quantization.

Ex. 2.4 Show that the kth moment can be written in the language of Second Quantization as

$$\big\langle \dot{\varnothing}\big|\big(a^\dagger a\big)^k\big|\mathcal{M}(t)\big\rangle = \mathbb{E}\big[N^k(t)\big|N(t_0)\big].$$

Ex. 2.5 Consider the two dimensional vector space $\mathbb{R}^2$ with the euclidean inner product $\langle\cdot,\cdot\rangle$. Use the orthonormal basis

$$e_1 = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\1\end{pmatrix} \qquad e_2 = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\-1\end{pmatrix}$$

to show that $\sum_k e_k\langle e_k,\cdot\rangle$ is the identity matrix.

Ex. 2.6 Prove that $a^\dagger$ does not have a right eigenvector in the vector space of analytic functions.

Ex. 2.7 Operators that act in a linear space can be written using a basis and its dual basis. Write the annihilation and creation operators a and $a^\dagger$ in the form

$$a = \sum_{j,k=0}^{\infty} A_{j,k}|j\rangle\langle k| \qquad \text{and} \qquad a^\dagger = \sum_{j,k=0}^{\infty} A^\dagger_{j,k}|j\rangle\langle k|,$$

i.e. find the values of $A_{j,k}$ and $A^\dagger_{j,k}$. Find the analogous form of the combined operator $a^\dagger a$.

Ex. 2.8

a) Find the operator for measuring the 2nd, 3rd and 4th moment and 2nd, 3rd, and 4th factorial moment at an intermediate time t_0 in terms of $a^\dagger$ and a. What is their normal ordered form?

b) Find the path integral expression for $\mathbb{E}[N^2(t_2)N^2(t_1)|N(t_0)]$.

Chapter 3

Doi-Peliti Field Theory

At the end of the previous chapter, we found the path integral

$$\langle \bullet \rangle = \int \bullet \, e^{\mathcal{A}[\widetilde{\phi},\phi]} \mathcal{D}[\widetilde{\phi},\phi], \tag{2.87}$$

with action

$$\mathcal{A}[\widetilde{\phi},\phi] := -\int_{-\infty}^{\infty} \widetilde{\phi}(t) \frac{\mathrm{d}}{\mathrm{d}t}\phi(t) - \mathcal{L}[\widetilde{\phi}(t),\phi(t)]\,\mathrm{d}t. \tag{2.86}$$

But we didn't know what to do with it. In this chapter, we will make explicit calculations and look at several examples that we considered earlier in the form of Master Equations. In particular, we will also learn how to use Feynman diagrams to make our lives easier.

3.1 Feynman diagrams

First, we put off any interpretation of the process to the section on example processes, Sec. 3.2. Let's assume, we want to calculate $\langle \phi(t_1)\phi^\dagger(t_0)\rangle$, which means we put a particle into the system at time t_0 and calculate the first moment of the particle number at time t_1. We need to figure out how to calculate

$$\langle \phi(t_1)\phi^\dagger(t_0)\rangle = \int \phi(t_1)\phi^\dagger(t_0)\, e^{-\int_{-\infty}^{\infty} \widetilde{\phi}(t)\frac{\mathrm{d}}{\mathrm{d}t}\phi(t) - \mathcal{L}[\widetilde{\phi},\phi]\mathrm{d}t} \mathcal{D}[\widetilde{\phi},\phi]. \tag{3.1}$$

As the exponential contains $\widetilde{\phi}$, we split the initialization accordingly $\langle \phi(t_1)\phi^\dagger(t_0)\rangle = \langle \phi(t_1)\widetilde{\phi}(t_0)\rangle + \langle \phi(t_1)\rangle$. Next, we use functional derivatives, i.e. instead of differentiating with respect to variables, we differentiate with respect to functions ϕ and $\widetilde{\phi}$. Functional differentiation is done analogously to the usual differentiation: it is based on the difference quotient. Let's say we have functional $F[\phi]$ and we nudge function ϕ in direction of

a different function by adding a small perturbation function ϵh, where $\epsilon \in \mathbb{R}$ is a small parameter and h is a function. Then, the functional derivative of F with respect to ϕ in direction of h is defined as

$$\frac{\delta F[\phi]}{\delta \phi}(h) = \lim_{\epsilon \to 0} \frac{F[\phi + \epsilon h] - F[\phi]}{\epsilon}, \tag{3.2}$$

assuming that all parts are well defined. The most common choice for h is the δ-function. Let's calculate an example (assuming $\mathcal{L} = 0$):

$$\frac{\delta \mathcal{A}[\widetilde{\phi}, \phi]}{\delta \widetilde{\phi}}(\delta(t)) = \lim_{\epsilon \to 0} \frac{-\int_{-\infty}^{\infty} (\widetilde{\phi}(t) + \epsilon\delta(t)) \frac{\mathrm{d}}{\mathrm{d}t}\phi(t)\mathrm{d}t + \int_{-\infty}^{\infty} \widetilde{\phi}(t) \frac{\mathrm{d}}{\mathrm{d}t}\phi(t)\mathrm{d}t}{\epsilon} \tag{3.3}$$

$$= -\int_{-\infty}^{\infty} \delta(t) \frac{\mathrm{d}}{\mathrm{d}t}\phi(t)\mathrm{d}t = -\dot{\phi}(0). \tag{3.4}$$

Because functional differentiation is also based on the difference quotient, the results look very similar, and we can quickly adapt our muscle memory for usual differentiation to also work for functional differentiation. In the following, the direction h will always be a δ-function and we are going to write $\frac{\delta}{\delta J(t_n)}$ for the functional derivative with respect to J in the direction of $\delta(t - t_n)$.

Exercise 3.1 Let $S[f]$ and $T[f|$ be the following functionals

$$S[f] = \int_{-\infty}^{\infty} \exp\big(-f^2(x)\big)\mathrm{d}x, \qquad T[f] = \exp\left(-\int_{-\infty}^{\infty} f^2(x)\mathrm{d}x\right),$$

calculate the functional derivatives of $S[f]$ and $T[f]$ in direction $h(x)$.

Going back to our original problem, Eq. (3.1), we can calculate $\langle \phi(t_1)\widetilde{\phi}(t_0)\rangle$ and $\langle \phi(t_1)\rangle$ using functional derivatives as follows:

$$\langle \phi(t_1)\rangle = \frac{\delta}{\delta J(t_1)} \int e^{-\int_{-\infty}^{\infty} \widetilde{\phi}(t)\frac{\mathrm{d}}{\mathrm{d}t}\phi(t) - \mathcal{L}[\widetilde{\phi},\phi] - J(t)\phi(t)\,\mathrm{d}t} \mathcal{D}[\phi^\dagger, \phi]\Big|_{J=0} \tag{3.5}$$

$$\langle \phi(t_1)\widetilde{\phi}(t_0)\rangle = \frac{\delta}{\delta J(t_1)} \frac{\delta}{\delta \widetilde{J}(t_0)} \int e^{-\int_{-\infty}^{\infty} \widetilde{\phi}(t)\frac{\mathrm{d}}{\mathrm{d}t}\phi(t) - \mathcal{L}[\widetilde{\phi},\phi] - J(t)\phi(t) - \widetilde{J}(t)\widetilde{\phi}(t)\,\mathrm{d}t} \mathcal{D}[\phi^\dagger, \phi]\Big|_{\substack{J=0 \\ \widetilde{J}=0}} \tag{3.6}$$

This approach can be generalized to any observable and initialization. For example $\langle \phi^{n_2}(t_2)\phi^{n_1}(t_1)\widetilde{\phi}^{n_0}(t_0)\rangle$ can be calculated by using $\frac{\delta^{n_2}}{\delta J^{n_2}(t_2)}$, $\frac{\delta^{n_1}}{\delta J^{n_1}(t_1)}$ and $\frac{\delta^{n_0}}{\delta \widetilde{J}^{n_0}(t_0)}$ and evaluating the result at $J = 0$ and $\widetilde{J} = 0$.

Thus we have reduced the problem to evaluating the path integral without initializations and measurements but with additional terms in the exponential function.

A further simplification can be achieved by splitting $\mathcal{L}[\widetilde{\phi}, \phi]$ into a bilinear part that has terms of the form $\widetilde{\phi}\phi$ and other terms, which we will call interaction terms. These other terms will be grouped into $\mathcal{L}_{\text{int}}[\widetilde{\phi}, \phi]$ ('int' for interaction). Furthermore, we group the existing term of $\widetilde{\phi}\frac{\mathrm{d}}{\mathrm{d}t}\phi$ together with the bilinear terms from $\mathcal{L}$. They form together an expression of the form $\widetilde{\phi}\big(\frac{\mathrm{d}}{\mathrm{d}t}+r\big)\phi$, where r is a placeholder for whatever the exact bilinear term was in $\mathcal{L}$. The promised simplification consists of splitting up the exponential as follows

$$e^{-\int_{-\infty}^{\infty} \widetilde{\phi}(t)\frac{\mathrm{d}}{\mathrm{d}t}\phi(t) - \mathcal{L}[\widetilde{\phi},\phi] - J(t)\phi(t) - \widetilde{J}(t)\widetilde{\phi}(t)\,\mathrm{d}t} = \tag{3.7}$$

$$= e^{-\int_{-\infty}^{\infty} \widetilde{\phi}(t)\left(\frac{\mathrm{d}}{\mathrm{d}t}+r\right)\phi(t) - J(t)\phi(t) - \widetilde{J}(t)\widetilde{\phi}(t)\,\mathrm{d}t} \sum_{k=0}^{\infty} \frac{1}{k!}\left(\int_{-\infty}^{\infty} \mathcal{L}_{\text{int}}[\widetilde{\phi}, \phi]\mathrm{d}s\right)^k, \tag{3.8}$$

and treating the terms in the sum as if they were observables or initializations, i.e. we use $\frac{\delta}{\delta J}$ and $\frac{\delta}{\delta \widetilde{J}}$ again. The time variable s is simply introduced to make a clearer separation between the integrals. In fact, when we consider $k > 1$, we actually have k distinct integrals over $\mathcal{L}_{\text{int}}$, which we will distinguish by using integration variables $s_1, s_2, \ldots$.

We are left with evaluating the following path integral:

$$\int e^{-\int_{-\infty}^{\infty} \widetilde{\phi}(t)\left(\frac{\mathrm{d}}{\mathrm{d}t}+r\right)\phi(t) - J(t)\phi(t) - \widetilde{J}(t)\widetilde{\phi}(t)\,\mathrm{d}t} \mathcal{D}[\widetilde{\phi}, \phi] = e^{-\int_{-\infty}^{\infty} \widetilde{J}(t)(\frac{\mathrm{d}}{\mathrm{d}t}+r)^{-1}J(t)\mathrm{d}t}, \tag{3.9}$$

but wait a second! Where does this result come from and what does $(\frac{\mathrm{d}}{\mathrm{d}t} + r)^{-1}$ mean?

In order to understand this result, let's consider the analogous case for integrals over variables. We have variable $x \in \mathbb{C}$ and an integral over $\exp(-\bar{x}Px + yx + \bar{y}\bar{x})$, where $y \in \mathbb{C}$ are dummy variables emulating J:

$$\int e^{-\bar{x}Px + yx + \bar{y}\bar{x}} \frac{\mathrm{d}x\mathrm{d}\bar{x}}{\pi} = \int e^{-|(\sqrt{P}x - \bar{y}/\sqrt{P})|^2} \frac{\mathrm{d}x\mathrm{d}\bar{x}}{\pi} e^{\bar{y}P^{-1}y} = e^{\bar{y}P^{-1}y} \tag{3.10}$$

However, this result does not completely match with our situation in the path integral in several respects!

