FIELD THEORY TECHNIQUES IN THE ANALYSIS OF CLASSICAL REACTION-DIFFUSION SYSTEMS

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1 Introduction

Since the seminal works of Fisher, Wilson, and others on the underlying structure of field theory in the 1970's, as exemplified by [1, 2], the physics community has witnessed an explosive development of field-theoretic methods with applications in many branches of physics. In the area of condensed matter, for example, field-theoretical approaches are becoming almost indispensable [3]. Since it was developed primarily to handle quantum

interactions of elementary particles, an area rife with probability, its success in statistical physics might not have been entirely unanticipated, but the elegance and adaptability of the framework to classical calculations is certainly worth admiring. We will omit the modifier "quantum" when talking about field theory from now on, as all of our calculations will lack the defining characteristic of quantum probability. We will be dealing with entirely classical Kolmogorovian probability and not quantum probability amplitudes.

The primary focus of this paper will be a subclass of classical statistical systems that readily subject themselves to field theoretic analysis, reaction-diffusion systems (sometimes referred to as RD systems from now on). The basic idea of these systems is best exposed with an intuitive picture of one or several types of particles, such as molecules of chemical compounds, immersed in a liquid or other setting, undergoing ordinary Brownian diffusion. In addition there are reactions between these particles, analogous to chemical reactions, in which two or more particles, after they have come into close proximity of each other, react to produce a new set of particles, e.g. a third type of molecule.[1] The basic types of questions we will be interested in are closely related to the notion of *universality*, the independence of phenomena on their microscopic details. Field theory comes very handy in calculating asymptotic decay exponents of reactant densities in great generality, covering a wide range of seemingly distinct physical situations. There is still notable dependence on qualitatively different initial conditions and the techniques presented in this thesis are also suited to calculating the evolution characteristics of specific configurations, but as mentioned above they also seem to excel in their generality. Through the renormalisation group flow, field theory also becomes a powerful tool for studying scaling relations. There are of course countless other mathematical tools with which one can approach RD systems and about as many parameters that can be tuned

[1] If the reader is left unmoved by this intuitive, but inherently chemical illustration, I should point out that the formalism presented in this dissertation has also been applied to the recombination of holes and electrons in semiconductors [4] and the annihilation of primordial magnetic monopoles in the early Universe [5].

in the analysis. Some of these are presented in section 2 in which RD systems are further introduced, pre-field-theoretical approaches are discussed and their limitations, as well as occasional benefits, are presented.

In section 3the field theoretic description of reaction-diffusion, originally due to Doi[6] and then revived by Peliti[7], is introduced with emphasis on renormalisation group techniques. I believe the procedure has great pedagogical value as it allows one to appreciate the structure of field theory in a classical setting. Since quantum physics has the potential to obscure calculations of perfectly observable phenomena for a lot of people, a classical analogue of QFT is useful in gaining an intuitive grasp on field theory calculations and in recognising the elements of field theory that have nothing to do with quantum phenomena but rather probability in general. Having said that, the correspondence should not be taken too far, as there are key differences involved as well, which I will attempt to point out, and the whole lot of similarities could be considered to be largely a consequence of using functional integration in both quantum and classical field theory. It could be argued that functional integration is a much more fundamental mathematical underpinning of both variants of field theory.

In the following section 4 I will present some key theoretical and experimental results in the field, though the latter are quite scarce. Fortunately the former make up for that fact as there are links to other important areas of modern statistical physics, and physics in general, interspersed throughout the field. There is a particularly strong connection to percolation, more specifically directed percolation and to a lesser degree directed isotropic percolation. It has been found that a mesoscopic action related to a certain branching and decaying process is equivalent to a stochastic process describing directed percolation. This process also undergoes a phase transition as the individual reaction rates are independently varied. As we are using field-theoretic techniques, identifying critical exponents of the phase transition is a breeze. And there are many other systems exhibiting such and potentially much richer phase transition behaviour,

alongside numerous other properties of interest. After roughly covering the universality class of directed percolation, I will then present what might be called classical results in the field, data relating to the annihilation of two particles of different species. This is by far not trivial, yet serves as a good illustration of our adopted formalism. I will continue by tackling a less typical field, diffusion-reaction systems on complex networks. This is a relatively young field, active only during the last 10 years or so and I will attempt to present a concise summary of its achievements up to now. Theoretical considerations are rounded up with an exposition of Lévy flights which are a type of superdiffusive motion, important in itself, but that also enable us to consider cases where the field-theoretical results converge extremely well, thus providing a valuable testing ground. I will attempt to supplement the list of theoretical results with my own insights and I will finally list some open problems and possible directions of further research in section 5.

This review is largely based on a review by Howard et al. [8] and the references contained therein. The theoretical machinery is based on standard introductory accounts of field theory [9, 10] and the exposition of renormalisation and renormalisation group flows along with critical exponents in the classic textbook by Peskin & Schroeder [11]. The latter operates within a quantum setting, but the techniques covered are perfectly applicable to our procedures. The specific application of the field formalism to RD systems is mostly based on Cardy's lecture notes, available online.[12]

2 Reaction-Diffusion systems

2.1 Reaction-diffusion preliminaries

There are numerous processes in nature that fall conveniently under the reaction-diffusion paradigm. First and foremost the type of process we are dealing with is characterised by the types of particles involved. We could have, say, three species of particles as in

the example above. These particles then undergo reactions such as $A + B \to C$ or $A + A \to B + C$. There can of course be an arbitrary number of particle species, though most theoretical results focus on small numbers of these. Each reaction has an associated rate. A system of N particle species is specified by a list of all of its reactions, of the form $\sum_{j=1}^{N} k_j A_j \to \sum_{j=1}^{N} l_j A_j$, along with their rates. Let there be altogether M reactions. The k_j and l_j for the i-th reaction can be put in a matrix (k_{ij}, l_{ij}) of dimensions $M \times 2N$ with no two rows the same. This fully captures the reaction data.

The rate for a reaction is defined so that if it were the only reaction taking place and there were no stochastic fluctuations, the local particle densities $a_j(t)$ would satisfy

$$\partial_t a_i(t) = -\lambda (k_i - l_i) \prod_{j=1}^{N} a_j(t)^{k_j} \tag{1}$$

The parameter λ is the rate. E.g. in a two particle annihilation $A + B \to 0$ we would have $\partial_t a = -\lambda ab$ and $\partial_t b = -\lambda ab$.

The equation defining λ above is also called the mean field approximation. This neglects possible statistical fluctuations as irrelevant. In fact each reaction-diffusion a parameter range for which this approximation is valid in order to be able to define a renormalisation group expansion [8]. Most often it is justified above a so-called *critical dimension*. The derivation of it is shown in Section 2.1.1. The mean field approximation is usually taken to be true locally but can also be taken to hold globally, i.e. for the averaged particle densities, when the particles are homogeneously mixed.

An important property of the mean field approximation is that it comprises the *tree-level* sum of Feynman diagrams, as it satisfies the corresponding Dyson equation [8]. This might seem cryptic now but it will be important in obtaining results for asymptotic properties of $A + A \to 0$.

The particles also diffuse, so each species is characterised by its diffusion constant D_{A_j}.

The latter is technically defined through the correlations in a stochastic Langevin equation dual to our field theory description, of the noise term at different times, but can be thought of as the quantity such that the average distance traveled by a particle undergoing diffusion after time t is$2\sqrt{Dt}$.

The simplest and most analytically accessible reactions are single-species, of which some have been studied very extensively and are sometimes referred to by their name, e.g. annihilation $A+A \to 0$ and coagulation $A+A \to A$. [8]_We can build a very complete and accessible theoretical picture for processes of type $kA \to lA$ with $k > l$ which we shall do as an example in the next section. These of course do not fit the chemical analogy very well. They might still thrive in slightly more convoluted biological or sociological analogies, but are at any rate useful for elucidating the basic concepts of our framework.

As mentioned in the introduction we will be primarily interested in asymptotic scaling exponents and amplitudes for long times and large distances. These apply to the densities of reacting particles as well as the magnitudes of fluctuations. Some of these are sometimes tractable throughout the evolution of the system. In multi-species reactions final distributions sometimes demonstrate interesting phenomena such as segregation or depletion. These results can depend strongly on system parameters, some of which are listed in section 2.3.

2.1.1 Critical dimension

For simple reaction-diffusion processes, the dimension above which fluctuations become important is easily determined by considering the properties of random walks in d dimensions, which is what diffusion amounts to. Two random walkers are almost certainly going to meet in finite time in $d = 1$ or $d = 2$ dimensions, while they are almost certainly not going to meet in $d \geq 3$ dimensions. We thus identify d_c as the critical dimension. This additionally sheds light on the universality of the process. In dimensions $d \leq 2$, the

asymptotic properties of the process, that is properties at late times, when the particles are very distant from each other and we can ignore any microscopic length scales, are completely determined by the probability of two faraway random walkers diffusing into each other, a universal quantity. Above the critical dimension particles would almost certainly never meet and hence there would be no reaction had it not been for their microscopic details, notably length scales. With the introduction of these universality is lost.

In a reaction with three reacting particles $d_c = 1$, as three random walkers are likely to meet in a finite time only in $d = 1$.

Later we will be able obtain the critical dimension from the scaling of the coupling in our action, which in general depends on dimension. Beneath the critical dimension we will obtain IR divergences, while above it we will have ultraviolet divergences and both exactly at d_c. It can be thus shown that the critical dimension for a $kA \to lA$ reaction is $d_c = 2/(k-1)$.[8]

2.2 Mathematical approaches

There are several alternatives to field theory in approaching these types of problems. It should be noted straight away that we are primarily interested in systems out of equilibrium. In a lot of reaction-diffusion systems of interest the equilibrium condition is rather boring anyway, e.g. in pair annihilation $A + A \to 0$ the steady state is either an empty lattice or one diffusing particle. In cases where we are nevertheless interested in the equilibrium statistics, there are very elegant and powerful techniques at our disposals, such as the various canonical ensembles.

However in the more interesting case of analysing the approach to equilibrium we have as of yet less knowledge and consequently methods at our disposal. There is of course Monte Carlo simulation, which, in most areas of RD systems, serves as a substitute

for experimental verification of analytical findings and can also be used to solve specific brute force without any interference of analytical results. It can also be used with a pure research mindset to discover new phenomena. It is usually defined on a lattice with a characteristic spacing. It will be useful to first consider the dynamics on a lattice with particles hopping between lattice sites and reacting when on the same site with given probabilities in our field theoretic approach as well. Only later will we take a continuum limit and transform particle numbers into slightly more abstract particle densities.

The remaining techniques do not require a lattice. For two reacting particles, as in e.g. annihilation, we can define a stochastic Langevin equation and proceed with stochastic calculus analysis. There are two types of such Langevin equations, the mesoscopic, whose validity diminishes as we move further out of equilibrium and hinges on the a priori identification of slow variables[13, 8]. Nevertheless, they can yield important additional insight and are also amenable_to being solved with the tools of stochastic calculus in the region of their validity. For reactions of no more than two particles we can also obtain a different Langevin equation, analogous to that for the evolution of particle densities, directly from field-theoretic action ([8], sec. 3.5). It turns out that this describes a complex quantity, so the presence of a field-theoretical framework seems necessary for its consistent interpretation, but regardless of that, it doubtlessly increases our calculational possibilities.

Mean field theory is for all practical purposes exact above the critical dimension. It is usually much simpler than any of the other available analytical methods. A more involved approximation is that of Smoluchowski [14, 15], roughly corresponding to an extended mean field formalism with an additional mean two-point correlation function. This can also be used below critical dimension in specific cases. It is a very successful approximation in theories where propagators and fields do not get renormalized. The prime examples of RD processes, $A + A \to 0$ and $A + B \to 0$ are such, so Smoluchowski theory can be applied to them.

2.3 Tunable parameters

There is an abundance of tweakable parameters in the problems described above. First we can choose whether we're analysing a continuum or lattice, in discrete or continuous time. In this thesis we will mostly be concerned with spatial and temporal continuums, as they provide the most straightforward route to universal results and are the natural setting of field theory calculations. When utilising the Doi-Peliti field-theoretical formalism we will however always pass to the continuum through an intermediate stage on a lattice. The parameters of the lattice are thus important as well. In fact we will touch upon an area where the lattice structure is of utmost importance, while discussing RD processes on complex networks in section 4.3.

As for the lattice properties, we can tweak the lattice type, making it either (hyper-)cubic or triangular, for example. We can also modify occupancy restrictions, e.g. we would allow at most n particles at a site or reduce the probabilty of hopping to a site with many particles on it already. A rough continuum analogue of occupancy restrictions is the size of the reaction region, i.e. how close particles have to be to each other to react, or the radius of a hard-sphere particle, though these present one of the outstanding problems of the field-theoretic approach, as they haven't been adequately implemented yet.[2]

RD systems can be classified into groups of qualitatively different behaviour, closely related to their universality classes, the collection of critical exponents when there is a phase transition. The ones we will touch upon are directed percolation and its variants, branching and annihilating random walkers and simple systems without phase transitions [8] which we proceed to analyse in the following section. By adjusting the reactants and rates of typical representatives of these groups new interesting processes can be obtained.