First, we see that $\bar{x}$ is the complex conjugate of x but $\widetilde{\phi}$ is not exactly the complex conjugate of ϕ. That's true, but if we introduce $\widetilde{x} = \bar{x} - 1$, we get an extra e^{Px} compared to the path integral, don't we? Yes, but you might remember that we actually did have the exact equivalent in the path integral, see Eq. (2.77), and we absorbed it into the measure $\mathcal{D}$, which is a way of saying, we were hiding it.

Second, Eq. (3.10) uses y and $\bar{y}$ as complex conjugates, however, we didn't mention that J and $\widetilde{J}$ are related. I omitted the relation between J and $\widetilde{J}$ above (sorry about that) in order to argue here why they actually need to be related. However, it will turn out that their exact relation is actually not important, we only need that Eq. (3.9) is true for some relation between $\widetilde{J}$ and J.

Third, in a normal integral, the P in the bilinear part would be a number that can be inverted. But in the path integral setting we have to invert $(\mathrm{d}/\mathrm{d}t + r)$. How can that work? The trick is to use the Fourier transform, defined as follows

$$\phi(\omega) = \mathcal{F}[\phi](\omega) = \int_{-\infty}^{\infty} \phi(t) e^{i\omega t} \mathrm{d}t \tag{3.11}$$

$$\phi(t) = \mathcal{F}^{-1}[\phi](t) = \int_{-\infty}^{\infty} \phi(\omega) e^{-i\omega t} đ\omega, \tag{3.12}$$

where $đ\omega := \mathrm{d}\omega/(2\pi)$. This allows us to transform the bilinear part of $\mathcal{A}$:

$$\int_{-\infty}^{\infty} \widetilde{\phi}(t)\Big(\frac{\mathrm{d}}{\mathrm{d}t} + r\Big)\phi(t)\mathrm{d}t = \int_{\mathbb{R}^2} \widetilde{\phi}(\omega')\big(-i\omega + r\big)\phi(\omega)\delta(\omega + \omega')đ\omega đ\omega' \tag{3.13}$$

$$= \int_{-\infty}^{\infty} \widetilde{\phi}(-\omega)\big(-i\omega + r\big)\phi(\omega)đ\omega \tag{3.14}$$

where $\delta(\omega + \omega') = 2\pi\delta(\omega + \omega')$. In particular, we require that r is constant in time t, which makes it dimensionally a rate, and we therefore assume $r > 0$. Thus, in Fourier space, we know the inverse of $(-i\omega + r)$ and Eq. (3.9) becomes

$$\int e^{-\int_{-\infty}^{\infty} \widetilde{\phi}(t)\left(\frac{\mathrm{d}}{\mathrm{d}t}+r\right)\phi(t) - J(t)\phi(t) - \widetilde{J}(t)\widetilde{\phi}(t)\,\mathrm{d}t} \mathcal{D}[\widetilde{\phi}, \phi] = e^{\int_{-\infty}^{\infty} \frac{\widetilde{J}(-\omega)J(\omega)}{-i\omega+r} đ\omega}. \tag{3.15}$$

Hence, we can return to our original task and calculate $\langle \phi(t_1)\phi^\dagger(t_0)\rangle$ using functional derivatives with respect to J and $\widetilde{J}$. Our first step is to ignore the interaction part $\mathcal{L}_{\mathrm{int}}$, which is equivalent to considering only $k = 0$ in Eq. (3.8). We will make a note of this $k = 0$-choice by using subscripts on the angular brackets: $\langle \phi(t_1)\widetilde{\phi}(t_0)\rangle_\ell$ stands for considering the path integral with exponent $k = \ell$ in Eq. (3.8):

$$\langle \phi(t_1)\widetilde{\phi}(t_0)\rangle_0 = \frac{\delta}{\delta\widetilde{J}(t_0)}\frac{\delta}{\delta J(t_1)} \exp\left(\int_{-\infty}^{\infty} \frac{\widetilde{J}(-\omega)J(\omega)}{-i\omega + r} đ\omega\right)\Bigg|_{\substack{J=0\\ \widetilde{J}=0}} \tag{3.16}$$

$$= \int_{-\infty}^{\infty} \frac{e^{-i\omega(t_1 - t_0)}}{-i\omega + r} đ\omega = \Theta(t_1 - t_0)e^{-r(t_1 - t_0)}, \tag{3.17}$$

where the δ-function for t_0 and t_1 become in Fourier space exponential functions:

$$\mathcal{F}[\delta(t - t_0)](\omega) = e^{-i\omega t_0} \quad \text{and} \quad \mathcal{F}[\delta(t - t_1)](\omega) = e^{-i\omega t_1}, \tag{3.18}$$

however $\widetilde{J}$ has the argument $-\omega$, which leads to the different signs for the two times. The $\Theta(t_1 - t_0)$ is the so-called Heaviside function defined as

$$\Theta(t_1 - t_0) = \begin{cases} 1 & t_1 - t_0 \geq 0 \\ 0 & t_1 - t_0 < 0 \end{cases} \tag{3.19}$$

Eq. (3.17) is our first explicit example of a path integral calculation! It only consists of 1) an initialization at time t_0, 2) the measurement at time t_1 and the bilinear part of the action $\mathcal{A}$ connecting the two. It is represented by the simplest of Feynman diagrams: the straight line

$$\langle \phi(t_1)\widetilde{\phi}(t_0)\rangle_0 \hat{=} \quad t_1 \text{ ——— } t_0 \tag{3.20}$$

where the labels t_1 and t_0 at the two ends of the line are often omitted. All lines that will appear in any of the Feynman diagrams that follow can be reduced to the calculation we just performed. A line in a Feynman diagram and the terms it represents are usually called *bare propagator*, because they are the simplest way of connecting two times. However, what makes Feynman diagrams more interesting are vertices.

Vertices arise from interaction terms that we gathered in $\mathcal{L}_{\text{int}}[\widetilde{\phi}, \phi]$. For now we ignore their interpretation in terms of stochastic processes or physics but simply concentrate on how to do calculations if such terms exist.

One of the simplest interaction terms is $\mathcal{L}_{\text{int}}[\widetilde{\phi}, \phi] = \gamma\widetilde{\phi}$, where γ is a constant parameter. Let's say, we want to calculate $\langle \phi(t_1)\rangle$. Following Eq. (3.8), the first term we should look at is for $k = 0$, i.e. we ignore $\mathcal{L}_{\text{int}}[\widetilde{\phi}, \phi]$ and just work with the bilinear part of the action. This means in the first instance, we calculate $\langle \phi(t_1)\rangle_0$. Let's try that:

$$\langle \phi(t_1)\rangle_0 = \frac{\delta}{\delta J(t_1)} \exp\left(\int_{-\infty}^{\infty} \frac{\widetilde{J}(-\omega)J(\omega)}{-i\omega + r} \text{đ}\omega \right) \Bigg|_{\substack{J=0 \\ \widetilde{J}=0}} = \int_{-\infty}^{\infty} \frac{\widetilde{J}(-\omega)e^{-i\omega t_1}}{-i\omega + r} \text{đ}\omega \Bigg|_{\substack{J=0 \\ \widetilde{J}=0}} = 0 \tag{3.21}$$

Thus, we find $\langle \phi(t_1)\rangle_0 = 0$ as our initial approximation of $\langle \phi(t_1)\rangle$. Let's calculate the next-best approximation by calculating $\langle \phi(t_1)\rangle_1$. According to Eq. (3.8) for $k = 1$, $\langle \phi(t_1)\rangle_1$ can be written using our previous result for $\langle \phi(t_1)\widetilde{\phi}(t_0)\rangle_0$:

$$\langle \phi(t_1)\rangle_1 = \gamma \int_{-\infty}^{\infty} \langle \phi(t_1)\widetilde{\phi}(s)\rangle_0 \text{d}s, \tag{3.22}$$

and following Eq. (3.17), the integral can be evaluated as

$$\langle \phi(t_1)\rangle_1 = \gamma \int_{-\infty}^{t_1} e^{-r(t_1 - s)} \text{d}s = \frac{\gamma}{r} \tag{3.23}$$

The Feynman diagram of $\langle\phi(t_1)\rangle_1$ is almost as simple as the straight line:

$$\langle\phi(t_1)\rangle_1 \hat{=} \; t_1 \longrightarrow \times \tag{3.24}$$

where the cross symbolizes the one term $\gamma\widetilde{\phi}$ from the interaction term $\mathcal{L}_{\text{int}}[\widetilde{\phi},\phi]$.

Staying with the observable $\langle\phi(t_1)\rangle$ and the interaction term $\mathcal{L}_{\text{int}}[\widetilde{\phi},\phi] = \gamma\widetilde{\phi}$, what are the results for $\langle\phi(t_1)\rangle_k$ with $k \geq 2$?

For $k = 2$, Eq. (3.8), says we can reduce $\langle\phi(t_1)\rangle_2$ to

$$\langle\phi(t_1)\rangle_2 = \gamma^2 \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} \langle\phi(t_1)\widetilde{\phi}(s_1)\widetilde{\phi}(s_2)\rangle_0 \mathrm{d}s_1\mathrm{d}s_2 \tag{3.25}$$

Although we have not calculated $\langle\phi(t_1)\widetilde{\phi}(s_1)\widetilde{\phi}(s_2)\rangle_0$ before, we have the means to do so:

$$\langle\phi(t_1)\widetilde{\phi}(s_1)\widetilde{\phi}(s_2)\rangle_0 = \frac{\delta}{\delta J(t_1)}\frac{\delta}{\delta\widetilde{J}(s_1)}\frac{\delta}{\delta\widetilde{J}(s_2)} \exp\left(\int_{-\infty}^{\infty} \frac{\widetilde{J}(-\omega)J(\omega)}{-i\omega + r}\text{đ}\omega\right)\Bigg|_{\substack{J=0\\ \widetilde{J}=0}} = 0 \tag{3.26}$$

It turns out that $\langle\phi(t_1)\widetilde{\phi}(s_1)\widetilde{\phi}(s_2)\rangle_0 = 0$ because the number of (functional) derivatives with respect to J is not equal the number of (functional) derivatives with respect to $\widetilde{J}$. Evaluating at $J = 0$ and $\widetilde{J} = 0$ makes the result of the derivatives equal to zero. In fact, this is an extremely useful insight that will help us rule out many occurring terms when considering expansions in the interaction term.

Continuing with the evaluation of $\langle\phi(t_1)\rangle$ with interaction $\mathcal{L}_{\text{int}}[\widetilde{\phi},\phi] = \gamma\widetilde{\phi}$, the terms $\langle\phi(t_1)\rangle_k$ can be expressed in a similar way as $\langle\phi(t_1)\rangle_2$

$$\langle\phi(t_1)\rangle_k = \underbrace{\int_{-\infty}^{\infty}\cdots\int_{-\infty}^{\infty}}_{k \text{ terms}} \langle\phi(t_1)\widetilde{\phi}(s_1)\ldots\widetilde{\phi}(s_k)\rangle_0 \mathrm{d}s_1\ldots\mathrm{d}s_k = \begin{cases} \frac{\gamma}{r} & k = 1 \\ 0 & k \neq 1 \end{cases} \tag{3.27}$$

Again, the reason why $\langle\phi(t_1)\rangle_{k\neq 1} = 0$ is that the term involves one (functional) derivative with respect to J and $k \neq 1$ (functional) derivatives with respect to $\widetilde{J}$ of Eq. (3.15), followed by an evaluation at $J = 0$ and $\widetilde{J} = 0$.

This finishes the evaluation of $\langle\phi(t_1)\rangle$ in the case of $\mathcal{L}_{\text{int}}[\widetilde{\phi},\phi] = \gamma\widetilde{\phi}$. The solution is $\langle\phi(t_1)\rangle = \langle\phi(t_1)\rangle_1 = \frac{\gamma}{r}$. However, the found Feynman diagram, Eq. (3.24) is still a bit boring.

To get more interesting Feynman diagrams, let's consider the interaction terms $\mathcal{L}_{\text{int}}[\widetilde{\phi},\phi] = \alpha\widetilde{\phi}\phi^2 + \beta\widetilde{\phi}^2\phi$ and the observable $\langle\phi(t_1)\widetilde{\phi}(t_0)\rangle$. The first step is to calculate $\langle\phi(t_1)\widetilde{\phi}(t_0)\rangle_0$, which we did in Eq. (3.17). So we swiftly move on to calculating $\langle\phi(t_1)\widetilde{\phi}(t_0)\rangle_1$. Because

$\mathcal{L}_{\text{int}}[\widetilde{\phi}, \phi]$ is the sum of two terms and the path integral is linear, we can consider the terms separately:

$$\langle \phi(t_1)\widetilde{\phi}(t_0)\rangle_1 = \alpha \int_{-\infty}^{\infty} \underbrace{\langle \phi(t_1)\widetilde{\phi}(t_0)\widetilde{\phi}(s_1)\phi^2(s_1)\rangle_0}_{=0} \mathrm{d}s_1 + \beta \int_{-\infty}^{\infty} \underbrace{\langle \phi(t_1)\widetilde{\phi}(t_0)\widetilde{\phi}^2(s_1)\phi(s_1)\rangle_0}_{=0} \mathrm{d}s_1 \tag{3.28}$$

Both terms equal zero because the number of ϕ terms (and thus J-derivatives) is different to the number of $\widetilde{\phi}$ terms (and thus $\widetilde{J}$ derivatives).

Next, we need to consider $\langle \phi(t_1)\widetilde{\phi}(t_0)\rangle_2$, which contains three terms:

$$\langle \phi(t_1)\widetilde{\phi}(t_0)\rangle_2 = \alpha^2 \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} \underbrace{\langle \phi(t_1)\widetilde{\phi}(t_0)\widetilde{\phi}(s_1)\phi^2(s_1)\widetilde{\phi}(s_2)\phi^2(s_2)\rangle_0}_{=0} \mathrm{d}s_1\mathrm{d}s_2 \tag{3.29a}$$

$$= 2\alpha\beta \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} \langle \phi(t_1)\widetilde{\phi}(t_0)\widetilde{\phi}(s_1)\phi^2(s_1)\widetilde{\phi}^2(s_2)\phi(s_2)\rangle_0 \mathrm{d}s_1\mathrm{d}s_2 \tag{3.29b}$$

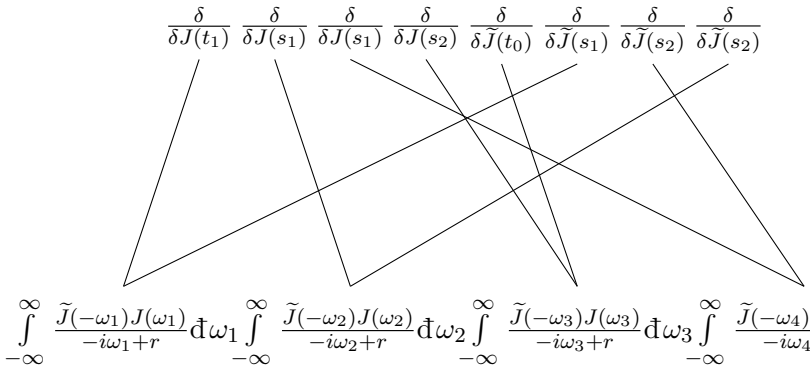
$$= \beta^2 \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} \underbrace{\langle \phi(t_1)\widetilde{\phi}(t_0)\widetilde{\phi}^2(s_1)\phi(s_1)\widetilde{\phi}^2(s_2)\phi(s_2)\rangle_0}_{=0} \mathrm{d}s_1\mathrm{d}s_2 \tag{3.29c}$$

While the first and third term equal zero because of unequal numbers of ϕs and $\widetilde{\phi}$s, the second term actually does have an equal number of them. Evaluating it involves four J derivatives and four $\widetilde{J}$ derivatives. Since we set J and $\widetilde{J}$ equal to zero afterwards, we can focus on Eq. (3.29b) and apply the corresponding number of functional derivatives to Eq. (3.15):

$$\begin{aligned}
&\langle \phi(t_1)\widetilde{\phi}(t_0)\widetilde{\phi}(s_1)\phi^2(s_1)\widetilde{\phi}^2(s_2)\phi(s_2)\rangle_0 = \\
&= \frac{\delta}{\delta J(t_1)}\frac{\delta^2}{\delta J^2(s_1)}\frac{\delta}{\delta J(s_2)}\frac{\delta}{\delta \widetilde{J}(t_0)}\frac{\delta^2}{\delta \widetilde{J}^2(s_2)}\frac{\delta}{\delta \widetilde{J}(s_1)} \exp\left(\int_{-\infty}^{\infty} \frac{\widetilde{J}(-\omega)J(\omega)}{-i\omega + r} \text{đ}\omega\right)\Bigg|_{\substack{J=0\\ \widetilde{J}=0}} \\
&= \frac{\delta}{\delta J(t_1)}\frac{\delta^2}{\delta J^2(s_1)}\frac{\delta}{\delta J(s_2)}\frac{\delta}{\delta \widetilde{J}(t_0)}\frac{\delta^2}{\delta \widetilde{J}^2(s_2)}\frac{\delta}{\delta \widetilde{J}(s_1)}\frac{1}{4!}\left(\int_{-\infty}^{\infty} \frac{\widetilde{J}(-\omega)J(\omega)}{-i\omega + r} \text{đ}\omega\right)^4\Bigg|_{\substack{J=0\\ \widetilde{J}=0}},
\end{aligned} \tag{3.30}$$

where we have to remember that the fourth power of the integral means that there are actually four integrals each with their own variable ω_1, ω_2, ω_3 and ω_4. Because of this, the derivatives create several slightly different expressions, each of which can be identified by the pairings of J- and $\widetilde{J}$-derivatives that were applied to the integrals. One

possible pairing is



(3.31)

where a line indicates that the derivative above is applied to the integral below.

Before we start counting how many such pairings exists for this example, let's evaluate the example pairing in Eq. (3.31):

$$\begin{aligned}
&\left(\frac{\delta}{\delta J(t_1)}\frac{\delta}{\delta \widetilde{J}(s_1)}\int \frac{\widetilde{J}(-\omega_1)J(\omega_1)}{-i\omega_1+r}\text{đ}\omega_1\right)\left(\frac{\delta}{\delta J(s_1)}\frac{\delta}{\delta \widetilde{J}(s_2)}\int \frac{\widetilde{J}(-\omega_2)J(\omega_2)}{-i\omega_2+r}\text{đ}\omega_2\right)\cdot \\
&\cdot\left(\frac{\delta}{\delta J(s_2)}\frac{\delta}{\delta \widetilde{J}(t_0)}\int \frac{\widetilde{J}(-\omega_3)J(\omega_3)}{-i\omega_3+r}\text{đ}\omega_3\right)\left(\frac{\delta}{\delta J(s_1)}\frac{\delta}{\delta \widetilde{J}(s_2)}\int \frac{\widetilde{J}(-\omega_4)J(\omega_4)}{-i\omega_4+r}\text{đ}\omega_4\right) = \\
&= \int \frac{e^{-i\omega_1(t_1-s_1)}}{-i\omega_1+r}\text{đ}\omega_1 \int \frac{e^{-i\omega_2(s_1-s_2)}}{-i\omega_2+r}\text{đ}\omega_2 \int \frac{e^{-i\omega_3(s_2-t_0)}}{-i\omega_3+r}\text{đ}\omega_3 \int \frac{e^{-i\omega_4(s_1-s_2)}}{-i\omega_4+r}\text{đ}\omega_4 \qquad (3.32)\\
&= \Theta(t_1-s_1)e^{-r(t_1-s_1)}\Theta(s_1-s_2)e^{-r(s_1-s_2)}\Theta(s_2-t_0)e^{-r(s_2-t_0)}\Theta(s_1-s_2)e^{-r(s_1-s_2)},
\end{aligned}$$

where the Heaviside functions create the time ordering of $t_1 > s_1 > s_2 > t_0$. This terms' contribution to $\langle\phi(t_1)\widetilde{\phi}(t_0)\rangle_2$ can now be determined by integrating over s_1 and s_2 and attaching the factor $2\alpha\beta$, see Eq. (3.29b):

$$2\alpha\beta \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} \Theta(t_1-s_1)\Theta(s_1-s_2)\Theta(s_2-t_0)e^{-r(t_1+s_1-s_2-t_0)}\text{d}s_2\text{d}s_1 = \qquad (3.33a)$$

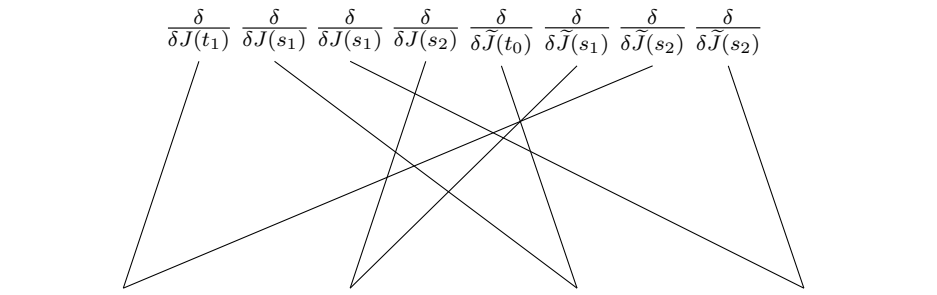
$$= 2\alpha\beta \int_{t_0}^{t_1}\int_{t_0}^{s_1} e^{-r(t_1+s_1-s_2-t_0)}\text{d}s_2\text{d}s_1 \qquad (3.33b)$$

$$= \frac{2\alpha\beta}{r}\int_{t_0}^{t_1}\left(e^{-r(t_1-t_0)} - e^{-r(t_1+s_1-2t_0)}\right)\text{d}s_1 \qquad (3.33c)$$

$$= \frac{2\alpha\beta}{r^2}\left(r(t_1-t_0)e^{-r(t_1-t_0)} + e^{-2r(t_1-t_0)} - e^{-r(t_1-t_0)}\right) \qquad (3.33d)$$

Thus, given that $t_1 > t_0$, we found an additional term in $\langle \phi(t_1)\widetilde{\phi}(t_0)\rangle$. However, there are potentially lots of pairing like the one in Eq. (3.31). How many are there and what terms do they correspond to?