[2] While it is true that Van Wijland [16] has introduced a method that allows us to treat hard-core potential particles bosonically so that they never appear on the same site, the particles can still pass through each other, which leads to notably erroneous results in 1 dimension.[8]

One can also introduce external elements with a more or less direct physical interpretation. One can consider systems with particle input in which the steady state becomes interesting as it is a driven out-of-equilibrium state. One can also introduce things like shear flows which contribute to the mixing of particles and thus add new terms to the path integral action. It is possible to generalise ordinary diffusion to Lévy flights which turns out to be very useful as we can consider cases when the convergence of the dimensional regularisation perturbation is much quicker than usually. Finally one can redefine the entire dynamics by moving the process to a complex network (simpler topological constructs more reminiscent of Euclidean space are also acceptable). These modifications and their implications will be elaborated on in section 4.

3 Field Theory in Reaction-Diffusion Systems

We will illustrate the translation of the problem into field-theory language on the example of the $A + A \to 0$ process. The main steps of the procedure are first considering particles on a discrete lattice with a probability distribution over the space of possible configurations of site occupation numbers. This can be worded in terms of states and the corresponding master equation can be interpreted as a quasi-Schrödinger equation. We then introduce creation and annihilation operators for individual sites and express all observables, including the quasi-Hamiltonian, in terms of these operators. What follows is an analogue of transforming the wavefunction formulation of quantum mechanics into Feynman's path integral approach. This step employs a clever trick that involves inserting a complete set of *coherent* states after each infinitesimal time interval, allowing us to replace the creation and annihilation operators with values of two distinct scalar fields. We can do the same for observables and calculate their expectation values by integrating over all configurations of the two fields. There are some unnecessary leftover terms from the initial and final contributions to the action which we can dispose of by

shifting one of the fields.

We then identify the part of the action bilinear in the fields as the free action, which is basically the action of pure diffusion, and expand the remaining terms in the exponential into a perturbation expansion, given that coupling constants are small[3]. We then analyse the appearance of ultraviolet and infrared divergences with respect to the dimension. We set scale dependent renormalisation conditions, calculate the beta function of the dimensionless coupling and identify a non-trivial IR-stable fixed point that finally yields the IR scaling laws which are what we are after.

3.1 Setting up field theory on the lattice

3.1.1 States and normalisation

Consider first particles residing on a lattice. The particles can hop to neighbouring sites and if there are several particles at the same site they have a given probability of annihilating. The idea is to introduce states analogous to wavevectors in second-quantized quantum theories. Our basis states will correspond to distinct sets of occupation numbers of lattice sites. Consider, for example, a somewhat artificial scenario with three lattice sites. Our basis vectors will then be labeled $|\{n_1, n_2, n_3\}\rangle$ with $n_i = 0, 1, 2, \ldots$ Of course if there is a conserved number of particles N only basis states with $\sum_i n_i = N$ will be allowed and there might be other constraints. Physical states are then associated with vectors of the form

$$|\psi\rangle \quad = \quad \sum_{\vec{n}} P\left(\vec{n}\right) |\vec{n}\rangle \tag{2}$$

[3]The coupling constants could easily be dimensionful and so we cannot speak of them being large or small just yet, but rather have to wait until we introduce the dimensionless coupling $g_0 = (\lambda_0/D)\,\kappa^{-2\epsilon/d_c}$ with κ an arbitrary momentum scale. Since κ is completely arbitrary and since we are guaranteed that this expression becomes small with time due to the RG flow we can conclude that such an expansion is justified.

with the constraint that

$$\sum_{\vec{n}} P\left(\vec{n}\right) = 1 \tag{3}$$

where $\vec{n}$ is a vector in a space of dimension equal to the number of lattice sites. We will interpret $P\left(\vec{n}\right)$ as the probability that the system is in state $|\vec{n}\rangle$. From the constraint we can recognise the principal difference from quantum computations in that we are not dealing with probability amplitudes but direct probabilities. Our normalisation must thus differ from the quantum conventions.

Our goal is to write a master equation for the evolution of the states and interpret it as a quasi-Schrödinger equation. We are looking for an expression of the form

$$\frac{\mathrm{d}}{\mathrm{d}t} |\psi\rangle = -H |\psi\rangle \tag{4}$$

We have to introduce some further structure resembling second-quantized theories before we can continue. We can think of global states as tensor products of individual lattice site states. In our three site example this means $|\{n_1, n_2, n_3\}\rangle = |n_1\rangle_1 |n_2\rangle_2 |n_3\rangle_3$. Label the state with no particles $|0\rangle$ and introduce creation and annihilation operators $a_i^\dagger$ and a_i satisfying

$$\left[a_i, a_j^\dagger\right] = \delta_{ij} \tag{5}$$

with other commutators vanishing. Finally define

$$|n\rangle_i = \left(a_i^\dagger\right)^n |0\rangle \tag{6}$$

Again note the non-standard normalisation.

3.1.2 Generating the Hamiltonian

With this formalism in place we can start recasting known master equations into Hamiltonian form. Let us consider the master equation for particles hopping form one lattice site to another unidirectionally. This case is very simple to generalize to bidirectional hopping between several pairs of neighbouring sites. Let $P(n_1, n_2)$ denote the probability that the system is in state $|n_1, n_2\rangle$. The probability for hopping from site 1 to site 2 is proportional to a constant rate D and the number of particles at site 1. We thus have:

$$\frac{\mathrm{d}}{\mathrm{d}t}P(n_1, n_2) = \lambda(n_1+1)P(n_1+1, n_2-1) - \lambda n_1 P(n_1, n_2) \tag{7}$$

Recalling the definition of our state, we can write its evolution as

$$\begin{aligned}
\frac{\mathrm{d}}{\mathrm{d}t}|\psi\rangle &= \sum_{n_1=n_2=0}^{\infty}\frac{\mathrm{d}}{\mathrm{d}t}P(n_1, n_2)|n_1, n_2\rangle \\
&= \sum\left(D(n_1+1)P(n_1+1, n_2-1) - Dn_1P(n_1, n_2)\right)|n_1, n_2\rangle \\
&= \sum Dn_1P(n_1, n_2)|n_1-1, n_2+1\rangle - \sum Dn_1P(n_1, n_2)|n_1, n_2\rangle \\
&= D\left(a_2^\dagger a_1 - a_1^\dagger a_1\right)\sum P(n_1, n_2)|n_1, n_2\rangle = -H|\psi\rangle
\end{aligned} \tag{8}$$

In the third line we have renamed summation indices and used $a_i|\ldots, n_i, \ldots\rangle = \\ = n_i|\ldots, n_i-1, \ldots\rangle$ and $a_i^\dagger|\ldots, n_i, \ldots\rangle = |\ldots, n_i+1, \ldots\rangle$ in the fourth line. These identities follow from the definition of n states and the commutation relations of a. We see the Hamiltonian equals $H = -\lambda\left(a_2^\dagger - a_1^\dagger\right)a_1$. In the bidirectional case it equals $H = \lambda\left(a_2^\dagger - a_1^\dagger\right)(a_2 - a_1)$ and when there are more than two lattice sites we obtain the diffusion Hamiltonian in its most general form:[4]

[4]It might not be immediately clear that we can add different Hamiltonians together. We can do so

$$H_{\text{diff}} = D \sum_{\langle ij \rangle} \left(a_i^\dagger - a_j^\dagger \right) (a_i - a_j) \tag{9}$$

where the sum is taken over pairs of neighbouring sites.

The second relevant process is pair annihilation at a single site and by similar proportionality arguments as for particle hopping we deduce its master equation to be

$$\frac{\mathrm{d}}{\mathrm{d}t} P_n = \mu \, (n+2) \, (n+1) \, P_{n+2} - \mu n \, (n-1) \, P_n \tag{10}$$

By again differentiating $|\psi\rangle = \sum P_n \, |n\rangle$ with respect to t, shifting the summation indices and using properties of a's and $a^\dagger$'s we obtain the annihilation Hamiltonian for a single site, $H_i = -\lambda \left(1 - a_i^{\dagger 2} \right) a_i^2$. The complete Hamiltonian for our lattice model is then:

$$H = H_{\text{diff}} - \sum_i \lambda \left(1 - a_i^{\dagger 2} \right) a_i^2 \tag{11}$$

In fact it is easy to generalise these observations to a Hamiltonian of a general reaction $k_A A \ldots \to l_A A \ldots$

$$\frac{\mathrm{d}}{\mathrm{d}t} P_n = \mu \frac{(n+k-l)!}{(n-l)!} P_{en+k-l} - \mu \frac{n!}{(n-k)!} P_n \tag{12}$$

Upon going through the differentiation of $|\psi\rangle$ again we can derive the following heuristic rule. For each $kA \to lA$ reaction we get two normal-ordered terms in the quasi-Hamiltonian, multiplied by the rate μ. The first one is always positive and represents only the left hand side of the equation, $a^{\dagger k} a^k$. There will always be the same number of creation and annihilation operators in this term as the information is basically duplicated. The second term is negative and takes into account both sides of the equation,

because the only constraint Hamiltonians have to obey, the conservation of total probabilty, is linear and homogeneous. Viewing Hamiltonians as linear operators on the vector space of states in the basis identified near the beginning of this section we can phrase the constraint as $\sum_\alpha H_{\alpha\beta} = 0$._See Cardy [12]. This will obviously be satisfied by any linear combination of appropriate Hamiltonians.

$-a^{\dagger l}a^k$. It can be shown [8] that this generalises to equations with several participating species, i.e. for equation $A + B + C \rightarrow D + 2A$ at rate ι we would obtain a quasi-Hamiltonian term $\iota\left(abc - d^\dagger a^{\dagger 2} abc\right)$. This heuristic rule will be useful in later analysis of more complex reactions.

3.1.3 Initial conditions

It is physically reasonable to consider initial conditions where the number of particles at each site is described by an independent Poissonian distribution. This means we have excluded scenarios where there is, for example, a known number of particles present in the entire lattice, as the probabilty distributions must then be appropriately correlated to satisfy this global constraint. However this is hardly a severe blow for our programme of deducing asymptotic scaling laws. In addition we would probably use other mathematical tools in cases where the system is small enough for the overall number of particles to be tractable. For a large number of sites the overall deviation from the mean number of particles will also be relatively small. At any rate, independent Poissonian distributions seem justified. The nice thing about these is that they can be quantum mechanically compactly represented by coherent states, i.e. eigenstates of the annihilation operator. We thus have:

$$|\psi\left(t=0\right)\rangle = \prod_i \mathrm{e}^{\rho_0}\mathrm{e}^{-\rho_0 a_j^\dagger}|0\rangle \tag{13}$$

The normalisation again differs from quantum conventions. ρ_0 is the average number of particles per site.

In the subsequent steps of the derivation the following identities, which follow from the commutation relations 5, are used ubiquitously:

$$\begin{aligned} \mathrm{e}^{\phi^* a}\,\mathrm{F}\left(a,\,a^\dagger\right) &= \mathrm{F}\left(a,\,a^\dagger+\phi^*\right)\mathrm{e}^{\phi^* a} \\ \mathrm{F}\left(a,\,a^\dagger\right)\mathrm{e}^{\phi a^\dagger} &= \mathrm{e}^{\phi a^\dagger}\mathrm{F}\left(a+\phi,\,a^\dagger\right) \end{aligned} \tag{14}$$

We must also define the expectation values of observables in our formalism. All the observables that we will consider can be thought of as depending on the number of particles, though we might need a Fourier transform or two along the way. Therefore the basis vectors $\bigotimes_i |n_i\rangle$ are "eigenstates" of the observable and we can consider our observables to be operators acting on $|\psi\rangle = \sum P(\vec{n})\,|\vec{n}\rangle$ as

$$A\,|\psi\rangle = \sum A(\vec{n})\,P(\vec{n})\,|\vec{n}\rangle \tag{15}$$

To obtain the average $\overline{A} = \sum A(\vec{n})\,P(\vec{n})$ we must project $A\,|\psi\rangle$ onto a reference bra. In our normalisation conventions this turns out to be $\langle 0|\prod \mathrm{e}^{a_j}$. The complete expression for averages of observables is thus

$$\overline{A} = \langle 0|\prod \mathrm{e}^{a_j} A \mathrm{e}^{-Ht}\,|\psi(0)\rangle \tag{16}$$

This expression will now be converted into path integral form.

3.2 Path integrals

As in ordinary accounts of deriving Feynman path integrals from the wavefunction formulation of quantum mechanics, we first acknowledge the limit

$$\mathrm{e}^{-Ht} = \lim_{\delta t \to 0} (1 - H\,\delta t)^{t/\delta t} \tag{17}$$

and proceed by writing the e^{-Ht} in 16 as a product of $t/\delta t$ terms of the form $\left(1 - H\left(a,\, a^\dagger\right)\delta t\right)$. As usual we insert a complete set of states between each pair of factors, only this time we insert a set of coherent states of the form

$$1 = \int \frac{\mathrm{d}\phi\,\mathrm{d}\phi^*}{2\pi} \mathrm{e}^{-\phi\phi^*} \mathrm{e}^{\phi a^\dagger} \left|0\right\rangle \left\langle 0\right| \mathrm{e}^{\phi^* a} \tag{18}$$

This is for one lattice site, whereas we actually insert a product for all the sites. The integration measure equals $\mathrm{d}\phi\mathrm{d}\phi^* = \mathrm{d}(\mathrm{Re}\,\phi)\,\mathrm{d}\,(\mathrm{Im}\,\phi)$, but it is useful to formally consider ϕ and ϕ^* as independent quantities, as they will be interpreted as such later. Doing so is rather analogous to regarding the two as independent in a quantum complex scalar field theory and so should not be problematic. The fields ϕ and ϕ^* will also carry a time label indicating at which point in the product expansion of the exponent 17 they were inserted.