Let's count possible pairings: For the ω_1-integral, we can choose from 4 J derivatives and from 4 $\widetilde{J}$ derivatives. Once they are chosen, then we move on to the ω_2-integral, for which there are 3 J- and 3 $\widetilde{J}$-derivatives left. For the ω_3-integral, we have choice out of two derivatives for each type of derivative. Thus there are $(4!)^2 = 576$ possible pairings. This seems like a combinatorial nightmare! However, there are two lifelines for us: 1) we treated the 4 integrals as distinguishable in our counting of all possible pairings. However, which of them is the ω_1-integral and which one the ω_3-integral doesn't matter. We could relabel them and still get the same result. This gives us a reduction by 4! and leaves us with 24 possible pairings. Furthermore, this repetition of 4! cancels nicely with the factor 1/4! in Eq. (3.30) 2) A closer look will show us that almost all of them equal zero. In fact, our choice above, Eq. (3.31), seems to be one of the lucky few that are not zero. Let's look at a different pairing:



(3.34)

$$\int_{-\infty}^{\infty} \frac{\widetilde{J}(-\omega_1)J(\omega_1)}{-i\omega_1+r} đ\omega_1 \int_{-\infty}^{\infty} \frac{\widetilde{J}(-\omega_2)J(\omega_2)}{-i\omega_2+r} đ\omega_2 \int_{-\infty}^{\infty} \frac{\widetilde{J}(-\omega_3)J(\omega_3)}{-i\omega_3+r} đ\omega_3 \int_{-\infty}^{\infty} \frac{\widetilde{J}(-\omega_4)J(\omega_4)}{-i\omega_4+r} đ\omega_4$$

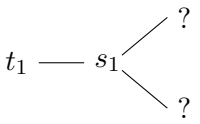
$$\hat{=}\Theta(t_1 - s_2)e^{-r(t_1-s_2)}\Theta(s_1 - t_0)e^{-r(s_1-t_0)}\Theta(s_1 - s_2)e^{-r(s_1-s_2)}\Theta(s_2 - s_1)e^{-r(s_2-s_1)}$$

which equals zero once we integrate over s_1 and s_2 because the third Heaviside function imposes $s_1 \geq s_2$ and the fourth imposes $s_2 \geq s_1$. Since there is no δ-function at $s_1 = s_2$, the integral equals zero.

In this example, we see that time-ordering is a crucial component in determining whether a pairing results in a non-zero contribution. What is fixed is that $t_1 > t_0$, but what are the options for s_1 and s_2? Since t_1 appears in the J-derivative, we pair it with a $\widetilde{J}$-derivative, and the time associated with that $\widetilde{J}$-derivative will be smaller than t_1 according to Eq. (3.17). Analogously, whatever J-derivative is paired with the $\widetilde{J}(t_0)$ derivative, its associated time must be larger than t_0. Let's go through some options in a graphic way: **on the left, we put larger times and on the right smaller times**:

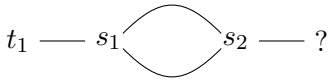
- Let's connect t_1 with s_1 such that $t_1 \geq s_1$. But s_1 is also associated with two J-derivatives which both need to be paired with other $\widetilde{J}$-derivatives. Their associated

times will be smaller than s_1. So we draw two lines from s_1 to other times.



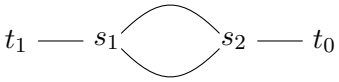
(3.35)

The only available $\widetilde{J}$-derivatives are associated with t_0 (once available) or s_2 (twice available). First, let's replicate our first pairing example, Eq. (3.31), where both $J(s_1)$-derivatives were paired with $\widetilde{J}(s_2)$-derivatives. To show this, we bend both lines down to meet at time s_2:



(3.36)

Finally, there is only one pairing left, which connects the $J(s_2)$-derivative with the $\widetilde{J}(t_0)$-derivative. We show that last connection as the straight line on the right:



(3.37)

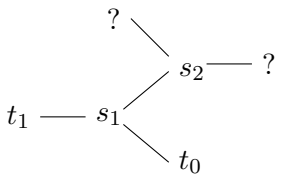
It turns out that drawing the time-ordering in diagrams is the easiest way of determining allowed pairings. We stylize them a little bit and call them *Feynman diagrams*:

(3.38)

In particular, we can associate to each node a specific term in the interaction part $\mathcal{L}_{\text{int}}[\widetilde{\phi}, \phi] = \alpha\widetilde{\phi}\phi^2 + \beta\widetilde{\phi}^2\phi$. The left node was due to the three (functional) derivatives associated with s_1, which came from the term $\alpha\widetilde{\phi}\phi^2$. To clarify this, it is common the write α next to the node. Analogously, the right node was due to the three (functional) derivatives associated with s_2, which came from the term $\beta\widetilde{\phi}^2\phi$, and which could be clarified by drawing β next to the right node:

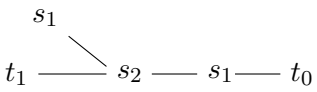
One important observation is that when pairing a $J(s_1)$-derivative with a $\widetilde{J}(s_2)$-derivative, we had two identical options. This means the resulting term actually appears twice in the set of all possible pairings but it's associated with the same Feynman diagram. This factor is called a *symmetry factor* and needs to be remembered once we focus only on drawing diagrams instead of thinking about pairings of functional derivatives:

- What about other pairings and their diagrams? Let's jump back to the situation in Eq. (3.35). We had the option to pair one of the $J(s_1)$-derivatives with the $\widetilde{J}(t_0)$-derivatives. This option leaves a $J(s_2)$ derivative and a $\widetilde{J}(s_2)$ derivative, which don't have any other derivatives to pair with.



(3.39)

which shows that this attempted time-ordering doesn't work. Let's consider the tried time-ordering from Eq. (3.34). If we follow the same sketch rules as before, we find



(3.40)

The attempt at drawing the time-ordering fails since s_1 appears on the left of s_2 and on the right of s_2. The failure to draw the time-ordering, which really is the failure to draw Feynman diagrams, represents pairings which result in zero-contributions to the observable.

We can formalize this insight as follows. We represent $\alpha\widetilde{\phi}\phi^2$ by nodes of the form  and we represent $\beta\widetilde{\phi}^2\phi$ by nodes of the form  . Then for $\langle\phi(t_1)\widetilde{\phi}(t_0)\rangle_k$, we can use at most k such nodes to create (Feynman) diagrams that have t_1 on the left and t_0 on the right. Every admissible diagram represents a pairing of J- and $\widetilde{J}$-derivatives for which time-ordering works.

For $k = 1$, we could only use either  or  but not both. Hence, we would be unable to draw a complete diagram.

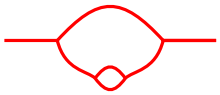
For $k = 2$, choosing one of the nodes twice would not allow us to create a diagram either. That's why the terms in Eq. (3.29a) and (3.29c) equalled zero. So we need to pick one of each type of node, for which we found the Feynman diagram with one loop, Eq. (3.38). This is the only admissible diagram for $k = 2$. It came with a symmetry factor of 2.

For odd k, we realize that no diagram can be drawn because we always end up with loose ends.

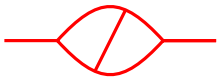
For $k = 4$, things get interesting. All of a sudden, we have several options when we pick

each type of node twice:

(3.41a)



(3.41b)



(3.41c)

In particular, the only relevant differences are topological differences between diagrams. If I can deform one diagram continuously into another one without crossing nodes, then they represent the same term.

So far, we have evaluated more complicated diagrams by reducing them to diagrams corresponding to expressions of the form $\langle \dots \rangle_0$ which are integrated over all internal/interaction times, which we denoted above by $s_1, s_2, \dots$. However, we can get the results quicker by observing how the interaction times actually appear in explicit calculations. In Eq. (3.32), s_1 only appeared in exponentials, which can be combined to $e^{is_1(\omega_1-\omega_2-\omega_4)}$. Thus, integrating over s_1 at that stage would have given us a factor $\delta(\omega_1 - \omega_2 - \omega_4) = 2\pi\delta(\omega_1 - \omega_2 - \omega_4)$. Analogously for s_2 in Eq. (3.32), exponentials can be combined and integrating over s_2 would have given us a factor $\delta(\omega_2 - \omega_3 + \omega_4)$. As all internal times are represented by nodes in the Feynman diagrams, we can deduce that nodes actually represent δ functions of the in- and outgoing lines of the node. Each line is associated with a propagator and an ω_i variable.

Let's summarizes the process of how to calculate an observable $\langle \mathcal{O} \rangle_k$ at kth order in the interaction terms:

1. How to get Feynman diagrams
   - each $\phi(t_j)$ in the observable $\mathcal{O}$ is drawn as a left end point of a line
   - each $\widetilde{\phi}(t_j)$ in the observable $\mathcal{O}$ is drawn as a right end point of a line
   - for $\langle \mathcal{O} \rangle_k$, we take k terms from $\mathcal{L}_{\text{int}}[\widetilde{\phi}, \phi]$, each is represented by a node. The term $\widetilde{\phi}^n \phi^m$ is represented by a node with m lines coming in from the right, and n lines going out to the left. For example $\widetilde{\phi}^3\phi^2$ will be drawn as  . The special case of $\widetilde{\phi}$ will be drawn as  . Nodes represent interaction terms.
   - nodes and end points are connected by lines which are not allowed to change the left-right direction. For example, when we follow a line that initially goes from right to left, it can not bend over to go then from left to right. This rule is to ensure time-ordering is followed.
2. How to get calculable terms from Feynman diagrams

- for every line, write $\frac{1}{-i\omega_j + r}$ where j is an index used to distinguish between different ωs from different lines.
- for every node, write δ(outgoing ωs $-$ ingoing ωs), where by ingoing, we mean lines going into the node from the right, and by outgoing we mean lines leaving the node to the left. For example, for the node  , we associated with the lines on the left the variables ω_1, ω_2 and ω_3, while we associated with the lines on the right the variables ω_4 and ω_5. Then the node represents the term $2\pi\delta(\omega_1 + \omega_2 + \omega_3 - \omega_4 - \omega_5)$. We should also multiply by the parameter that is associated with the interaction term which the node represents
- end points are associated with specific times. If it's a left end point associated with time t_1, we multiply the resulting term by $e^{-i\omega_1 t_1}$, where ω_1 is the variable belonging to the line connected to the end point. If it's a right end point associated with time t_0, we multiply by $e^{i\omega_0 t_0}$, where ω_1 is the variable belonging to the line connected to that end point.
- integrate over all ωs
- multiply by the symmetry factor, which is the number of ways in which you can connect nodes and lines and get topologically the same diagram, if lines and stumps of nodes were actually distinguishable.

This is hard to wrap your head around. A good way of understanding these steps is to do a few explicit examples and compare the calculations to the rules here. In the next section, we are going to present several examples.

3.2 Examples

This section picks up the examples that we introduced and discussed in Chapter 1 on Master Equations and which we continued to describe as PDEs of the probability generating function in Chapter 2 on Second Quantization. Now we are going to look at them from a field theoretic perspective.

3.2.1 Extinction and Spontaneous creation

The Master for extinction and spontaneous creation was derived in Eq. (1.21) and read

$$\frac{\partial}{\partial t}P\big(N(t)\big|N(t_0)\big) = \epsilon(N(t)+1)P\big(N(t)+1\big|N(t_0)\big) - \epsilon N(t)P\big(N(t)\big|N(t_0)\big) \tag{1.21}$$

$$+ \gamma P\big(N(t)-1\big|N(t_0)\big) - \gamma P\big(N(t)\big|N(t_0)\big). \tag{1.22}$$

The corresponding PDE for the probability generating function was derived in Eq. (2.8a)

$$\frac{\partial}{\partial}\mathcal{M}(z,t) = \left(\epsilon(1-z)\frac{\mathrm{d}}{\mathrm{d}z} + \gamma(z-1)\right)\mathcal{M}(z,t), \tag{2.8a}$$

and using the language of Second Quantization we can write the same PDE as

$$\frac{\partial}{\partial t}|\mathcal{M}(t)\rangle = \Big(\epsilon(1-a^\dagger)a + \gamma(a^\dagger - 1)\Big)\,|\mathcal{M}(t)\rangle \tag{3.42}$$

$$= \left(-\epsilon\widetilde{a}a + \gamma\widetilde{a}\right)|\mathcal{M}(t)\rangle, \tag{3.43}$$

where in the last line, we simply used the Doi-shift $a^\dagger = \widetilde{a} + 1$, which we introduced in Sec. (2.2). In particular, we identify $\mathcal{L}[a^\dagger, a] = -\epsilon\widetilde{a}a + \gamma\widetilde{a}$.

Following the derivation of the path integral, we can immediately write down our field-theoretic action, using Eq. (2.86):

$$\mathcal{A}[\widetilde{\phi}, \phi] := -\int_{-\infty}^{\infty} \widetilde{\phi}(t)\left(\frac{\mathrm{d}}{\mathrm{d}t} + \epsilon\right)\phi(t) - \gamma\widetilde{\phi}\,\mathrm{d}t, \tag{3.44}$$

and we can start calculating observables!

As there is spontaneous creation in the system, we expect a non-empty steady state. Therefore, we start our calculations by measuring the expected number of particles at time t_1. The expected number of particles is measured by $\langle\text{☼}|a|\mathcal{M}(t_1)\rangle$ in the Second Quantization picture, see Eq. (2.26). In the field theory, this becomes $\langle\phi(t_1)\rangle$, which we calculated above in Eq. (3.23)

$$\mathbb{E}[N(t)] = \langle\phi(t_1)\rangle \mathrel{\hat{=}} \longrightarrow\!\times \quad = \frac{\gamma}{\epsilon} \tag{3.23}$$

What about the 2nd moment? According to Eq. (2.27), the 2nd moment can be written as $\langle\text{☼}|(a^\dagger a)^2|\mathcal{M}(t_1)\rangle$. Enforcing normal ordering, we get $\mathbb{E}[N^2(t)] = \langle\text{☼}|a^2|\mathcal{M}(t_1)\rangle + \langle\text{☼}|a|\mathcal{M}(t_1)\rangle$. Hence, in the field theory we calculate

$$\mathbb{E}[N^2(t)] = \langle\phi^2(t_1)\rangle + \langle\phi(t_1)\rangle. \tag{3.45}$$

Luckily, we have already calculated $\langle\phi(t_1)\rangle = \gamma/\epsilon$ and can focus on $\langle\phi^2(t_1)\rangle$. In Sec. 3.1 on Feynman diagrams, we found that we need to consider all possible diagrams that end in two lines on the left – representing $\phi^2(t_1)$ – and only have 'nodes' of the form $\longrightarrow\!\times$ – representing $\gamma\widetilde{\phi}$. After some doodling, we can see that there is only a single option:

$$\langle\phi^2(t_1)\rangle \mathrel{\hat{=}} \begin{array}{l}\longrightarrow\!\times\\ \longrightarrow\!\times\end{array} \quad = \langle\phi(t_1)\rangle^2 = \left(\frac{\gamma}{\epsilon}\right)^2. \tag{3.46}$$

Thus, the 2nd moment equals $\mathbb{E}[N^2(t)] = \gamma^2/\epsilon^2 + \gamma/\epsilon$.

Remembering the relation between moments and factorial moments, Eqs. (2.26) and (2.27), we realize that we actually calculated the 2nd factorial moment in Eq. (3.46). Furthermore, we can generalize our doodling and counting of ways how to connect lines to the

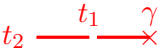
kth factorial moment:

$$\mathbb{E}[(N(t))_k] = \langle \phi^k(t_1)\rangle \hat{=} \quad = \langle \phi(t_1)\rangle^k = \left(\frac{\gamma}{\epsilon}\right)^k. \tag{3.47}$$

The skeptical reader might think, that this could have been found fairly easily by different means, in particular, extracting this from the Master Equation would be have been a manageable task – and you are right!

In order to show-off some of the strengths of Doi-Peliti field theory, we calculate correlation functions. The simplest correlation function is $\mathbb{E}[N(t_2)N(t_1)]$ which correlates the mean particle number at time t_1 with the mean particle number at time t_2. On the level of Second Quantization, this is expressed as $\langle \text{☼}|ae^{\mathcal{L}[a^\dagger,a](t_2-t_1)}a^\dagger a|\mathcal{M}(t_1)\rangle$, and therefore in the field theory, it corresponds to $\langle\phi(t_2)\phi^\dagger(t_1)\phi(t_1)\rangle = \langle\phi(t_2)\widetilde{\phi}(t_1)\phi(t_1)\rangle + \langle\phi(t_2)\phi(t_1)\rangle$. Here, the last term $\langle\phi(t_2)\phi(t_1)\rangle$ isn't actually different to $\langle\phi^2(t_1)\rangle$, which we can deduce from purely topological considerations. We therefore focus on calculating $\langle\phi(t_2)\widetilde{\phi}(t_1)\phi(t_1)\rangle$. Assuming $t_2 > t_1$, we find:

$$\langle\phi(t_2)\widetilde{\phi}(t_1)\phi(t_1)\rangle \hat{=} \quad = \Theta(t_2-t_1)\frac{\gamma}{\epsilon}e^{-\epsilon(t_2-t_1)}, \tag{3.48}$$



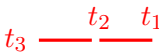
where we included time labels and the node label for convenience. Furthermore, we drew a little gap at time t_1 to show that a line ends at t_1 and another line start at t_1. Also note that we could have chosen $t_1 > t_2$ and would have gotten the same result with interchanged t_1 and t_2. Hence the correlation function is

$$\mathbb{E}[N(t_2)N(t_1)] = \left(\frac{\gamma}{\epsilon}\right)^2 + \frac{\gamma}{\epsilon}e^{-\epsilon|t_2-t_1|}, \tag{3.49}$$

where we recover the previously found result for the 2nd moment if we set $t_2 = t_1$. Such correlation functions are typically quite difficult to extract from a Master Equation. Doi-Peliti field theory provides a method that – once learned – allows swift calculations of correlation functions. Food for thought: How would you calculate the correlation in Eq. (3.49) directly from a Master Equation?

We can also consider higher order correlation functions. The easiest next step would be to calculate $\mathbb{E}[N(t_3)N(t_2)N(t_1)]$, which equals to $\langle\phi(t_3)\phi^\dagger(t_2)\phi(t_2)\phi^\dagger(t_1)\phi(t_1)\rangle$ in the field theory. Once the Doi-shift $\phi^\dagger = \widetilde{\phi} + 1$ is done, the one of the new objects is $\langle\phi(t_3)\widetilde{\phi}(t_2)\phi(t_2)\widetilde{\phi}(t_1)\phi(t_1)\rangle$. Assuming $t_3 > t_2 > t_1$, we find:

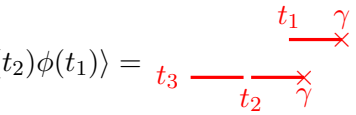
$$\langle\phi(t_3)\widetilde{\phi}(t_2)\phi(t_2)\widetilde{\phi}(t_1)\phi(t_1)\rangle \hat{=} \quad \tag{3.50}$$



$$= \Theta(t_3-t_2)\Theta(t_2-t_1)\frac{\gamma}{\epsilon}e^{-\epsilon(t_3-t_2)}e^{-\epsilon(t_2-t_1)}. \tag{3.51}$$

Another new term is $\langle \phi(t_3)\widetilde{\phi}(t_2)\phi(t_2)\phi(t_1)\rangle$. Assuming $t_3 > t_2 > t_1$, we find

$$\langle \phi(t_3)\widetilde{\phi}(t_2)\phi(t_2)\phi(t_1)\rangle = \quad = \Theta(t_3 - t_2)\frac{\gamma^2}{\epsilon^2}e^{-\epsilon(t_3-t_2)}, \tag{3.52}$$



There are several diagrams like the ones in Eqs. (3.50) and (3.52) depending on the ordering of the times. When we sum over all $3! = 6$ possible time-orderings, the diagrams can be associated with the resulting terms

$$\hat{=} \frac{\gamma}{\epsilon}e^{-\epsilon(t_{\max}-t_{\min})} \tag{3.53}$$

$$\hat{=} \frac{\gamma^2}{\epsilon^2}\left(e^{-\epsilon|t_3-t_2|} + e^{-\epsilon|t_1-t_2|} + e^{-\epsilon|t_3-t_1|}\right) \tag{3.54}$$

Together with the result from Eq. (3.47), the three-time correlation function can be identified as

$$\mathbb{E}[N(t_3)N(t_2)N(t_1)] = \frac{\gamma^3}{\epsilon^3} + \frac{\gamma^2}{\epsilon^2}\left(e^{-\epsilon|t_2-t_3|} + e^{-\epsilon|t_1-t_2|} + e^{-\epsilon|t_1-t_3|}\right) + \frac{\gamma}{\epsilon}e^{-\epsilon(t_{\max}-t_{\min})} \tag{3.55}$$

So far we have only measured the system in steady state. Let's try to push the system out of the steady state and see how it converges back.

As first example, let's add a particle to the system and measure the mean particle number afterwards. In probabilisitic terms, this can be expressed as $\mathbb{E}[N(t_1)|N(t_0^+) = N(t_0^-)+1]$. How do we do this in the field theory? In Sec. 2.3.5, we found that adding a particle at time t_0 simply means that we add $\phi^\dagger(t_0)$ in the path integral:

$$\mathbb{E}[N(t_1)|N(t_0^+) = N(t_0^-) + 1] = \langle \phi(t_1)\phi^\dagger(t_0)\rangle = \langle \phi(t_1)\widetilde{\phi}(t_0)\rangle + \langle \phi(t_1)\rangle, \tag{3.56}$$

where t_0^+ is the one-sided limit of appraoching t_0 from above, while t_0^- is the one-sided limit for approaching t_0 from below. The $\langle \phi(t_1)\rangle$ was calculated before in Eq. (3.23) and the term $\langle \phi(t_1)\widetilde{\phi}(t_0)\rangle$ was also calculated before in Eq. (3.17). Thus, the result is

$$\mathbb{E}[N(t_1)|N(t_0^+) = N(t_0^-) + 1] = \langle \phi(t_1)\phi^\dagger(t_0)\rangle = \Theta(t_1 - t_0)e^{-\epsilon(t_1-t_0)} + \frac{\gamma}{\epsilon}. \tag{3.57}$$

The result shows that if we add a particle to the steady state, the system returns to the steady state on the time scale of a single particle extinction. This is not surprising since particles don't interact, they go extinct and are created independently of the other particles in the system.

Another interesting manipulation of the steady state could be to enforce an empty system at some time t_0. In Sec. 2.3.5, we found that this can be achieved by adding $e^{-\widetilde{\phi}(t_0)\phi(t_0)}$

as initialization. If we are interested in calculating the mean particle number at time $t_1 > t_0$, then we need to calculate:

$$\mathbb{E}[N(t_1)|N(t_0)=0] = \left\langle \phi(t_1) e^{-\widetilde{\phi}(t_0)\phi(t_0)} \right\rangle = \sum_{k=0}^{\infty} \frac{(-1)^k}{k!} \left\langle \phi(t_1) \left(\widetilde{\phi}(t_0)\phi(t_0) \right)^k \right\rangle, \quad (3.58)$$

however, given the possible topologies of the system's Feynman graphs, we can see that the right-end point representing $\widetilde{\phi}(t_0)$ cannot link to any left-end point for $k > 1$. Hence only $k = 0$ and $k = 1$ give non-zero contributions:

$$\mathbb{E}[N(t_1)|N(t_0)=0] = \langle \phi(t_1) \rangle - \langle \phi(t_1)\widetilde{\phi}(t_0)\phi(t_0) \rangle = \frac{\gamma}{\epsilon} \left(1 - e^{-\epsilon(t_1 - t_0)} \right), \quad (3.59)$$

where we used the previously calculated results from Eq. (3.23) and (3.48). Thus we see that the convergence to the steady state is determined by the time scale of the extinction ϵ, i.e. if we ask questions such as 'How long does it take to reach x% of the steady state particle number?', the answer only depends on ϵ and not on γ.