The motivation for inserting coherent instead of some other states is that they fit nicely into our second-quantized formalism, as a and $a^\dagger$ even appear in their definition, so we are justified in hoping this might simplify our calculation significantly. Since the ρ_0 in the exponent of the initial state corresponds to the average number of particles per lattice or, in other words and in anticipation of taking the continuum limit, to the generalized particle density, we see that the ϕ fields will roughly correspond to particle densities at a given time and location. The coherent states are in fact overcomplete but one can easily show that the inserted sets are exactly complete. For this and a more detailed derivation of the following few results the reader is directed to [17].

Due to the inserted states, Eq. 16 will consist of a large number of factors of the form

$$\mathrm{e}^{-\phi(t+\delta t)\phi^*(t+\delta t)} \left\langle 0\right| \mathrm{e}^{\phi^*(t+\delta t)a} \left(1 - H\left(a,\, a^\dagger\right)\delta t\right) \mathrm{e}^{\phi(t)a^\dagger} \left|0\right\rangle \tag{19}$$

along with the contributions from the first and the last time slice which need to be taken

care of separately. By using relations 14 to commute the exponents involving a and $a^\dagger$ all the way through the expression where they give $\mathrm{e}^{\phi^*(t+\delta t)a}\left|0\right\rangle = 1$ and similarly on the $\langle 0|$ side of the expression, we obtain

$$\mathrm{e}^{-\phi(t+\delta t)\phi^*(t+\delta t)}\mathrm{e}^{\phi(t)\phi^*(t+\delta t)}\left\langle 0\right| 1 - H\left(a+\phi\left(t\right),\, a^\dagger+\phi^*\left(t+\delta t\right)\right)\delta t\left|0\right\rangle \tag{20}$$

By taking into account that the Hamiltonians are normal ordered, as can be seen from 9 and 11 and as is further advocated in [8], we can drop the a and $a^\dagger$ terms from the Hamiltonian altogether and retain only the ϕ and ϕ^* fields. Since these are c-numbers we can also eliminate the bracketing $\langle 0|0\rangle = 1$ factors. Because δt is infinitesimal we can also reexponentiate the $1 - H\delta t$ term, yielding final factors of the form

$$\mathrm{e}^{-\phi^*(t+\delta t)(\phi(t+\delta t)-\phi(t))}\mathrm{e}^{-H(\phi(t),\,\phi^*(t+\delta t))\delta t} \overset{\delta t\to 0}{=} \mathrm{e}^{-(\phi^*(t)\partial_t\phi(t)+H(\phi(t),\,\phi^*(t)))\delta t} \tag{21}$$

These will feature in the final result for 16 in a long chain of similar factors and one such chain for each lattice site. Since we're multiplying exponentials the product of factors will be absorbed into a sum of their exponents and in the limit $\delta t \to 0$ this will change into an integral over time. We can still schematically discuss only one lattice site and only in the very end extend the result to several sites, even though the factors are not entirely independent - the Hamiltonians include pairwise interactions between particles at different lattice sites. Nevertheless, these only appear in very benign places and do not affect the argument. Abbreviating $\frac{\mathrm{d}\phi\,\mathrm{d}\phi^*}{2\pi}$ by $đ\phi$, we see that 16 will be of the form

$$\begin{aligned}
\overline{A} &= \mathcal{N}^{-1}\int\int đ\phi\left(t\right)đ\phi\left(\delta t\right)\left\langle 0\right|\mathrm{e}^{a}A\mathrm{e}^{-\phi(t)\phi^*(t)}\mathrm{e}^{\phi(t)a^\dagger}\left|0\right\rangle\cdot & (22)\\
&\quad\cdot\exp\left(-\int \mathrm{d}t\,\left(\phi^*\left(t\right)\partial_t\phi\left(t\right)+H\left(\phi\left(t\right),\,\phi^*\left(t\right)\right)\right)\right)\left\langle 0\right|\mathrm{e}^{\phi^*(\delta t)a}\mathrm{e}^{\rho_0}\mathrm{e}^{-\rho_0 a^\dagger}\left|0\right\rangle & (23)\\
&= \mathcal{N}^{-1}\int \mathcal{D}\phi\mathcal{D}\phi^* A\,\exp\left(-S\left[\phi,\,\phi^*\right]\right) & (24)
\end{aligned}$$

The functional S is readily interpreted as an action and it contains the time integral from 22 as well as terms coming from the initial and final factors that are discussed to some length in section 3.3 of [8]. These cancel for various reasons, one of them being causality of the propagators. There is also a more stubborn $-\phi(t)$ factor that has to be eliminated by a field shift $\phi^* \to \phi^* + 1$. Let us forget about it for now and implement it in a few lines. The field ϕ^* is to be treated as independent from now on and so can be relabeled to avoid confusion, $\phi^* \overset{\text{relabel}}{\to} \tilde{\phi}$. The only additional term left over is $-\tilde{\phi}(0)\,\rho_0$ which imposes initial conditions.

Finally let us take into account the spatial extent of the fields ϕ and $\tilde{\phi}$ by multiplying the functional integrals for individual lattice sites together. We obtain

$$\overline{A} = \mathcal{N}^{-1} \left(\prod_i \int \mathcal{D}\phi_i \mathcal{D}\tilde{\phi}_i \right) A\, \mathrm{e}^{-S\left(\vec{\phi}(t), \vec{\tilde{\phi}}(t)\right)} \tag{25}$$

$$S\left(\vec{\phi}(t)\,, \vec{\tilde{\phi}}(t)\right) = \sum_i \int \mathrm{d}t \, \left(\tilde{\phi}_i \partial_t \phi_i - \lambda \left(1 - \tilde{\phi}_i^2\right) \phi_i^2 \right) + D \sum_{\langle ij \rangle} \int \mathrm{d}t \, \left(\tilde{\phi}_i - \tilde{\phi}_j \right) (\phi_i - \phi_j) \tag{26}$$

Here we have explicitly written out H as the full Hamiltonian from Eq. 11. Let us now take a continuum limit by promoting ϕ and $\tilde{\phi}$ from (roughly) the average number of particles per lattice site to roughly the average particle density. For simplicity let's assume we are working in a d-dimensional (hyper)cubic lattice with spacing h. Then $\phi_i(t) \to \phi(x,\, t)\, h^d$ in the vicinity of x_i, the location of the i-th lattice site in the newly established coordinate system, while $\tilde{\phi}_i(t) \to \tilde{\phi}(x,\, t)$. The sums are promoted to integrals , $\sum_i \to \int \mathrm{d}^d x\, h^{-d}$, and field differences are promoted to gradients with constants rescaling to absorb potential factors of h floating around.[5] The full action,

[5] We have chosen $\phi_i(t) \to \phi(x,\, t)\, h^d$ because of convention and because it is at times convenient to think of ϕ as a particle density and the response field $\tilde{\phi}$ as merely an artifact of our calculation. But the allusion of ϕ to the particle density should not be taken too far, as it is in fact in general complex. What is true is that its expectation value is the expected particle density [12]. We could have thus also chosen $\phi_i \to \phi h^a$, $\tilde{\phi}_i \to \tilde{\phi} h^b$ with the only constraint, enforced by the diffusion term, that $a + b = d$. The rest of the dimensions can be absorbed into parameters such as λ.

e.g. the argument of the exponential in 25, thus becomes

$$S\left[\phi,\tilde{\phi}\right]=\int \mathrm{d}^{d}x\int \mathrm{d}t\,\left(\tilde{\phi}\partial_{t}\phi+D\nabla\tilde{\phi}\nabla\phi-\lambda\left(1-\tilde{\phi}^{2}\right)\phi^{2}\right) \tag{27}$$

We can integrate the gradient term by parts to get $\nabla\tilde{\phi}\nabla\phi\rightarrow-\tilde{\phi}\nabla^{2}\phi$. Recall from a couple of paragraphs ago that we still have to perform the shift $\tilde{\phi}\rightarrow\tilde{\phi}+1$ to get rid of a final term and that an initial term is thus left over. This is caused by the first term in the action, which we can consequently leave unchanged. This leaves us with the final expressions

$$\begin{aligned} S\left[\phi,\tilde{\phi}\right] &= \int \mathrm{d}^{d}x\int\left(\mathrm{d}t\,\left(\tilde{\phi}\left(\partial_{t}-D\nabla^{2}\right)\phi+2\lambda\tilde{\phi}\phi^{2}+\lambda\tilde{\phi}^{2}\phi^{2}\right)-\tilde{\phi}\left(0\right)\rho_{0}\right) \\ \overline{A} &= \mathcal{N}^{-1}\int\mathcal{D}\phi\mathcal{D}\tilde{\phi}A\left[\phi,\,\tilde{\phi}\right]\mathrm{e}^{-S\left[\phi,\tilde{\phi}\right]} \end{aligned} \tag{28}$$

Finally note that the normalisation factor $\mathcal{N}$ in 22 is determined by demanding $\overline{1}=1$, so $\mathcal{N}=\int\mathcal{D}\phi\mathcal{D}\tilde{\phi}\mathrm{e}^{-S\left[\phi,\tilde{\phi}\right]}$.

A word on general $kA\rightarrow lA$ reactions. As we have mentioned below equation 12, the reactive parts of their Hamiltonians look like

$$H_{react}=\lambda_{0}\sum\left(a_{i}^{\dagger k}-a_{i}^{\dagger l}\right)a_{i}^{k} \tag{29}$$

upon substituting $a\rightarrow\phi$, $a^{\dagger}\rightarrow\tilde{\phi}+1$ and some elementary algebraic manipulation we obtain reactive terms in the action of the form

$$\sum_{i=1}^{k}\lambda_{i}\tilde{\phi}^{i}\phi^{k} \tag{30}$$

with

$$\lambda_i = \begin{cases} \lambda_0 \left(\binom{k}{i} - \binom{l}{i} \right) & i \leq l \\ \lambda_0 \binom{k}{i} & i > l \end{cases} \tag{31}$$

We can interpret this as a set of Feynman vertices, which are however all related through λ_0 and thus undergo the same renormalization. This is good since we do not wish to introduce new parameters upon renormalisation and somewhat equivalent to analysing Lagrangians with broken symmetry.[6]

3.3 Expansion in terms of Feynman diagrams

The most insightful part of deriving the field theory formalism is the instating of perturbation theory and the ensuing Feynman diagrams. There are at least two equivalently powerful ways of thinking about diagrams when implementing them. We will occasionally be using a partially Fourier transformed propagator $G_0(\vec{p}, t)$ which will make expressions look like multidimensional convolutions and will thus emphasize the role of G as a Green's function and elucidate some structure of perturbative calculations. We of course again encounter ultraviolet divergences due to unbounded internal momenta in loop calculations, which we can regulate by absorbing the poles into the couplings. What's more surprising is that we also encounter infra-red divergences for $\vec{p} \to 0$ (which we shall assume throughout this section when needed) and $\omega \to 0$ which corresponds to long times $t \to \infty$. From our physical intuition we do not expect meek tabletop diffusion experiments to explode if we wait long enough, so these infra-red divergences have to be regulated. This is achieved by means of summing the perturbation series at an earlier time, when it converges, and using the running couplings of renormalisation group flows, quantitatively got at by solving the Callan-Symanzik equation for the particle density,

[6] The shift $\tilde{\phi} \to \phi^* + 1$ is in fact not completely harmless. It can conceal e.g. inversion symmetry $\tilde{\phi} \to -\tilde{\phi}$ and in some cases, e.g. with branching and annihilating random walkers (section 6.4 of [8]), this is not always optimal as it can lead us down the wrong path.

to investigate its asymptotic infra-red behaviour, which turns out to be regular. RD systems also offer a curious way to intuitively approach renormalisation group (RG) flows, since the couplings are literally flowing in time.

3.3.1 Feynman diagrams from the action

The standard way of approaching Feynman diagrams is to consider the part of the action bilinear in fields ϕ and $\tilde{\phi}$ as the action of the free theory, expanding the rest of the action as a perturbation series in the small coupling constants and averaging with respect to the Gaussian free action. This yields all the convenient properties of Gaussian integration at our disposal, including Wick's theorem. Continuing the derivation for $A + A \to 0$, we can read the propagator and interaction vertices directly from the action in 28. It is a well know theorem that the propagator is the inverse of the bilinear functional form in the quadratic term of the action, the free action. The propagator in our case is purely diffusive and is straightforward to calculate by ordinary inversion in Fourier space which yields

$$G(p;\, t) = \int \mathrm{d}^d p\, \mathrm{e}^{ip\cdot x} \left\langle \tilde{\phi}(x,\, t)\,,\, \phi(0,\, 0) \right\rangle = \mathrm{e}^{-Dp^2 t} \Theta(t) \tag{32}$$

There are two distinct vertices represented in figure_1._The interesting thing about processes without branching, which cover a wide array of distinct natural phenomena, is that the propagator and hence both the diffusivity D and the field strength of ϕ, $\tilde{\phi}$ do not get renormalised. In $A + A \to 0$ this is evident from the fact that all vertices require two $\tilde{\phi}$ input fields while the propagator only provides one such output branch. Consequently there is no way of forming any loops within propagators. As has been mentioned before, this is the reason approximations of the Smoluchowski type are so successful in capturing the essence of RD calculations.