So far we have explored various options to derive moments and correlation functions for the particle system. Are we able to extract probabilities for specific particle numbers as well? Yes! The trick is to realize that the probability generating function can be regarded as the factorial moment generating function:

$$\mathcal{M}(z) = \sum_{N=0}^{\infty} P(N) z^N = \sum_{k=0}^{\infty} \frac{\mathbb{E}[(N)_k]}{k!} (z-1)^k \quad (3.60)$$

$$= \sum_{k=0}^{\infty} \frac{1}{k!} \left(\frac{\gamma}{\epsilon}(z-1) \right)^k = e^{\frac{\gamma}{\epsilon}(z-1)}, \quad (3.61)$$

where the zeroth factorial moment is defined as $(N)_0 = 1$, and where we use the previously found result for the kth factorial moment, Eq. (3.47). This recovers the result of Eq. (2.8c), where we tried to solve the steady-state version of the PDE for $\mathcal{M}$. Using z-derivatives and evaluating at $z = 0$, we can now recover the steady state probability distribution, which we found in Sec. 1.3.3.

What we were unable to do so far was the derivation of the time-dependent probability generating function and the time-dependent probability distribution. However, we are able to calculate them in the field theory by simply calculating the time-dependent factorial moments.

In the case of adding a particle to the steady state, the kth factorial moment is

$$\mathbb{E}[(N(t))_k | N(t_0^+) = N(t_0^-) + 1] = \langle \phi^k(t_1)\phi^\dagger(t_0) \rangle = \Theta(t_1 - t_0) k \frac{\gamma^{k-1}}{\epsilon^{k-1}} e^{-\epsilon(t-t_0)} + \frac{\gamma^k}{\epsilon^k}, \quad (3.62)$$

resulting in a probability generating function of

$$\mathcal{M}(z,t) = e^{\frac{\gamma}{\epsilon}(z-1)} + \Theta(t-t_0)(z-1) e^{\frac{\gamma}{\epsilon}(z-1) - \epsilon(t-t_0)}, \quad (3.63)$$

which solves the process' PDE

$$\frac{\partial}{\partial t}\mathcal{M}(z,t) = \left(\gamma(z-1) + \epsilon(1-z)\frac{\partial}{\partial z}\right)\mathcal{M}(z,t), \tag{3.64}$$

with initial condition 'steady state +1 particle at time t_0'.

In the case of enforcing an empty system at time t_0, the kth factorial moment is

$$\mathbb{E}[(N(t))_k | N(t_0)=0] = \left\langle \phi^k(t) e^{-\widetilde{\phi}(t_0)\phi(t_0)} \right\rangle = \left(\frac{\gamma}{\epsilon}\left(1 - e^{-\epsilon(t-t_0)}\right)\right)^k. \tag{3.65}$$

Thus $\mathcal{M}(z,t)$ equals

$$\mathcal{M}(z,t) = e^{\frac{\gamma}{\epsilon}(1-e^{-\epsilon(t-t_0)})(z-1)}, \tag{3.66}$$

which is another solution of the PDE in Eq. (3.64), but now with initial condition 'empty system at time t_0', i.e. $M(z,0)=1$.

Exercise 3.2 For the process of extinction and spontaneous creation, show that the kth factorial moment of the particle number at time t, given that the system was empty at time t_0 equals

$$\mathbb{E}[(N(t))_k | N(t_0)=0] = \left\langle \phi^k(t) e^{-\widetilde{\phi}(t_0)\phi(t_0)} \right\rangle = \left(\frac{\gamma}{\epsilon}\left(1 - e^{-\epsilon(t-t_0)}\right)\right)^k. \tag{3.65}$$

3.2.2 Coagulation, Extinction and Spontaneous Creation

In Sec. 1.3.4, we considered a single-particle system with coagulation, extinction and spontaneous creation. Back in that section, we were stuck on calculating the steady state distribution of particle numbers. Let's revisit that system using the field theory.

Its Master equation is given by

$$\begin{aligned}\frac{\partial}{\partial t}P\big(N(t)\big|N(t_0)\big) =& \epsilon(N(t)+1)P\big(N(t)+1\big|N(t_0)\big) - \epsilon N(t)P\big(N(t)\big|N(t_0)\big) \\ &+ \gamma P\big(N(t)-1\big|N(t_0)\big) - \gamma P\big(N(t)\big|N(t_0)\big) \\ &+ \lambda\binom{N(t)+1}{2}P\big(N(t)+1\big|N(t_0)\big) - \lambda\binom{N(t)}{2}P\big(N(t)\big|N(t_0)\big),\end{aligned} \tag{1.29}$$

from which we can derive the PDE of the probability generating function:

$$\mathcal{M}(z,t) = \left(\epsilon(1-z)\frac{\mathrm{d}}{\mathrm{d}z} + \gamma(z-1) + \frac{\lambda}{2}(z-z^2)\frac{\mathrm{d}^2}{\mathrm{d}z^2}\right)\mathcal{M}(z,t), \tag{3.67}$$

which in turn can be written in the language of Second Quantization:

$$|\mathcal{M}(t)\rangle = \underbrace{\left(\epsilon(1-a^\dagger)a + \gamma(a^\dagger - 1) + \frac{\lambda}{2}(a^\dagger - a^{\dagger 2})a^2\right)}_{=\mathcal{L}[a^\dagger, a]} |\mathcal{M}(t)\rangle. \tag{3.68}$$

Since $\mathcal{L}[a^\dagger, a]$ is normal ordered, we can go ahead and write our action, see Eq. (2.86):

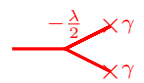
$$\mathcal{A}[\widetilde{\phi}, \phi] = -\int_{-\infty}^{\infty} \widetilde{\phi}(t)\left(\frac{\mathrm{d}}{\mathrm{d}t} + \epsilon\right)\phi(t) - \gamma\widetilde{\phi} + \frac{\lambda}{2}\left(\widetilde{\phi}(t) + \widetilde{\phi}^2(t)\right)\phi^2(t)\,\mathrm{d}t. \tag{3.69}$$

Our main tool in analyzing moments will be Feynman diagrams. What will be their components? The interaction part are represented by the following nodes

(3.70)

With the action at hand, we can try to calculate the expected particle number. Given that there is a spontaneous creation process in the system, a steady state particle distribution will establish itself and we don't need to initialize the system explicitly. Hence, we want to calculate $\mathbb{E}[N] = \langle\phi\rangle$. From our previous calculation in Eq. (3.21), we know that $\langle\phi\rangle_0 = 0$. This is our zeroth approximation to the expected steady state particle number – and its a pretty bad one. So let's move on to the next best approximation, given by $\langle\phi\rangle_1$. We calculated this term in Eq. (3.23) and found that $\langle\phi\rangle_1 = \gamma/\epsilon$. This approximation only takes extinction and spontaneous creation into account, but still ignores coagulation.

The next correction to the expected particle number would come from $\langle\phi\rangle_2$. However, when we try to draw Feynman diagrams with exactly 2 nodes and a single left-end line, we fail. Hence $\langle\phi\rangle_2 = 0$. The next addition to the approximation is therefore $\langle\phi\rangle_3$. Here, we can combine two γ nodes and one node that has two incoming lines from the left and one outgoing line to the right:

$$\langle\phi(t)\rangle_3 \hat{=}$$ 

$$= -2\frac{\lambda\gamma^2}{2}\int \frac{\delta(\omega_1 - \omega_2 - \omega_3)\delta(\omega_2)\delta(\omega_3)e^{-i\omega_1 t}}{(-i\omega_1 + \epsilon)(-i\omega_2 + \epsilon)(-i\omega_3 + \epsilon)}\text{đ}\omega_1\text{đ}\omega_2\text{đ}\omega_3 \tag{3.71a}$$

$$= -\frac{\lambda\gamma^2}{\epsilon^3}, \tag{3.71b}$$

where each node represented one $\delta(\dots) = 2\pi\delta(\dots)$ (and its parameter), each line represented one factor $1/(-i\omega + \epsilon)$ and the left-end line stump represented $e^{-i\omega_1 t}$. The factor 2 is the symmetry factor.

Hence, our improved approximation of the expected particle number in steady state is

$$\mathbb{E}[N] = \frac{\gamma}{\epsilon}\left(1 - \frac{\lambda\gamma}{\epsilon^2} + \dots\right) \tag{3.72}$$

The new contribution takes coagulation into account and therefore reduces our previous approximation which only accounted for extinction and spontaneous creation. However, we also have a problem now. What if $(1 - \lambda\gamma/\epsilon^2) < 0$? Would that mean that our next-best approximation to the expected particle number is negative? What it really means is that our approximation hasn't taken a sufficient number of interaction terms into account. This is a notorious problem in any field theory. Let's see what happens if we continue to take more terms into account.

Next up is $\langle\phi\rangle_4$, represented by all the Feynman diagrams with 4 nodes. Luckily, there is only one:

$$\langle\phi(t)\rangle_4 \hat{=} \tag{3.73a}$$

$$= 4\frac{\lambda^2\gamma^2}{4}\int \frac{\delta(\omega_1-\omega_2-\omega_3)\delta(\omega_2+\omega_3-\omega_4-\omega_5)\delta(\omega_4)\delta(\omega_5)e^{-i\omega_1 t}}{(-i\omega_1+\epsilon)(-i\omega_2+\epsilon)(-i\omega_3+\epsilon)(-i\omega_4+\epsilon)(-i\omega_5+\epsilon)}đ\omega_1 đ\omega_2 đ\omega_3 đ\omega_4 đ\omega_5 \tag{3.73b}$$

$$= \frac{\lambda^2\gamma^2}{\epsilon^3}\int \frac{đ\omega_2}{(-i\omega_2+\epsilon)(i\omega_2+\epsilon)} \tag{3.73c}$$

$$= \frac{\lambda^2\gamma^2}{2\epsilon^4}, \tag{3.73d}$$

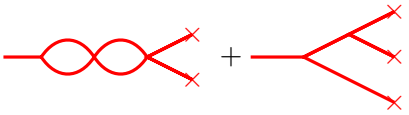
Hence, the next-level approximation equals

$$\mathbb{E}[N] = \frac{\gamma}{\epsilon}\left(1 - \frac{\lambda\gamma}{\epsilon^2} + \frac{\lambda^2\gamma}{2\epsilon^3} + \dots\right) \tag{3.74}$$

There is understandable curiosity about trying to interpret the meaning of these Feynman diagrams with regards to the physical processes. However, this is a futile exercise or at least one that leads to many hand-wavy arguments. Try to resist this temptation and simply regard the diagrams as a useful tool for calculating approximations.

The next term is $\langle\phi\rangle_5$. It's our first example of a term that is represented by two topologically different diagrams:

$$\langle\phi(t)\rangle_5 \hat{=}$$



(3.75)

Comparing the left diagram (with two loops) with the diagram in Eq. (3.73a), we realize that there is a diagrammatic pattern emerging. Every term that allows one more node to be drawn will contain a diagram that is a chain of loops which end on left in a line stump and on the right in two source nodes.

Exercise 3.3 Consider the action

$$\mathcal{A}[\widetilde{\phi},\phi] = -\int_{-\infty}^{\infty} \widetilde{\phi}(t)\left(\frac{\mathrm{d}}{\mathrm{d}t}+\epsilon\right)\phi(t) - \gamma\widetilde{\phi} + \frac{\lambda}{2}\widetilde{\phi}(t)\phi^2(t) + \frac{\kappa}{2}\widetilde{\phi}^2(t)\phi^2(t)\,\mathrm{d}t.$$

Calculate the term I that is represented by the following Feynman diagram:

$I \mathrel{\hat{=}}$ 

However, that's not the only emerging diagram pattern. If we compare the right diagram in Eq. (3.75) (without loops) with the diagram in Eq. (3.71a), every term that allows two more nodes to be drawn will contain a diagram that looks like a tree rotated by 90 degrees.

Trying to understand all the emerging topological patterns can be a lot of work. However, as they are linked to parameters of the action, we can make useful approximations. For example, if we were to focus on all terms in $\langle\phi(t)\rangle$ which have at most a factor γ^2, then the accuracy can be quantified by the Landau Big-O notation as $\mathcal{O}(\gamma^3)$. The diagrams that remain relevant are exactly those that form a chain of loops as seen in the left diagram in Eq. (3.75). Summing over all contributions that are loop chains is called a *Dyson sum*:

$$I_{\mathrm{Dy}} \mathrel{\hat{=}} \quad + \quad + \quad + \ldots \tag{3.76a}$$

$$= -\frac{\lambda\gamma^2}{\epsilon^3}\sum_{k=0}^{\infty}\left(\int_{-\infty}^{\infty}\frac{-\lambda\text{đ}\omega}{(-i\omega+\epsilon)(i\omega+\epsilon)}\right)^k \tag{3.76b}$$

$$= -\frac{\lambda\gamma^2}{\epsilon^2}\frac{2}{2\epsilon+\lambda} \tag{3.76c}$$

Hence the expected particle number can be approximated as

$$\mathbb{E}[N] = \frac{\gamma}{\epsilon}\left(1 - \frac{2\lambda\gamma}{\epsilon(2\epsilon+\lambda)}\right) + \mathcal{O}(\gamma^3) \tag{3.77}$$

We can now interpret this first result. As expected, the coagulation process lowers the expected number of particles in the system compared to the system which only has extinction and spontaneous creation. We can also see that if $\epsilon \gg \gamma$, then our correction to γ/ϵ becomes less significant. This can be explained by considering that a dominant extinction process will make the appearance of a pair of particles very unlikely, which implies that coagulation will occur even less often. A third extreme would be the consideration of $\lambda \to \infty$, which means that as soon as there is a pair, coagulation kicks in and turns the pair into a single particle.

The diagrammatic sum in Eq. (3.76a) does not only represent the fact the we sum in the arithmetic sense lots of terms, but it also can be interpreted as a way of thinking about effective interactions in contrast to microscopic interactions. More explicitly, we observe that the interaction represented by  , with its original parameter $-\lambda/2$, can be replaced by the same vertex with a adjusted parameter to account for all the loops! Comparing Eq. (3.71a) with Eq. (3.76c), we see that if we replace the parameter for vertex  with $-\epsilon\lambda/(2\epsilon+\lambda) =: \lambda_R$, then we can forget about all the extra loops that we have summed over in Eq. (3.76a).

Physically λ_R can be interpreted as an additional effective extinction process in the system that only works once there are at least two particles. Given two particles, the probability that one of them is lost due to coagulation rather than extinction equals $\lambda/(2\epsilon+\lambda)$, where the rate 2ϵ is the extinction rate for the two particle state. This probability is exactly how the original extinction rate ϵ is scaled in λ_R!

The index R in λ_R stands for *Renormalisation*. Usually the word renormalisation is used in connection with spatial processes where the system can be scaled (i.e. we can zoom out) and from the new perspective the system's behaviour can be explained based on the microscopic description by adjusting the parameters of the interactions. Continuous phase transitions then occur when the system behaves in the same way at all length scales, i.e. at a fixed point of the renormalisation procedure.

In the present case however, there is no space. What does renormalisation do? An understandable guess would be that we now scaling in time. However, we immediately can discard that as well because all the parameters in the system (ϵ, γ, and λ) have the dimension of a rate. Hence, they would scale in the same way.

3.2.3 Diffusion and Extinction

In Sec. 1.4, the Master Equation was adapted to model processes in space, such as diffusion. How does this approach translate to the field theory? On a d-dimensional square lattice with lattice constant h, the Master Equation for diffusion is

$$\frac{\partial}{\partial t}P\big(N\big|N_0\big) = \frac{D}{h^2}\sum_{x\in X}\sum_{\substack{y\in X\\ |x-y|=h}}\Big((N_x+1)P\big(N+1_x-1_y\big|N_0\big) - N_xP\big(N\big|N_0\big)\Big), \quad (1.42)$$

which can be transformed into a PDE for the probability generating function

$$\frac{\partial}{\partial t}\mathcal{M}(z,t) = \frac{D}{h^2}\sum_{x\in X}\sum_{\substack{y\in X\\ |x-y|=h}}(z_y-z_x)\frac{\mathrm{d}}{\mathrm{d}z_x}\mathcal{M}(z,t). \quad (3.78)$$

We can make use of the isotropy of the system to generate a more symmetric looking version of this equation:

$$\frac{\partial}{\partial t}\mathcal{M}(z,t) = \frac{D}{2h^2}\sum_{x\in X}\sum_{\substack{y\in X\\ |x-y|=h}} (z_y - z_x)\left(\frac{\mathrm{d}}{\mathrm{d}z_x} - \frac{\mathrm{d}}{\mathrm{d}z_y}\right)\mathcal{M}(z,t). \tag{3.79}$$

In the language of second quantization, this equals

$$\frac{\partial}{\partial t}|\mathcal{M}(t)\rangle = \frac{D}{2h^2}\sum_{x\in X}\sum_{\substack{y\in X\\ |x-y|=h}} (\widetilde{a}_y - \widetilde{a}_x)\,(a_x - a_y)\,|\mathcal{M}(t)\rangle, \tag{3.80}$$

where the Doi shift $a^\dagger = \widetilde{a} + 1$ does not affect the shape of the equation. Hence, we can derive the action of the corresponding field theory:

$$\mathcal{A}[\widetilde{\phi},\phi] = -\sum_{x\in X}\int_{-\infty}^{\infty} \widetilde{\phi}_x(t)\frac{\mathrm{d}}{\mathrm{d}t}\phi_x(t) + \frac{D}{2h^2}\sum_{\substack{y\in X\\ |x-y|=h}}\left(\widetilde{\phi}_x(t) - \widetilde{\phi}_y(t)\right)\left(\phi_x(t) - \phi_y(t)\right)\,\mathrm{d}t \tag{3.81}$$

$$= -\sum_{x\in X} h^d\int_{-\infty}^{\infty} \widetilde{\phi}_x(t)\frac{\mathrm{d}}{\mathrm{d}t}\frac{\phi_x(t)}{h^d} + \frac{D}{2}\sum_{\substack{y\in X\\ |x-y|=h}}\frac{\left(\widetilde{\phi}_x(t) - \widetilde{\phi}_y(t)\right)}{h}\frac{\left(\frac{\phi_x(t)}{h^d} - \frac{\phi_y(t)}{h^d}\right)}{h}\,\mathrm{d}t, \tag{3.82}$$

where in the second line, we have simply moved the h^2 into the sum to find the difference quotients for $\widetilde{\phi}$ and ϕ. Furthermore, we have multiplied the sum by h^d but also divided every ocurrance of ϕ by h^d, which makes ϕ/h^d a density. Taking the spatial continuum limit $h \to 0$ turns the difference quotients into spatial derivatives, while the sum over X becomes an integral. The sum over nearest neighbours produces a factor 2 for each of the d directions and finally we rename the continuum limit of ϕ/h^d to ϕ, but have to remember going forward that it's now a density. The result of the continuum limit is therefore

$$\mathcal{A}[\widetilde{\phi},\phi] = -\int_{x\in\mathbb{R}^d}\int_{-\infty}^{\infty} \widetilde{\phi}(x,t)\frac{\mathrm{d}}{\mathrm{d}t}\phi(x,t) + D\nabla\widetilde{\phi}(x,t)\cdot\nabla\phi(x,t)\,\mathrm{d}t\mathrm{d}^d x \tag{3.83}$$

$$= -\int_{x\in\mathbb{R}^d}\int_{-\infty}^{\infty} \widetilde{\phi}(x,t)\frac{\mathrm{d}}{\mathrm{d}t}\phi(x,t) - D\widetilde{\phi}(x,t)\Delta\phi(x,t)\,\mathrm{d}t\mathrm{d}^d x, \tag{3.84}$$

where we assume that $\phi \to 0$ as $|x| \to \infty$. Eq. (3.84) shows that the diffusion process add an additional term to the bilinear part of the action which involves a spatial derivative. Just as in Eq. (3.9), we have to ask ourselves how to calculate the inverse of operator of $\mathrm{d}/\mathrm{d}t - D\Delta$. The answer is again: Fourier transforms! Our Fourier transforms that

include space and time are

$$\phi(k,\omega) = \mathcal{F}[\phi](k,\omega) = \int_{\mathbb{R}^d}\int_{-\infty}^{\infty} \phi(x,t) e^{i\omega t - ik\cdot x} \mathrm{d}t \mathrm{d}^d x \tag{3.85}$$

$$\phi(x,t) = \mathcal{F}^{-1}[\phi](x,t) = \int_{\mathbb{R}^d}\int_{-\infty}^{\infty} \phi(k,\omega) e^{-i\omega t + ik\cdot x} đ\omega đ^d k, \tag{3.86}$$

where $đ\omega = 2\pi \mathrm{d}\omega$ and $đ^d k = (2\pi)^d \mathrm{d}^d k$.

Equipped with this Fourier transform, we can express the action as

$$\mathcal{A}[\widetilde{\phi},\phi] = -\int_{x\in\mathbb{R}^d}\int_{-\infty}^{\infty} \widetilde{\phi}(-k,-\omega)(-i\omega)\phi(k,\omega) + D\widetilde{\phi}(-k,-\omega)k^2\phi(k,\omega)\, đ\omega đ^d k, \tag{3.87}$$

where $k^2 = k\cdot k = |k|^2$. If we now include extinction with rate ϵ into the action, Eq. (3.44), then the entire action equals

$$\mathcal{A}[\widetilde{\phi},\phi] = -\int_{x\in\mathbb{R}^d}\int_{-\infty}^{\infty} \widetilde{\phi}(-k,-\omega)(-i\omega + Dk^2 + \epsilon)\phi(k,\omega)\, đ\omega đ^d k. \tag{3.88}$$

In a first step, we analyze the bare propagator, i.e. we create a particle and measure its density at a later point in time:

$$\langle \phi(x,t)\phi^\dagger(x_0,t_0)\rangle = \langle \phi(t)\widetilde{\phi}(t_0)\rangle \mathrel{\hat{=}} \text{———} \tag{3.89}$$

$$= \int_{\mathbb{R}^d}\int_{-\infty}^{\infty} \frac{e^{-i\omega(t-t_0)+ik(x-x_0)}}{-i\omega + Dk^2 + \epsilon} đ\omega đ^d k \tag{3.90}$$

$$= \Theta(t-t_0) e^{-\epsilon(t-t_0)} \int_{\mathbb{R}^d} e^{-Dk^2(t-t_0)+ik(x-x_0)} đ^d k \tag{3.91}$$

$$= \Theta(t-t_0) \frac{e^{-\epsilon(t-t_0) - \frac{|x-x_0|^2}{4D(t-t_0)}}}{(4\pi D(t-t_0))^{\frac{d}{2}}}. \tag{3.92}$$

We find the particle density that is the product of the normal distribution in d dimensions with an exponential decay with rate ϵ. As time progresses, the particle density becomes gradually wider or blurred, which means we know less and less about the position of the particle. In fact, the spatial variance equals $2D(t-t_0)$ which increases linearly with time. In the other extreme, when $t \to t_0^+$, the distribution becomes a $\delta(x-x_0)$ function, i.e. at the initial time, we know exactly where the particle is. Furthermore, if we were to

ask what the probability is to find the particle anywhere in the system, then we would have to integrate the function over the entire space, which results in

$$P\big(\text{particle in system}\big|\text{it was at } x_0 \text{ at } t_0\big) = \int_{\mathbb{R}^d} \langle \phi(x,t)\phi^\dagger(x_0,t_0)\rangle \mathrm{d}^d x = \Theta(t-t_0)e^{-\epsilon(t-t_0)}. \tag{3.93}$$

The function $\langle \phi(x,t)\phi^\dagger(x_0,t_0)\rangle$ is the time-dependent probability distribution of the position of the particle with the caveat that probability is not conserved because the particle might go extinct. Probability conservation can be restored by extending the space to include a special 'position' for the extinct particle.