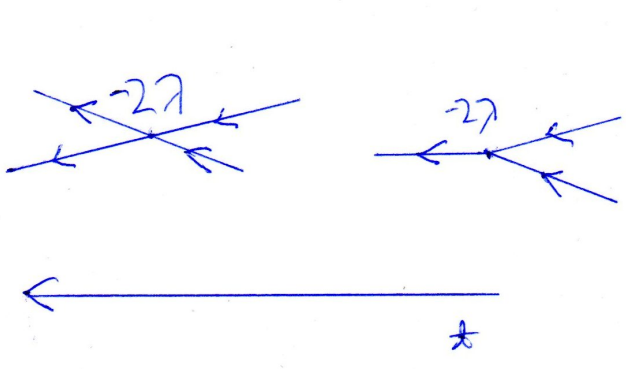

Figure 1: The vertices of the theory described by action 28. Time is flowing right to left, as marked. We will adopt this convention throughout this text.

3.3.2 Feynman diagrams from Green's functions

A conceptually different approach for systems close enough to equilibrium is to transform the field theory description of the system into a corresponding Langevin equation, that is a stochastic differential equation for the field ϕ, usually with multiplicative noise. This is only possible in systems with reactions of at most two input reactants. There is a straightforward mapping between an action, such as in 28, and a corresponding Langevin equation. Demonstrating its validity is not difficult, but involves some long and cumbersome functional integration calculations. The reader is directed to [12] for a more complete derivation. The Langevin equation in the $A + A \to 0$ case is

$$\partial_t \phi - D\nabla^2 \phi = -2\lambda\phi^2 + \xi + \rho_0 \delta(t) \tag{33}$$

where ξ is a Gaussian noise term characterised by

$$\langle \xi(x', t')\, \xi(x, t) \rangle = -2\lambda\phi^2 \delta(x' - x)(t' - t) \tag{34}$$

By again using the diffusive propagator G, e.g. Green's function of the diffusive differ-

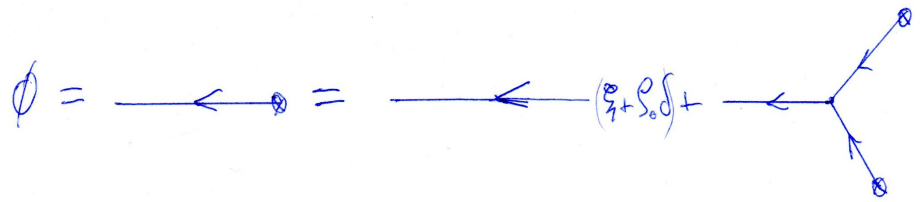

Figure 2: The recursive definition of ϕ.

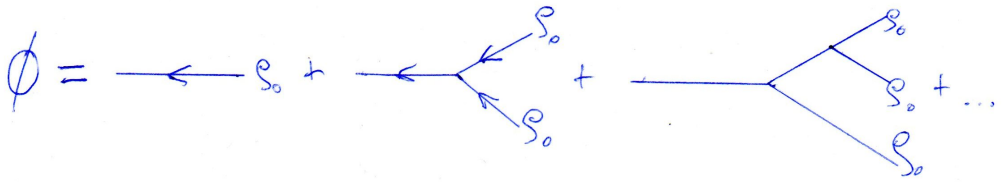

Figure 3: Sum of tree level diagrams with an arbitrary number of initial fields.

ential operator in Eq. 33, we can formally write the solution as

$$\phi(x,\,t) = \int G(x - x';\,t - t')\left(-2\lambda\phi(x',\,t')^2 + \xi(x',\,t') + \rho_0\delta(t')\right) \tag{35}$$

This lends itself to a recursive definition, which can be neatly presented diagrammatically as in figure 2. These diagrams are exactly the Feynman diagrams.

The noise terms in Eq. 35 refer to a specific realisation of the noise that we can know nothing about unless it's measured. In the case of no noise the, ϕ is equal to the sum of all tree diagrams beginning with any number of ρ_0 terms, as in figure 3, which is thus seen to roughly correspond to the mean-field analysis. In the case of noise we can analyse the average value $\langle\phi(x,\,t)\rangle$. As can be seen if we expand 35 to a couple of terms we soon get terms involving products of the noise at different times. Since the noise is Gaussian, a variant of Wick's theorem holds, schematically $\langle\xi^{2n}\rangle = \sum_{\text{all pairings}}\langle\xi^2\rangle^n$ and we know the form of the right hand side from 34. This gives rise to a new interaction vertex with two outgoing lines, as $\langle\xi^2\rangle \propto \phi^2$ corresponding to the leftmost vertex in figure 1.

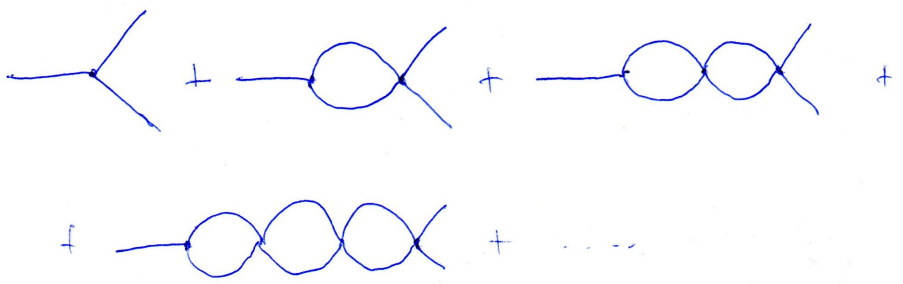

Figure 4: Sum over loops for the renormalisation of the three point vertex in $A + A \to 0$

This somewhat more intuitive approach to Feynman diagrams will be best demonstrated in the next section when we calculate the renormalised coupling associated with λ.

3.4 Renormalisation

In $A + A \to 0$, all of the possible loop corrections to say the three point vertex are rather easy to visualise and can remarkably be summed exactly. This sum is shown in figure 4. Going into Fourier space, the convolutions associated with the diagrams transform into products whereas the sum stays in place due to the linearity of the Fourier transform. The entire string is a summable geometric series. But we need not limit ourselves to the case of double particle same-species annihilation. This situation arises in any $kA \to lA$ type of reaction. The loop expansion of a single vertex in a $kA \to lA$ reaction is similar to that shown in figure 4, just that there are now k instead of 2 propagators connecting each pair of adjacent vertices. Let us review the general procedure for any reaction of this type.

We are interested in the spatially homogeneous case, which is a valid assumption even in the two species segregated case, as the characteristic sizes of segregation zones are much bigger than distances between individual particles. Taking $\omega \to 0$ as well we encounter the IR divergences when the dimensionality of the system $d < 2$. as the critical dimension of the system is $d_c = 2$.

3.4.1 Loop integral and scaling

The addition of loops and the subsequent renormalisation of vertices with k ingoing and m outgoing legs is described by a vertex function $\Gamma^{(m,k)}(t)$, where t is the total time-span of the propagators of which it is composed, the horizontal distance in figure 4 At tree level it is just $\lambda_m \propto \lambda_0$. Denote the single loop integral from t_1 to t_2 as $I(t_2 - t_1)$. It is a rather complicated expression, consisting of an integral over $k-1$ independent d-dimensional momentum vectors of the product of k momentum-dependent propagators from $t_1$to t_2. We then have:

$$\Gamma^{(m,k)}(t_2 - t_1) = \lambda_m \delta(t_2 - t_1) - \lambda_m \lambda_0 I(t_2 - t_1) + \lambda_m \lambda_0^2 \int_{t_1}^{t_2} \mathrm{d}t' I(t_2 - t') I(t' - t_1) - \dots \tag{36}$$

The following results are quoted from [8] $I(t) = B_k (Dt)^{-d/d_c}$ where $B_k = k! k^{-d/2} (4\pi)^{-d/d_c}$ and $d_c = 2/(k-1)$.

Instead of going to momentum space by Fourier transforming, [8]use the Laplace transform[7] which also turns convolutions into products, but is in this case somewhat simpler. They thus obtain the Laplace transformed vertex function as

$$\tilde{\Gamma}^{(m,k)}(s) = \frac{\lambda_m}{1 + \lambda_0 \tilde{I}(s)}; \qquad \tilde{I}(s) = B_k \Gamma(\epsilon/d_c) D^{-d/d_c} s^{-\epsilon/d_c} \tag{37}$$

where $\epsilon = d_c - d$ and the Γ function in $\tilde{I}(s)$ is Euler's gamma unfortunately sharing a label with the vertex function. The statements $t \to \infty$ and $s \to 0$ are equivalent so the divergence $\tilde{\Gamma}^{(m,k)}$ in the latter case is the UV divergence.

We must then introduce a dimensionless coupling. Before we do so, a comment about scaling dimensions of quantities appearing in our framework is in order. Let us consider

[7]The Laplace transform $\tilde{g}(s)$ of a function $g(t)$ is defined as $\tilde{g}(s) = \int_0^\infty g(t) \mathrm{e}^{-st} \mathrm{d}t$

an arbitrary momentum scale κ. Distances scale inversely to momentum, as in ordinary quantum field theory, but since this is a diffusive setting with characteristic length $\sim (Dt)^{1/2}$, times scale as κ^{-2}. The action must be dimensionless and hence, since there is no relevant scale to compare it to, invariant under scaling. So all terms under the integral in the action must scale as κ^{d+2}. Our continuum limit conventions under Eq. 25 imply that ϕ scales as κ^d and that $\tilde{\phi}$ is invariant. From the interaction terms in the action we can thus deduce that the effective coupling λ_0/D must scale as $\kappa^{2-(k-1)d}$. Taking into account $\epsilon = d_c - d$ and $d_c = 2/(k-1)$ this is equivalent to $\kappa^{2\epsilon/d_c}$.

3.4.2 Dimensionless coupling and its beta function

We can thus introduce a dimensionless parameter $g_0 = (\lambda_0/D)\,\kappa^{-2\epsilon/d_c}$, corresponding to bare dimensionful parameters. The value of the momentum scale κ doesn't matter, what will matter in a moment is that it varies with time in diffusive fashion as $\kappa \sim t^{-1/2}$. For the time being we continue defining the theory "at momentum κ" by defining the renormalised coupling g_R as

$$g_R = \tilde{\Gamma}^{(k,k)}\left(D\kappa^2\right)\kappa^{-2\epsilon/d_c}/D = Z_g g_0 \tag{38}$$

where $Z_g^{-1} = 1 + g_0 B_k \Gamma(\epsilon/d_c)$. This is analogous to defining renormalisation conditions at spacelike momenta of magnitude typical for the problem at hand, but for infrared divergences.

We continue our march towards quantitative renormalisation group results, most notably in the form of a solution of the Callan-Symanzik equation, by noticing that particle densities must be independent of the renormalisation scale κ. In the case of a single species let us denote its density by a. Then we have

$$\left(\kappa\frac{\partial}{\partial\kappa}+\beta_g\left(g_R\right)\frac{\partial}{\partial g_R}\right)a\left(t,\,n_0,\,\kappa,\,g_R\right) \tag{39}$$

where n_0 is the initial density, previously denoted ρ_0. In the most general case we would have to include D among the arguments as well, but we have seen that it is not renormalised in the type of reactions we're interested so this is not necessary. β_g is the standard β function, which in our case can be computed explicitly from Eq. 38:

$$\beta_g\left(g_R\right)=\kappa\frac{\partial}{\partial\kappa}g_R=2g_R\left(-\frac{\epsilon}{d_c}+B_k\Gamma\left(1+\frac{\epsilon}{d_c}\right)g_R\right) \tag{40}$$

The crucial insight here is that it has an infrared stable fixed point at

$$g_R^*=\left(B_k\Gamma\left(\frac{\epsilon}{d_c}\right)\right)^{-1}\sim\mathcal{O}\left(\epsilon\right) \tag{41}$$

As we will see shortly, running couplings will all reach this fixed point in subcritical dimensions, regardless of their initial value, for long times and this will non-trivially affect their asymptotic time dependences.