As the system does not have any interaction terms, higher moments and correlation functions can be calculated exactly. However, we are now working with particle densities instead of particle numbers, which means that we have to specify whether we want to calculate the expected particle number, moments or correlations over the entire space or only a subspace. Furthermore, we have to adjust our understanding of probabilities to accommodate the apparent loss of conservation of probability. Let's consider a few example situations, which all start by assuming that one particle was put into the system at position x_0 and time t_0. Then,

- the expected particle number in the entire system at time $t \geq t_0$ equals

$$\mathbb{E}[N(t)|N(x_0,t_0)=1] = \int_{\mathbb{R}^d} \langle \phi(x,t)\phi^\dagger(x_0,t_0)\rangle \mathrm{d}^d x = e^{-\epsilon(t-t_0)} \tag{3.94}$$

- the expected particle number in subspace $V \subset \mathbb{R}^d$ equals

$$\mathbb{E}_V[N(t)|N(x_0,t_0)=1] = \int_{V} \langle \phi(x,t)\phi^\dagger(x_0,t_0)\rangle \mathrm{d}^d x \tag{3.95}$$

  For example in 2 dimensions, the expected particle number at time $t \geq t_0$ in a circle C of radius R centered at x_0 equals

$$\mathbb{E}_C[N(t)|N(x_0,t_0)=1] = e^{-\epsilon(t-t_0)}\left(1 - e^{-\frac{R^2}{4D(t-t_0)}}\right) \tag{3.96}$$

- the expected particle position at time $t \geq t_0$ equals

$$\mathbb{E}[X(t)|X(t_0)=x_0] = \int_{\mathbb{R}^d} x\langle \phi(x,t)\phi^\dagger(x_0,t_0)\rangle \mathrm{d}^d x = x_0 e^{-\epsilon(t-t_0)}, \tag{3.97}$$

  due to the symmetry of the Gaussian in Eq. (3.92). This seems odd. Surely, because of the symmetry of the diffusive movement, the particle should stay on

average at its initial position. Why does it look like it's converging towards the origin as $\lim_{t\to\infty} x_0 e^{-\epsilon(t-t_0)} = 0$? The reason for this strange behavior is that we set up each position as its own particle species in Sec. 1.4. Therefore, we should interpret the x_0 and the $e^{-\epsilon(t-t_0)}$ in Eq. (3.97) as bananas and apples: The mean position of the particle is x_0, while the probability for the spatial mean to be non-zero equals $e^{-\epsilon(t-t_0)}$. Hence, we have to make a distinction between the number 0 and the origin position O. A useful image is that of a manifold. The particle moves on a manifold for which we use an intuitive coordinate map onto the real space $\mathbb{R}^d$. Using the coordinate map, we can define differentiation and integration on the manifold[1]. Unfortunately, this is not the end of it: higher moments and correlations make this distinction between mere numbers and actual positions even harder.

- the second moment of the position at time $t \geq t_0$ in $\mathbb{R}^d$ equals

$$\mathbb{E}_V[X^2(t)|X(t_0) = x_0] = \int_{\mathbb{R}^d} x^2 \langle \phi(x,t)\phi^\dagger(x_0,t_0)\rangle \mathrm{d}^d x \tag{3.98}$$

$$= 2D(t-t_0)e^{-\epsilon(t-t_0)} + x_0^2 e^{-2\epsilon(t-t_0)}, \tag{3.99}$$

3.2.4 Diffusion, Extinction and Coagulation

In continuous space, we defined the annihilation field ϕ to be a density.

3.2.5 Diffusion, Extinction and Spontaneous Creation

Exercises

Ex. 3.1 Let $S[f]$ and $T[f|$ be the following functionals

$$S[f] = \int_{-\infty}^{\infty} \exp\bigl(-f^2(x)\bigr)\mathrm{d}x, \qquad T[f] = \exp\left(-\int_{-\infty}^{\infty} f^2(x)\mathrm{d}x\right),$$

calculate the functional derivatives of $S[f]$ and $T[f]$ in direction $h(x)$.

Ex. 3.2 For the process of extinction and spontaneous creation of a single particle species, assume that the system was empty at time t_0. Show that the kth factorial moment of the particle number at time t equals

$$\mathbb{E}[(N(t))_k|N(t_0) = 0] = \left\langle \phi^k(t) e^{-\widetilde{\phi}(t_0)\phi(t_0)} \right\rangle = \left(\frac{\gamma}{\epsilon}\left(1 - e^{-\epsilon(t-t_0)}\right)\right)^k.$$

1. The construction of differentiation and integration on a manifold based on the differentiation and integration on a different space (here $\mathbb{R}^d$) is called pullback in differential geometry. The expected position $x_0 e^{-\epsilon(t-t_0)}$ should be read as $x\delta(x-x_0)e^{-\epsilon(t-t_0)}$

Ex. 3.3 Consider the action

$$\mathcal{A}[\widetilde{\phi},\phi] = -\int_{-\infty}^{\infty} \widetilde{\phi}(t)\left(\frac{\mathrm{d}}{\mathrm{d}t}+\epsilon\right)\phi(t) - \gamma\widetilde{\phi} + \frac{\lambda}{2}\widetilde{\phi}(t)\phi^2(t) + \frac{\kappa}{2}\widetilde{\phi}^2(t)\phi^2(t)\,\mathrm{d}t.$$

Calculate the term I that is represented by the following Feynman diagram:

$I \mathrel{\hat{=}}$ 

3.2.6 What happens without the Doi-shift?

One common source of confusion is the Doi-shift. In the field-theory, it is defined as a shift in the creation field $\phi^\dagger = \widetilde{\phi} + 1$ and implies a different appearance of the action. Although the full path-integral will be unchanged with or without the Doi-shift, approximations to the full path-integral might lead to different results, which we will explore in this section.

The key process to consider in this context is the extinction process, Sec. 1.3.1. Let's denote the action with the Doi-shift by $\mathcal{A}$ and without the Doi-shift by $\mathcal{A}^\dagger$. They are given by

$$\mathcal{A} = -\int_{-\infty}^{\infty} \widetilde{\phi}\left(\frac{\partial}{\partial t}+\epsilon\right)\phi\,\mathrm{d}t \qquad \mathcal{A}^\dagger = -\int_{-\infty}^{\infty} \phi^\dagger\left(\frac{\partial}{\partial t}+\epsilon\right)\phi - \epsilon\phi\,\mathrm{d}t \tag{3.100}$$

We can use both actions to calculate the moments of the particle number. For example, if the system is initialised with a single particle, we find

$$\mathbb{E}[N(t)|N(0)=1] = \langle\phi(t)\phi^\dagger(0)\rangle_{\mathcal{A}} = \langle\phi(t)\widetilde{\phi}(0)\rangle_{\mathcal{A}} + \underbrace{\langle\phi(t)\rangle_{\mathcal{A}}}_{=0} = \Theta(t)e^{-\epsilon t} \tag{3.101}$$

$$\mathbb{E}[N(t)|N(0)=1] = \langle\phi(t)\phi^\dagger(0)\rangle_{\mathcal{A}^\dagger} = \Theta(t)e^{-\epsilon t} \tag{3.102}$$

Reassuringly, both actions give the same result and the action without the Doi-shift seems to even lead to simpler calculations in this case. However, this is misleading because as soon as other processes are involved, the Doi-shift reveals its advantage.

Let's consider the process of extinction and spontaneous creation. The actions for this process are

$$\mathcal{A} = -\int_{-\infty}^{\infty} \widetilde{\phi}\left(\frac{\partial}{\partial t}+\epsilon\right)\phi - \gamma\widetilde{\phi}\,\mathrm{d}t \tag{3.103}$$

$$\mathcal{A}^\dagger = -\int_{-\infty}^{\infty} \phi^\dagger\left(\frac{\partial}{\partial t}+\epsilon\right)\phi - \epsilon\phi - \gamma(\phi^\dagger - 1)\,\mathrm{d}t \tag{3.104}$$

The action $A^\dagger$ contains the term $-\gamma$ which is integrated over all time. This is a divergent integral but one could argue that we can continue to use it if we regard the content of the action as tempered distributions, which we should do anyways because we require that it can be Fourier-transformed. Ignoring that we are leaving well-defined mathematical ground, the Fourier-transformed non-shifted action is

$$\mathcal{A}^\dagger = -\int \phi^\dagger(\omega')\left(-i\omega+\epsilon\right)\phi(\omega)\delta(\omega+\omega')đ\omega' - \epsilon\phi(\omega)\delta(\omega) - \gamma\phi^\dagger(\omega)\delta(\omega) + \gamma\delta^2(\omega)đ\omega, \tag{3.105}$$

This action contains a square of a δ-function, which makes the action ill-defined. But can we still make sense of it in a limiting process since the δ-function is a limit to a sequence of functions with measure 1, i.e. can we replace the δ-functions by the sequence for now and postpone taking the limit to the very end? Yes, and we will see that the sequence that represents the square of a δ-function actually cancels with an equally ill-defined expansion in the interaction term! In particular, we find ourselves in a situation where the order in which we take limits matters.

As the process contains spontaneous creation, we don't need to initialise the system explicitly with any particles. We calculate the first moment of the particle number as follows

$$\mathbb{E}[N(t)] = \langle\phi(t)\rangle_{\mathcal{A}} \hat{=} \quad = \frac{\gamma}{\epsilon} \tag{3.106}$$

$$\mathbb{E}[N(t)] = \langle\phi(t)\rangle_{\mathcal{A}^\dagger} \hat{=} \quad + \quad + \quad + \ldots \tag{3.107}$$

But what are the contributions of the form ?

$$\hat{=} \int_{\mathbb{R}^2} \frac{\gamma\epsilon\delta(\omega)\delta(\omega+\omega')\delta(\omega')đ\omega đ\omega'}{-i\omega+\epsilon} = \int_{-\infty}^{\infty} \gamma\delta^2(\omega)đ\omega \tag{3.108}$$

Here, the squre of the δ-function appears again. Inspired by the terminology in Quantum Field Theory, we call contributions like in Eq. (3.108) vacuum contributions.

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