3.4.3 Callan-Symanzik equation and running couplings

Returning to the scale independence equation 39, we note that dimensional analysis yields a suggested form of the particle density:

$$a\left(t,\,n_0,\,\kappa,\,g_R\right)=\kappa^d\hat{a}\left(t/t_0,\,n_0/\kappa^d,\,g_R\right)=\kappa^d\hat{a}\left(Dt\kappa^2,\,n_0/\kappa^d,\,g_R\right) \tag{42}$$

where $t_0=1/\left(D\kappa^2\right)$. The form of κ dependence of the first and second term tell us we can exchange $\kappa\frac{\partial}{\partial\kappa}$ with $2t\frac{\partial}{\partial t}-dn_0\frac{\partial}{\partial n_0}$. We also obtain a d from the κ^d before the dimensionless $\hat{a}$ function. Inserting this into equation 39 yields the final form of the Callan Symanzik equation.

$$\left(2t\frac{\partial}{\partial t} - dn_0\frac{\partial}{\partial n_0} + \beta_g\left(g_R\right)\frac{\partial}{\partial g_R} + d\right)a\left(t,\, n_0,\, \kappa,\, g_R\right) = 0 \tag{43}$$

This is solved by the method of characteristics as described in any standard textbook covering RG techniques.$\log t^{1/2}$ is the parameter with respect to which the couplings will run. We will have two running couplings, $\tilde{g}_R\left(t\right)$, technically $\tilde{g}_R\left(\log t^{1/2}\right)$, but this is rather cluttered, with an implicit dependence on the initially chosen g_R, and $\tilde{n}_0\left(t\right)$, again with an implicit n_0 dependence. The running couplings satisfy equations

$$\frac{\mathrm{d}\tilde{n_0}}{\mathrm{d}\log t^{1/2}} = d\tilde{n_0}; \qquad \frac{\mathrm{d}\tilde{g_R}}{\mathrm{d}\log t^{1/2}} = -\beta_g\left(\tilde{g}_R\right) \tag{44}$$

for which exact solutions can easily be found:

$$\begin{aligned} \tilde{n}_0\left(t\right) &= \left(t/t_0\right)^{d/2} n_0 \\ \tilde{g}_R\left(t\right) &= g_R^*\left(1 + \frac{g_R^* - g_R}{g_R}\left(\frac{t_0}{t}\right)^{\epsilon/d_c}\right)^{-1} \end{aligned} \tag{45}$$

Thus we have confirmed the statement that $\tilde{g}_R\left(t\right) \to g_R^*$ as $t \to \infty$ regardless of initial conditions $\tilde{n}_0\left(t_0\right) = n_0$, $\tilde{g}_R\left(t_0\right) = g_R$

The additional d in the CS equation gives us the following relation

$$a\left(t,\, n_0,\, t_0,\, g_R\right) = \left(\frac{t_0}{t}\right)^{d/2} a'\left(\tilde{n}_0\left(t\right),\, \tilde{g}_R\left(t\right)\right) \tag{46}$$

where a' is a function that needs to be determined in a characteristic method of characteristics fashion. We could obtain an expansion in $\tilde{g}_R$ of a at some early time as there is no sign of infrared divergences then and set the dependence of a' on $\tilde{g}_R\left(t\right)$ so that when $\tilde{g}_R\left(t\right)$ is expressed in terms of g_R as per Eq. 45, the two expressions match to the

desired order. We must however come up with an exact a' dependence on $\tilde{n}_0$ since this diverges for late times and a perturbation expansion is thus no good.

An idea that turns out to work is to insert the sum of all tree-level diagrams that, as we briefly commented on in section 2, roughly coincides with the mean-field behaviour. For a $kA \to lA$ reaction the mean field equation is simply

$$\partial_t a = -\lambda_0 (k-l) a^k \tag{47}$$

which has an analytic solution

$$a(t) = \frac{a_0}{\left(1 + a_0^{k-1} (k-1)(k-l)\lambda_0 t\right)^{1/(k-1)}} \tag{48}$$

with asymptotic behaviour independent of initial conditions. Taking into account the time dependence of the effective reaction rate $\lambda(t) \sim D(\kappa(t))^{2\epsilon/d_c} \tilde{g_R}(t) = D(Dt)^{-\epsilon/d_c} \tilde{g}_R(t)$ the idea is thus to consider an a' of the form

$$a'(n, g) = \frac{n}{\left(1 + n^{k-1} (k-1)(k-l)(Dt)^{1-\epsilon/d_c} g\right)^{1/(k-1)}} \tag{49}$$

Then the inverse dependences of $\tilde{n}_0$ on n_0 and a on a' cancel and the final form of the result is

$$a(t) = \frac{n_0}{\left(1 + n_0^{2/d_c} (k-1)(k-l) g_R^* (Dt)^{d/d_c}\right)^{d_c/2}} \to \tilde{A}_{kl} (Dt)^{-d/2} \tag{50}$$

Here $\tilde{A}_{kl}$ is a universal amplitude that depends only on the dimensionality of the problem. Adding higher loop-order diagrams turns out to modify only the amplitude and provides an expansion in successive powers of ϵ, but the uniform RG flow for all cou-

plings guarantees that the exponent stays the same and it is therefore determined solely by the tree-level diagrams.

3.4.4 Asymptotic decay exponents and amplitude

Some inspiring results can already be obtained from only the form of the effective coupling, $\lambda(t) \sim D(Dt)^{-\epsilon/d_c}\,\tilde{g}_R(t)$. For $d > d_c \Rightarrow \epsilon < 0$, $\tilde{g}_R(t) \sim t^{\epsilon/d_c}$ for long times and so asymptotically tends to a constant value. Below the critical dimension, $\tilde{g}_R(t)$ flows to g_R^* relatively fast, so the asymptotic effective rate dependence is of the form $\lambda(t) \sim D(Dt)^{-\epsilon/d_c}\,g_R^*$. At the critical dimension we have instead $\lambda(t) \sim \frac{D}{\log(t/t_0)}$.

Replacing constant λ's in mean field equations, such as Eq. 47, with expressions of the above time dependence agrees with asymptotic particle densities obtained with completely different techniques for $k = 2$ and $k = 3$, $d = d_c = 1$. These results are

$$a(t) \sim \begin{cases} (8\pi Dt)^{1/2} & k = 2,\ d = 1 \\ \frac{\log(Dt)}{8\pi Dt} & k = 2,\ d = 2 \\ \left(\frac{\log(Dt)}{Dt}\right)^{1/2} & k = 3,\ d = 1 \end{cases} \tag{51}$$

The $k = 2$ results were obtained by Bramson and Griffeath by analytical methods. [18]

This is the final output of our analysis. The most important and also the most field-theoretic piece of information obtained is confirmation that the decay amplitude is universal, independent of microscopic details. The ϵ series is poorly convergent in the only physical dimension below the critical dimension, $d = 1$, so it has to be calculated using other methods, but it would be very hard to obtain even a hint of universality using other methods.

4 Theoretical Results and Further Applications

The RD formalism hasn't been developed to address any pressing issues in need of a quick resolution and can as such be seen as an exercise in Mathematics, or rather Mathematical Physics, due to the large amount of approximations involved. Due to its intuitive nature it seems that the formalism is just calling for applications and like most intuitive mathematical models it has spawned countless picturesque analogies in the literature. And there truly is no limit to how picturesque things can get. The results of an $A + A \to A$ reaction along with a much slower $A + A \to 0$ in $d = 2$ on a bounded elliptic region could be of much help to historians in shedding light on the everyday lives and deaths of blind gladiators, for example.

Suggestions for more serious applications are fortunately ever more frequent, as should be evident from the remainder of this section. Even if they were not, non-equilibrium processes, of which the reaction-diffusion systems are a part, constitute a much bigger part of our lives than ideal heat-baths, so their study appears rather natural. There are great theoretical insights to be had in pushing the frontiers of our understanding of non-equilibrium dynamics further. As will become obvious, modern research in the field is also plagued with a fair amount of rather obvious problems which dictate especially intensive directions of further investigation. These will also be touched upon in the closing section of this dissertation.

4.1 Percolation

4.1.1 Phase transitions

The RD phenomenology and especially the RG field-theoretic approaches are found to be intimately connected with other areas of modern statistical physics. Especially interesting are connections with directed percolation and the recent investigations into

branching and annihilating random walkers. Whereas the $kA \to lA$ processes of the previous section are pedagogically instructive, they are very specific. Particularly, due to there being no branching processes, the propagators and hence diffusion constants do not get renormalised.

A branching process alone is rather boring as it leads merely to a most likely exponential runaway increase in particle densities. When we add counterweight reactions reducing the numbers of particles things begin to look more interesting. In all but very specific cases the reaction rates of the competing reactions can be taken to be independent. This gives us a phase space in which interesting phase transitions can occur. These are characterised by a set of critical exponents, describing the power law behaviour of thermodynamic quantities as we approach the transition as measured by an appropriate parameter.

The same exponents can characterise a variety of physically seemingly distinct situations. This makes sense, as one of the properties of second order phase transitions, for which one can define critical exponents, is a diverging correlation length as we approach the critical point. At the critical point therefore the finite lengths involved in the accurate microscopic description of our system do not matter, as the dynamics and scaling are determined by an essentially infinite correlation length, similarly to what we encountered in investigating the origin of universal properties associated with the asymptotic decay of particles in section 2.1.1.

Sets of phenomena with equal universal quantities, such as critical exponents below critical dimension, are known as universality classes. The asymptotic densities and decay rates of many RD processes with tunable rates have been found to exhibit such critical behaviour. The universality classes encountered in RD research include the directed percolation class, associated with the reactions $A \to 0$ and $A \to A + A$, and the parity conserving class, associated with branching and annihilating random walkers with an even number of offspring, i.e. the reactions $A \to (m+1)\, A$ with even m. I will not

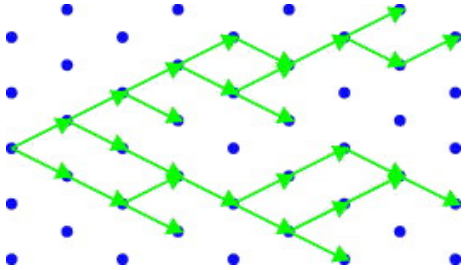

Figure 5: Directed bond percolation on a lattice. Time flows to the right. Image taken from [19]

repeat the actual calculations of critical exponents in this text, as without the comfort of an unrenormalised propagator, a larger number of parameters needs to be renormalised, 4 in particular for DP [19]. This leads to very long-winded and cumbersome algebra, particularly in the Callan Symanzik equation, so I will only outline the methods of calculation and the implications of the findings.

4.1.2 Percolation basics

Percolation primarily refers to phenomena associated with transport through porous media. When one has a lattice where each site can be either traversable or not and the probabilistic distribution of different types of sites is parametrized by a set of parameters, varying these parameters will often lead to a phase transition. In one of the phases, a fluid will not be able to traverse the entire length of the lattice, whereas in the other, there exists a path or a cluster along the entire lattice. The word percolation nowadays also refers to similar problems involving randomly populated lattices and traversability. For a summary, see e.g. [20]. In effect we speak of many types of percolation.

The type we are mostly concerned with in relation to RD processes is Directed Percolation (DP) and to a lesser degree Isotropic Percolation (IP). The former can most easily be illustrated in the following manner in two dimensions: suppose we have a rhombic lattice as shown in figure 5. There are diagonal bonds arranged randomly between lat-

tice sites. A bond corresponds to a traversable site in the example from the previous paragraph, so the lattice in our case is complementary to the lattice from the example (edges become vertices). Agents moving on this lattice can only move diagonally to the right and only if there is a bond present in one of the possible directions.

We can think of this percolation process as modeling a spreading of a disease. In fact many modern research articles use this terminology, both for the colourful imagery it incites and because most actual applications of the field are in epidemiology[8]. Directed bond percolation is sometimes also referred to as a *simple epidemic process* or *epidemic with recovery* [19]. We can think of the horizontal direction as time, flowing to the right, while the transverse dimension are, say, people arranged in 1 dimension. The propagating agents represent infections. In every time step the neighbours of an infected individual can get infected (branching bonds) or an individual may recover (terminating nodes).

A slightly more pessimistic version of this is the Isotropic Percolation, where the time direction is not incorporated into the lattice. Rather, infections, or bonds, spread out from a central seed. Again, branching represents infections of new carriers and the termination of bond sequences represents carriers who die on the spot and form untraversable debris. This universality class is not quite as studied and illustrative, so we shall focus on DP from now on.

These two processes connect with the field-theoretical study of RD processes in a rather remarkable way. The field-theoretical action that we assign to the aforementioned RD reactions associated with the DP universality class, analogous to the action in Eq. 28, first appeared in the study of elementary particles by the name of Reggeon field theory, a then "very powerful tool for studying the complex angular momentum structure of high energy scattering amplitudes" [21]. In two papers by Grassberger et al. [22, 23], the authors argued that the action is better viewed as a stochastic process (with the Langevin equation obtained from the action in the standard way [24]), a stochastic version of the

[8]See section 4.1.7

so called Schlögl's first reaction [25], $X + A \rightleftharpoons 2X$. They named the process after Gribov, a researcher in Reggeon Field Theory. A couple more papers established the equivalence between this process and a certain type of DP dynamics, including a very elegant exposition by Cardy and Sugar [26].

The correspondence has been verbalised in the slightly technical DP conjecture: "the critical behavior of an order parameter field with Markovian stochastic dynamics, decoupled from any other slow variable, that describes a transition from an active to an inactive, absorbing state (where all dynamics ceases) should be in the DP universality class" [19]. Because the RD approach with the appropriate reactions satisfies these criteria, it can be used to calculate the critical exponents.

4.1.3 Calculation of critical exponents by means of the reaction-diffusion paradigm

As we have mentioned before, there exist two reactions which upon adjusting their reaction rates give a second order phase transition in the DP universality class, that are therefore usually referred to as just DP. These are the spontaneous decay $A \to 0$, with reaction rate μ, corresponding to a terminating bond sequence, and the branching $A \to A + A$, with rate σ corresponding to an infection or a vertex with two bonds in figure 5.

The two regimes, active and absorbing, between which there is a phase transition, correspond to the cases $\sigma > \mu$, where the branching process dominates, and $\mu > \sigma$, where the decay dominates and the dynamics eventually dies out without any possibility of reactivating, respectively. The final state in the absorbing state is an empty lattice, while the active state would result in an exponential runaway if we don't impose additional restrictions. There's two ways of going about this, a) introducing additional annihilation/coagulation reactions and b) implementing site occupancy restrictions in the sense of Wijland [16]. Let us first consider a).

4.1.4 Directed percolation with regulating annihilation/coagulation

Let us therefore impose additional reactions $A+A \to (0,\, A)$ with rates $(\lambda,\, \lambda')$ and allow ourselves a general mean-field description at first, valid in supercritical dimensions. The mean field rate equation is now, referring to 1:

$$\partial_t a\,(t) = (\sigma - \mu)\, a\,(t) - \left(2\lambda + \lambda'\right) a\,(t)^2 \tag{52}$$

The final density can be calculated by setting $\partial_t a$ to 0 and finding the solutions to the right hand side. $a = 0$ corresponds to the absorbing state, while

$$a_\infty = \frac{\sigma - \mu}{2\lambda + \lambda'} \tag{53}$$

corresponds to the active state (this would have been negative in the absorbing state with $\sigma < \mu$). This is rather similar to ordinary annihilation/coagulation encountered in the previous section with the additional linear term and we can generalize this to a local mean field rate equation with standard diffusion. Let $r = (\mu - \sigma)/D$

$$\partial_t a\,(\vec{x},\, t) = -D\left(r - \nabla^2\right) a\,(\vec{x},\, t) - \left(2\lambda + \lambda'\right) a\,(t)^2 \tag{54}$$

We are interested in the correlation length ξ, which near a critical point will depend on the diffusive part. Observing the dimensions of parameters appearing in it we infer $\xi \sim |r|^{-1/2}$ and the corresponding time scale is $t_c \sim \xi^2/D$. We then define the critical exponents in standard fashion[8]:

$$\begin{aligned} \langle a_\infty \rangle \quad &\sim \quad (-r)^\beta \quad (r < 0)\,, \qquad \langle a\,(t) \rangle \sim t^{-\alpha} \;\; (r = 0) \\ \xi \quad &\sim |r|^{-v} \quad (r \neq 0)\,, \qquad t_c \sim \xi^2/D \sim |r|^{-z\nu} \quad (r \neq 0) \end{aligned} \tag{55}$$

From the mean field equations we can already establish mean field exponent values. We just need to additionally consider the α exponent. At $r = 0$, equation 54 becomes the equation for standard annihilation/coagulation and we know its time dependence to be t^{-1} in supercritical dimensions. Therefore:

$$\beta = 1,\, \alpha = 1,\, \nu = 1/2,\, z = 2 \tag{56}$$

We then use the heuristic arguments stated below Eq. 12 to write down the (unshifted) action for the set of reactions $A \to A + A$ with rate σ, $A \to 0$ with rate μ and $A + A \to (A,\, 0)$ with rates $(\lambda,\, \lambda')$:

$$\begin{aligned} S\left[\phi, \phi^*\right] \;=\; & \int \mathrm{d}^d x \int \mathrm{d}t \left(\phi^* \left(\partial_t - \nabla^2\right) \phi\mu \left(1 - \phi^*\right) \phi + \sigma \left(1 - \phi^*\right) \phi^* \phi \right. \\ & \left. -\lambda \left(1 - \phi^{*2}\right) \phi^2 - \lambda' \left(1 - \phi^*\right) \phi^* \phi^2 \right) \end{aligned}$$

plus initial and final terms which we can neglect due to the rapid fluctuations [8]. The shifted action with $\phi^* \to \tilde{\phi} + 1$ is then

$$\begin{aligned} S\left[\phi,\, \tilde{\phi}\right] \;=\; & \int \mathrm{d}^d x \int \mathrm{d}t (\tilde{\phi} \left(\partial_t + D \left(r - \nabla^2\right)\right) \phi - \sigma \tilde{\phi}^2 \phi + \\ & + \left(2\lambda + \lambda'\right) \tilde{\phi} \phi^2 + \left(\lambda + \lambda'\right) \tilde{\phi}^2 \phi^2) \end{aligned} \tag{57}$$

This turns out to be overdetailed as some of the terms are relatively irrelevant under RG transformations. We can also notice that the scaling is not optimal. Following similar basic Fourier transformation, inversion and inverse transformation step as for the $A + A \to 0$ annihilation propagator we find the tree level propagator to be

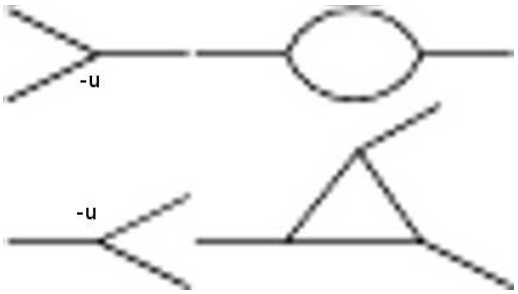

Figure 6: Left: vertices; Right: 1-loop diagrams of DP field theory. Taken from [8]

$$G_0\left(\vec{p},\,\omega\right)=\frac{1}{-i\omega+D\left(r+p^2\right)} \tag{58}$$

and its lowest loop order correction containing two three-point vertices, as shown in figure 6, one with coupling σ and one with coupling $2\lambda+\lambda'$. We would like both of these to scale equally under the RG transformations which would cause the one-loop propagator correction to scale equally (otherwise the scaling is complicated, not simply multiplicative). We can achieve this by choosing $\tilde{s}=\tilde{\phi}\sqrt{\left(2\lambda+\lambda'\right)/\sigma}$ and $s=\phi\sqrt{\sigma/\left(2\lambda+\lambda'\right)}$. The terms $-\sigma\tilde{\phi}^2\phi$ and $\left(2\lambda+\lambda'\right)\tilde{\phi}\phi^2$ then go into $u\left(s-\tilde{s}\right)\tilde{s}s$ while the $\left(\lambda+\lambda'\right)\tilde{\phi}^2\phi^2$ term remains in the form $\left(\lambda+\lambda'\right)\tilde{s}^2s^2$. $u=\sqrt{\sigma\left(2\lambda+\lambda'\right)}$ is the new effective coupling and it scales as $\kappa^{2-d/2}$. Similarly to the annihilation case we thus expect the critical dimension to be $d_c=4$. However we also find that the relative coupling, $\left(\lambda+\lambda'\right)/u$ scales as $\kappa^{-d/2}$ and becomes irrelevant under RG transformations, which means we can neglect the $\tilde{s}^2s^2$ terms altogether to obtain the final DP action.

$$S\left[s,\,\tilde{s}\right]=\int\mathrm{d}^dx\int\mathrm{d}t\,\left(\tilde{s}\left(\partial_t+D\left(r-\nabla^2\right)s-u\left(\tilde{s}-s\right)\tilde{s}s\right)\right) \tag{59}$$

This is also the action of the deprecated Reggeon field theory.

4.1.5 Van Wijland's occupancy restrictions

As we have said before we can also consider occupancy restrictions instead of additional coagulation/annihilation reactions. The beauty of DP lies in the fact that we obtain the same effective (sometimes called mesoscopic [8]) action. In numerical simulations occupancy restrictions are the simplest thing to implement, while they present a slightly more formidable challenge in the field-theoretical approach if we are not to clutter the action beyond recognition. One way of going about it is discarding the bosonic second-quantized framework we've been utilising throughout section 3 and implement fermionic annihilation and creation operators. Luckily there's a simple way in which we can retain the bosonic formalism, demonstrated by Van Wijland [16]. This was achieved by modifying the diffusion part of the quasi-Hamiltonian by including operator delta functions of the form $\delta_{\hat{a}_i^\dagger \hat{a}_i, n} |m\rangle = \delta_{m,n} |m\rangle$, representing the spatial exclusion due to the particles' hard-core potential. When passing to a coherent state representation, these have to be normal ordered, which is achieved by normal ordering its transformed form

$$\delta_{\hat{n},m} = \int_{-\pi}^{\pi} \frac{\mathrm{d}u}{2\pi} \mathrm{e}^{iu(\hat{n}-m)} \tag{60}$$

a considerable combinatorical exercise. For $m = 0, 1$ it turns out there are always exponentials left over which contribute to the action. In the case of processes $A \to (0,\, 2A)$, we obtain

$$S_{rest}\left[\phi,\, \tilde{\phi}\right] = \int \mathrm{d}^d x \int \mathrm{d}t \, \left(-\mu \left(1 - \tilde{\phi}\right) \phi \mathrm{e}^{-v\tilde{\phi}\phi} + \sigma \left(1 - \tilde{\phi}\right) \tilde{\phi}\phi \mathrm{e}^{-2v\tilde{\phi}\phi}\right) \tag{61}$$

omitting the diffusion part of the action. Originally, there are terms such as $\tilde{\phi}_i \phi_i$ present in the exponentials and v is a parameter that originates from taking the continuum limit. As $\tilde{\phi}_i \phi_i$ scales as κ^d, v thus scales as κ^{-d}, consequently goes to 0 after a couple of RG and this finally implies we can expand the exponential and retain only the first few

terms. By a suitable relabelling of coupling constants it turns out we recover the form of the effective Reggeon action 59.

This can be transformed into a Langevin equation of the form of the form

$$\partial_t s = D\left(\nabla^2 - r\right) s - us^2 + \eta \tag{62}$$

with a noise term η, $\langle\eta\rangle = 0$, $\langle\eta\left(\vec{x},\, t\right)\eta\left(\vec{x}',\, t'\right)\rangle = 2us\delta\left(\vec{x} - \vec{x}'\right)\delta\left(t - t'\right)$. This is a special case of a more general Langevin equation, namely

$$\partial_t s = D\left(\nabla^2 - R\left[s\right]\right) s + \eta, \qquad \left\langle\eta\left(\vec{x},\, t\right)\eta\left(\vec{x}',\, t'\right)\right\rangle = 2N\left[s\right] s\delta\left(\vec{x} - \vec{x}'\right)\delta\left(t - t'\right) \tag{63}$$

which represents the general Langevin equation for systems exhibiting active-absorbing phase transitions [19]. Thinking in terms of power expansions of $N\left[s\right]$ and $R\left[s\right]$ in powers of s, our case corresponds to the first few terms of each $N\left[s\right] = u + \ldots$ and $R\left[s\right] = r + us + \ldots$

4.1.6 Renormalisation

As said before we shall not go into the details of renormalisation here, only a qualitative account will be given. To one-loop order we can write down the loop integral which will consist of a product of two propagators of the type 58 with appropriate loop momenta and frequency such that they add up to the external momenta. Due to the diverging correlation length we the demand that $G\left(\vec{p} = 0,\, \omega = 0\right)$ diverges at the critical point, hence the trivial vertex function $\Gamma^{(1,1)}$, which can also be thought of as G^{-1}, must equal 0. We then invert the one-loop corrected G, demand that it equals 0 at $\vec{p},\, \omega = 0$ and hence obtain a constraint for the renormalised r_c of the critical point, which is easy

to solve to order $\mathcal{O}\left(u^2\right)$. We then introduce the true distance from the critical point, $r - r_c$ and rewrite the expression for a general $\Gamma^{(1,1)}\left(\vec{p}, \omega\right)$. We find three parameters need renormalising plus the field strength. We absorb all the UV divergences into their Z factors, which all contain appear as expansions of the quantity u^2/D^2 that we hence identify with the effective coupling with its renormalised dimensionless counterpart

$$v_R = Z_v v A_d \kappa^{d-4} \tag{64}$$

where A_d is a constant dependent on the dimensionality and $Z_v = Z_u^2/Z_D^2$, the latter being the multiplicative factors of u and D.

Now using dimensional analysis to exchange κ derivatives for derivatives with respect to the renormalised parameters D_R, τ_R and v_r, we can again write the Callan-Symanzik equation, analogous to 43, this time for the asymptotic density in the active phase and the propagator. For $d < d_c$ the β function yields a non-trivial fixed point $v_r^* = \epsilon/3 + \mathcal{O}\left(\epsilon^2\right)$. The upshot is that we can again obtain a scaling law in the vicinity of the fixed point, from which it is possible to infer the critical exponents 55 in terms of ϵ. To $\mathcal{O}\left(\epsilon\right)$ they turn out to be

$$\begin{aligned}
\beta &= 1 - \frac{\epsilon}{6} \\
\alpha &= 1 - \frac{\epsilon}{4} \\
v &= \frac{1}{2} + \frac{\epsilon}{16} \\
z &= 2 - \frac{\epsilon}{12}
\end{aligned}$$

As is standard with field-theoretic calculations, this firmly establishes universality, but does not converge or does so very poorly for physical dimensions $d = 1, 2, 3$ as $\epsilon = d_c - d = 4 - d$ is quite large there. It does however predict logarithmic corrections at

d_c [27, 28] and this agrees with the calculated values [29].

4.1.7 Further Applications

Most of these are epidemiological in nature, such as [30], that implements long-range time correlations, which can be interpreted as incubation times or [31] that implements immunisation. There has also been a lot of research into DP with several species. Upon introducing appropriate reactions coupling different species, one obtains multicriticality[32, 33], where species exhibit a hierarchy of phase transitions.

4.1.8 Branching and annihilating random walkers

I briefly present another curious set of reactions, that has attracted much attention, due to its defining yet another universality class. These are the so called branching and annihilating random walkers, the theory of which was largely established by Cardy and Täuber in [34] and [35]. These deal with similar equations, e.g. one has the branching process $A \to (m+1)\, A$ with rate σ and the annihilation process $kA \to 0$ with rate λ. In this case the mean field theory predicts only an active absorbing state, but $\sigma_c = 0$ can be thought of as a degenerate critical point, only approachable from one side, where the dynamics becomes that of ordinary annihilation. Due to the annihilation, one would expect the mean field discourse to be valid above $d_c = 2/(k-1)$, however this turns out to be false, as demonstrated by Monte-Carlo simulations [36].

Again using arguments from the end of section 3.1.2, we can arrive at an action for $k = 2$,

$$S\left[\phi, \tilde{\phi}\right] = \int \mathrm{d}^d x \int \mathrm{d}t \left(\tilde{\phi}\left(\partial_t - D\nabla^2\right)\phi + \left(1 - \tilde{\phi}^m\right)\tilde{\phi}\phi - \lambda\left(1 - \tilde{\phi}^2\right)\phi^2\right) \tag{65}$$

This gives a rich set of Feynman diagrams that must be renormalised but, more im-

portantly, also generate diagrams for all of the $A \to (m+1-l)\,A$ processes with small enough, even l. The renormalisation shifts are negative and proportional to to a combinatoric factor, which makes the branching process with the lowest number of products the most relevant. For odd m this is $A \to A + A$ and since the decay $A \to 0$ is also generated, we should expect this process to be in the DP universality class.

For m even things are drastically different as the parity of particle number is always conserved so the above processes cannot be generated. This process turns out to exhibit very interesting phase-space behaviour as it possesses an absorbing phase only below a certain inverted lower critical dimension, unlike with prototypical second-order phase transitions such as those of DP, where subcritical fluctuations prevent the phase transition from occurring [8].

4.2 Several-species reactions

While percolation, phase transitions, universality and the likes are all lively directions of intense research at the moment, with such diverse concepts as tricriticality and phase space topologies emerging [37, 38], one does not have to stray so considerably from the paradigm described in the previous section. A simple $A + B \to 0$ reaction already exhibits many effects not present in the original $A + A \to 0$ reaction, some of which have yet to receive appropriate analytic and numerical treatment. This is due to a conserved quantity, the difference of A and B reactant densities $a - b$, which can be thought of as a novel contribution to the zero-frequency Fourier mode, heavily influencing the late-time dynamics.

There seems to be a lack of consensus in the literature over what the critical dimension is. There are now two qualitative shifts in the asymptotic behaviour, one at $d = 2$, corresponding to the same shift we saw in the $A + A \to 0$ reaction, and a shift at $d = 4$ in the case of equal and homogeneous initial densities. I argue, along with [8], that

$d = 2$ should be regarded as the critical dimension, as the qualitative shift at $d = 4$ is also predicted by the mean field analysis. Let us proceed to describe these different asymptotic regimes.

4.2.1 Homogeneous initial conditions

Consider first the case when A and B particles are initially heavily and homogeneously mixed. In the unequal densities case suppose without loss of generality that $b_o > a_o$, where b_0 and a_0 are the initial densities of B and A particles, respectively. Then above $d = 2$ mean field equations yield the correct asymptotic behaviour of an exponential decay. The dynamics has been analysed by exact methods by Bramson and Lebowitz [39], who employed a continuous time technique on a lattice without occupation restrictions but with an infinite reaction rate so that particles annihilated immediately upon meeting at a site, and also by Blythe and Bray [40, 41]. These techniques can only provide rigorous upper and lower bonds, but in fortunate cases, such as these, they turn out to have an equal time dependence, which establishes the time dependence unambiguously. In the overlap of results from the above articles, the authors have obtained asymptotic exponents for all dimensionalities, which agree with mean field predictions for $d > d_c = 2$. The result is

$$a(t) \sim \begin{cases} \exp(-c_1 t) & d > d_c \\ \exp(-c_2 t/\ln t) & d = d_c \\ \exp\left(-c_3\sqrt{t}\right) & d < d_c \end{cases} \tag{66}$$

where the constants c_i haven't been determined. This is already qualitatively very different from the power-law decays of $A + A \to 0$.

In the case of equal densities these exact methods, along with [42], demonstrate that below $d = 4$, the asymptotic density is proportional to $t^{-d/4}$ and demonstrates *no*

transition at the critical dimension $d_c = 2$. For $d > 4$ the density goes as $\sim t^{-1}$.

This problem was first studied by Toussaint and Wilczek [43], who obtained the $t^{-d/4}$ result by assuming that in the initial equal densities case, only the fluctuations in the initial conditions are relevant to the final result and that after time t there will remain only particles that were initially dominant in all regions of linear scale up to the diffusion length, i.e. $\sim t^{1/2}$. This is also known as the segregation of particles. This assumption was later verified by Cardy and Lee's field-theoretical treatment of the equal initial densities case [44, 45]. Toussaint and Wilczek obtained the asymptotic result

$$a(t) \sim b(t) \sim \frac{\sqrt{n_0}}{\sqrt{\pi}\,(8\pi D t)^{d/4}} \tag{67}$$

The transition at $d = 4$ is best imagined in the way that both the $t^{-d/4}$ decay and the t^{-1} decay modes are present and that at late times the slower of the two dominates. Below $d = 4$, the former is slower, while for $d > 4$, the latter is.

The field theoretical machinery is very similar to the one used for the $A+A \to 0$ reaction. As can be read from the action, the reaction rate parameter λ still scales as κ^{2-d}, so $d_c = 2$. In fact the renormalisation of the diagrams is completely equivalent to the one encountered in the single-species case. The propagators cannot get renormalised as there are no branching diagrams and the renormalisation of a vertex is the same as shown in figure 4 just that one branch of each loop belongs to an A particle propagator and the other one to a B particle propagator. We also obtain the same results for the time dependence of the effective reaction rate due to the RG flow towards the fixed point for $d < d_c = 2$, $\lambda(t) \sim t^{-1+d/2}$ and $\lambda(t) \sim 1/\ln t$ for $d = d_c$. Plugging this into the tree-level, i.e. mean field expression for the densities yields exactly the results 66.

There have been many field-theoretical investigations into the problem, yet nobody has performed a full RG field-theoretical analysis of the case of unequal initial densities yet [8]. For equal densities, Cardy's and Lee's [44, 45] approach remains the norm.

They have constructed an effective theory that takes into account randomly generated "surface terms" that reflect the fluctuations in the initial state. However this is of little use below d_c, as the sum over initial terms has to be performed unperturbatively.[9]

In the analyses [40, 41], the terminology used often refers to A particles as diffusing through a sea of mobile traps, represented by B particles, much in the spirit of earlier investigations of particles diffusing through a sea of fixed randomly placed traps [47, 48]. This might have inspired investigations into the asymptotic decay properties of subdiffusive A particles in a sea of diffusive B traps, diffusive A particles in a sea of superdiffusive B traps and all such combinations. The case of superdiffusive motion will be covered to a certain extent in section 4.4, where we consider Lévy flights. In short, sub- or superdiffusive motion is characterised by the mean value of the particle displacement's squared increasing slower or faster than in ordinary diffusion, i.e $\langle l^2 \rangle \sim t$, respectively. We will instead have $\langle l^2 \rangle \sim t^\alpha$ with $\alpha < 1$ for subdiffusive and $\alpha > 1$ for superdiffusive motion. A variety of modified ensues. For example, the authors of [49] considered a diffusive particle propagating in the presence of subdiffusive traps with $\langle l^2 \rangle \sim t^\gamma$ and have found that for $\gamma \leq 2/(d+2)$ the asymptotic properties are exactly equal to those of fixed traps, $a(t) \sim \exp\left(-ct^{2/(d+2)}\right)$, similarly [50], while [51] have further classified the subdiffusive regimes with different values of γ, γ' of particles and traps.

There has also been work on a generalisation of the simple two particle reaction, that is $mA + nB \to 0$. The authors of [52] have found a $t^{-d/4}$ decay for $d < 4/(m+n-1)$, while Kwon et al. [53] have studied the case of driven particles with the restriction of hard-core repulsion, which in one dimension implies that particles cannot switch places, and found that densities decay as $t^{-(n+m)}$ in contrast to the predictions of any mean field model.

[9] Given the increasing amount of work on nonperturbative renormalisation group techniques, see e.g. [46], this might eventually become possible.

Let us also mention the case where the particles are diffusing amidst a shear flow, that is in a parallel velocity field where the magnitude of velocity is increasing in a direction transverse to the direction of the velocity itself, such as $\vec{v} = v_0 y \vec{x}$. The shear flow serves to mix the reactants better, which is a regime in which the original arguments by Toussaint and Wilczek, about asymptotic segregation, are particularly strong. This was studied in [54] in a field-theoretic setting, where the shear flow contributed terms of the form $\tilde{a} v_0 y \partial_x a$ and similarly for b to the action, serving to modify the propagator. It was established that for $t \ll t_c = v_0^{-1}$, the scaling is the same as without the shear flow, i.e. $\sim t^{-d/4}$, while at $t \gg t_c$ the densities scale as $t^{-(d+2)/4}$.

4.2.2 Heterogeneous initial conditions and other generalizations

There have also been studies where the A and B particles are initially segregated, separated by either a hyperplane [55] or a hyper-spherical boundary [56]. Let us first consider the former case. Here each half-space separates into three different regions: the reaction region of width ωat the interface where actual reactions are taking place, the depletion region of width υ besides the reaction region where there is a diminished density of particles, and the remaining half-space, where the density is still essentially equal to the initial density. It was calculated by [55] in the local mean field approximation that the reaction region grows as $\omega \sim t^{1/6}$, the depletion region as $\upsilon \sim t^{1/2}$ and the particle densities in the reaction region decay as $t^{-1/3}$.

We can also study cases where particles are flowing towards each other with currents of equal size J and opposite direction. The authors of [57] found that at long times the width of the reaction region scales as $\omega \sim J^{-1/3}$ and the reaction zone densities scale as $J^{2/3}$, still in mean field. There is a neat translation between the two systems since we can think of particles obtaining a velocity while traversing the depleted region in the first case. The particle current will then roughly equal $J \sim -\nabla a \approx -a_0/\upsilon \sim t^{-1/2}$, giving us a dictionary between the two cases.

A field-theoretic approach was then developed in [58] and in [59], the latter also generalizing it to $mA + nB \to 0$. RG methods yielded that for the case $d \leq 2$ the asymptotic behaviour is independent of the reaction rate, which gave credence to the above scaling results. Cardy and Lee [60]_also noticed that one can study reaction fronts arising from the asymptotic segregation in the case of equal initial densities and demonstrated that the width of the reaction zones becomes comparable with the width of the depletion zones as one approached $d \to 4$ from below, corresponding to the breakdown of segregation.

The case of the spherical boundary was covered in great detail by Shipilevsky [56, 61, 62, 63]. The results are too numerous and detailed to list here, but as an example, in [56] he demonstrated that at large enough numbers of A particles comprising an island in the B sea, a universal scenario arises: $\sim 4/5$ of the A particles are annihilated during the island's growth and the remaining $\sim 1/5$ during its collapse.

There has even been an investigation into the properties of reaction fronts in several scenarios with particles' diffusivity dependent on densities [64]. Altered asymptotic scaling exponents were obtained.

There have also been investigations into reactions with more than two species, that are too abundant to attempt to describe in detail in this dissertation. Let us just mention the directions of research. One can be interested in the asymptotic decay exponents and segregation properties of multi-species annihilation generalisations of the two species case, i.e. $A_i + A_j \to 0$ for $i, j = 0, 1, \ldots, q$, $i \neq j$, as in [65]. Another promising line of research are models of "vicious random walkers", where we have diffusing particles annihilating upon contact and we are interested in the probability of no annihilations having occurred yet, as in [66]. This line of research also overlaps with tackling difficult existential issues, such as those of [67].

4.3 Reaction-diffusion on complex networks

4.3.1 Brief introduction to complex networks[10]

Complex networks as a research field could be summarized as a physics-influenced approach on an ancient mathematical field, graph theory. It deals with sets of abstract point, not living in any imaginable metric or topological space, though they can be embedded in one if necessary, connected by edges. We will mostly be concerned with simple graphs, i.e. such that there can be at most one edge between any two vertices and such that no vertex can have an edge with itself. They will also be undirected, so that each edge can be traversed both ways. Another property that will mostly hold is that the graphs are sparse, i.e. that the number of edges E is of the same order of magnitude as the number of vertices N. The edges can carry additional properties, "weights". When we identify the points of the abstract graph with actual entities, these can represent distances between actual points in space, the number of minutes two individuals spent on the phone, etc. We can summarize the edges present with an adjacency matrix A_{ij}, whose fields are generated by

$$A_{ij} = \begin{cases} 1 & \text{points } i\text{and } j\text{are connected} \\ 0 & \text{points } i\text{and } j\text{are not connected} \end{cases} \tag{68}$$

If the edges are weighted, the weights are to be put in place of the 1's. Since we're dealing with undirected graphs A_{ij} is symmetric.

Two prototypical types of networks are important for the elucidation of the basic concepts we will be dealing with. The first is the regular d-dimensional lattice, which we can imagine as points on a hypercubic lattice embedded in a d-dimensional Euclidean space. The second is the random graph. There are actually many types of those, but consider

[10]This style of exposition of this section and the technical data is primarily based on [68].

first the homogeneous Erdős-Rényi type. This is generated by starting with a set of abstract points and then generating edges between them probabilistically - each possible edge has a probability p of being generated. In order to ensure the sparsity of the graph, p has to be of order $p \sim N/\frac{N(N+1)}{2} \sim 1/N$, where $\frac{N(N+1)}{2}$ is the number of all possible edges. In order to properly speak about random networks, we must in fact consider either an infinite network of this type or an ensemble of networks, otherwise we just get a specific network. But for real life purposes, classifying graphs as "random" when they posses properties of a typical representative of such ensembles will be completely adequate. We shall now describe these properties.

The most important differences between lattices and random networks arise when we study their *local structure* and *size*. We say that a network has a lot of local structure if for many points of the graph it holds true that neighbours of that point are themselves neighbours, e.g. on social networks a lot of friends of a given person often tend to be friends amongst each other as well. The actual quantitative measure of local structure can be defined in several ways [69], but a prototypical measure is a clustering coefficient at a point which is defined as follows: take the subnetwork composed of all the points connected to the given point but not the point itself. Then divide the number of edges in this subnetwork with the number of all possible edges.

A lattice has a lot of local structure, as is evident from any basic visualisation of it. Yet it requires a slight generalization of the clustering coefficient, as the simple definition from the previous paragraph return a misleading value of 0. The new definition considers the subnetwork generated by taking neighbours of neighbours except the original point instead of just neighbours. A random network, on the other hand, has a very small probability that neighbours of neighbours will be connected, essentially still the original p as nothing guarantees the closeness in any metric sense of two connected points.

For the other property, the size of the network, to be defined in a sensible manner, we must first ensure, that the network is connected, that is, following the edges of the graph

we can reach each point from each other point of the network. The lattice is clearly such, although we could have taken an infinite lattice and then the number of steps would not be finite, but to avoid such technicalities let us consider a periodic lattice, where the connectedness obviously holds. Random graphs, on the other hand, are not necessarily connected, but it has been shown by Erdős and Rényi[70] that there is an analogue of a phase transition above a certain threshold probability $p = N \ln(N)/2$ where the the network is very likely to be connected, not unlike in the description of directed percolation above.

With this interesting, but for our purposes irrelevant, technical result out of the way, let's proceed to define the size of the network. Again, several measures are in use [69]. Consider the measure of average shortest distance, in which the length of the shortest path for each pair of points is calculated, using e.g. Dijkstra's algorithm [71], and their arithmetic mean taken.

It turns out that lattices have large graph sizes that scale with the number of points roughly as $\sim N^{1/d}$. Random graphs turn out to be smaller, scaling only as $\ln N$[11]. If we tried embedding them in a metric space, regardless of the inappropriateness of such demeanor, we would have found that our space is riddled with wormholes connecting distant points. Thus the distance we need to travel on average is much shorter than in a more causality-friendly lattice.

There are also intermediate types of networks that traditional graph theory has not studied extensively but that became a central interest with the advent of the network perspective. These have a lot of local structure and yet their size is relatively small. Such networks are important as they represent a lot of real-life networks, though not necessarily in traditional areas of physics. Prime and by now thoroughly washed up

[11] It is interesting to sloppily interpret this result in the following way: random graphs are essentially dimensionless, but perhaps a more accurate statement would be, that they are analogous to an infinite-dimensional metric space. Rewrite $N^{1/d} = \left(\mathrm{e}^{\ln N}\right)^{1/d} = \mathrm{e}^{\frac{1}{d}\ln N}$. Since $d \to \infty$, $\frac{1}{d}\ln N \to 0$ for any N, we can expand the exponential to obtain $N^{1/d} \approx 1 + \frac{1}{d}\ln N \sim \ln N$.

examples include human social networks and the Internet, though there are also lesser known examples of protein networks and other subfields of biology. [72]. The prototypical way of constructing a random graph has been demonstrated by Watts and Strogatz [73], who considered a sort of double leveled lattice, where each point is connected to its ordinary lattice neighbours and the ordinary lattice neighbours of these. One then randomly rewires these edges to obtain a small world network.

But the most relevant type of network for reaction-diffusion systems is the so called-scale free network. The most important piece of introductory theoretical machinery of complex networks we will need is the *degree distribution* of a network. In a random graph different points will in general have different numbers of neighbours or edges emanating from them, called the *degree* of the vertex. The degree distribution is a map between natural numbers and the proportion of vertices in our network of this degree. Viewed as a property of the entire ensemble of random networks this becomes a probability distribution. An Erdős-Rényi graph will have a binomial, or in the limit of large N, Poissonian distribution:

$$n\left(k\right) = \mathrm{e}^{-\mu}\frac{\mu^{k}}{k!} \tag{69}$$

Here n is the probability mass function of the distribution itself, k is the degree and μ is the average degree. Due to the exponential fall off we can identify a largest value for which it is extremely unlikely that we will find a vertex with a higher degree in our network.

It has been found that the efficient solutions of many network-based problems require the existence of *hubs*, vertices with a much greater degree than average. Again, the world wide web is certainly such an example. This requires a heavy-tailed degree distribution, for which we can identify two characteristic values: the degree after which points of this degree will occur very rarely and the degree, after which there will be no more

such points. This is most simply realised through a power-law degree distribution, $n(k) \sim k^{-\gamma}$, with γ typically in the range $2 < \gamma < 3$ [74]. These graphs are also called scale free because they have no characteristic degree to distinguish them, also visible from the fact that ratios such as $n(2k)/n(k)$ are independent of k.

This however does not immediately imply that the networks will actually be invariant under a network analogy of renormalisation. This can be defined as grouping nearby vertices together, with their closeness described by an appropriate network measure, and taking the groups as vertices of a new graph. A lot of realistic networks are both scale-free (in the sense of a power law degree distribution) and small-world. Since the number of nodes increases exponentially with the size of a small-world network, such networks were thought to not exhibit self-similarity, as one would naively expect a power law relation in that case. It has been shown in [72] that self-similarity is nevertheless the case for many realistic networks. Such networks are often called *fractal* to distinguish them from the broader class of scale-free networks that have an underlying power law degree distribution but are not necessarily self similar. An important qualitative feature of such networks is that their hubs repel each other on all length scales, so that they end up being very dispersed[75]. Several synthetic scale-free networks, such as the example by Albert and Barabási [76], are not fractal [77].

It would also be convenient if while studying realistic weighted networks we would not always have to insert weights of edges by hand but rather would find a network-wide rule or relation that would connect them with other local and global properties of the graph. This has also been achieved, via the so-called *weight parameter θ,* through which the weight w_{ij} of an edge (inserted into the matrix A_{ij}, w_{ij} is just a temporary denotation) is defined as $w_{ij} = (k_i k_j)^{\theta}$, where k_i and k_j are the degrees of the adjoining vertices.[78] This is seen to hold true for classes of real-life networks.

4.3.2 Diffusion on complex networks

In section 3 before we took the continuum limit, our theory was defined on a regular hypercubic lattice. We can generalise this lattice to a complex network, but the rules for particle hopping between sites, i.e. diffusion, may now become local. Also it becomes obvious that it will become difficult to define continuous limits in most cases, except for those, where the vertices and edges are a subset of a triangulation of a topological space, and even then we are not obliged to think of it that way.

An important concept for defining diffusion is the Laplacian. In d-dimensional Euclidean space it is denoted by a squared nabla operator and denotes $\nabla^2 = \sum \frac{\partial^2}{\partial^2 \xi_i}$, where ξ_i are the labels of coordinates associated with a standard orthonormal Euclidean basis, $i = 1, \ldots, d$. The Laplacian is present in the ordinary continuous diffusion action term $\tilde{\phi}\left(\partial_t - D\nabla^2\right)\phi$ and it gets there through an integral by parts of the term $\nabla\tilde{\phi}\nabla\phi$, which in turn gets there through substituting a's and $a^\dagger$'s in the Hamiltonian and taking the continuum limit. Its origin is thus the diffusion term in the quasi-Hamiltonian, $H_{diff} = \mu \sum \left(a_i^\dagger - a_j^\dagger\right)(a_i - a_j)$. We could have already performed a discrete analogue of integration by parts, summation by parts, if you will, before taking the continuum limit. This is exactly what we will need for complex networks, as we most certainly will not introduce this limit. Let us thus delve deeper into this mathematical trick. If we have a 1-dimensional sequence x_i and we recursively define it's n'th difference as Δ^n (not to be confused with the Laplacian) as: $\Delta x_i = \Delta^1 x_i = x_{i+1} - x_i$ and $\Delta^{n+1} x_i = (\Delta^n x_{i+1} - \Delta^n x_i)$ then we have

$$\sum_i \Delta x_i \Delta y_i = \text{boundary terms} - \sum_i x_i \Delta^2 y_i \tag{70}$$

This is achieved by splitting the summation in half where each term gets its own factor of x, shifting the summation indices in the x_{i+1} term to change it to x_i and then bringing the two terms terms back together with the second difference of y_i appearing besides x_i.

This can be generalised to higher differences. The second difference is closely related to the Laplacian, denote it L, and so we shall argue that performing a similar trick in higher-dimensional analogues should yield the Laplacian. In equation form this means a sum over neighbours should yield $\sum \left(a_i^\dagger - a_j^\dagger\right)(a_i - a_j) \sim -\sum a_i^\dagger L_{ij} a_j$. Let us therefore try to implement this trick in the case of networks and see what we obtain. Let us drop the constant μ in the following derivation. Begin by noticing that

$$H_{diff} = \sum_{\langle ij \rangle} \left(a_i^\dagger - a_j^\dagger\right)(a_i - a_j) \tag{71}$$

where $\langle ij \rangle$ denote connected pairs can be rewritten more concretely with the adjacency matrix

$$\sum_{i,\,j} \left(a_i^\dagger - a_j^\dagger\right)(a_i - a_j)\, A_{ij} \tag{72}$$

This makes sense in the unweighted case, as it is simply 0 if the pair is not connected and 1 otherwise. In the connected case we can take this as part of the definition of the Laplacian. We now split the summation

$$H_{diff} = \sum_{i,\,j} a_i^\dagger (a_i - a_j)\, A_{ij} - \sum_{i,\,j} a_j^\dagger (a_i - a_j)\, A_{ij} \tag{73}$$

In the second term we switch the summation indices and take into account the undirectedness of the graph $A_{ij} = A_{ji}$ and get

$$\begin{aligned} H_{diff} &= \sum_{i,\,j} a_i^\dagger (a_i - a_j)\, A_{ij} - \sum_{i,\,j} a_i^\dagger (a_j - a_i)\, A_{ij} \\ &= 2\sum_{i,\,j} a_i^\dagger (a_i - a_j)\, A_{ij} = 2\sum_{i,\,j} a_i^\dagger a_i A_{ij} - 2\sum_{i,\,j} a_i^\dagger a_j A_{ij} \end{aligned}$$

In the first term of the last equation we could perform the summation over j and so obtain the degree of the i-th vertex k_i or, in cases of weighted graphs, the so called strength of the vertex s_i. But we want to retain the sum over all indices so substitute A_{ij} with $k_i\delta_{ij}$ where δ_{ij} is the usual Kronecker delta. We now have

$$H_{diff} = 2\sum_{i,\,j} a_i^\dagger a_i k_i \delta_{ij} - 2\sum_{i,\,j} a_i^\dagger a_j A_{ij} \tag{74}$$

and we can change an arbitrary number of i's into j's in the first term due to the delta enforcing equality. In order to obtain an expression of a relevant form change it to $\sum a_i^\dagger a_j k_j \delta_{ij}$. We can add the terms to get

$$H_{diff} = -2\sum_{i,\,j} a_i^\dagger \left(A_{ij} - \delta_{ij}k_i\right) a_j \tag{75}$$

We hence infer $L_{ij} = 2\left(A_{ij} - \delta_{ij}k_i\right)$. The factor of 2 is usually dropped [79] and in the case of weighted graphs we have $k_i \to s_i$.

To further strengthen the appropriateness of calling this quantity the Laplacian, let us consider a 1-dimensional lattice in ordinary Euclidean space with evenly spaced vertices. Suppose the n-th vertex has temperature T_n and we are trying to solve the diffusion equation in discrete time. Then in a single step we have $\Delta T_n = \Delta Q_n/C = \left(P_n - P_{n+1}\right)\Delta t/C$. But we also know that the heat current is proportional to the gradient of temperature $P_n = a\left(T_n - T_{n+1}\right)$. Tweaking the indices a bit and absorbing all the constants into D we obtain $\Delta T_n/\Delta t = D\left(T_{n+1} + T_{n-1} - 2T_n\right)$. We can think of the lattice as a network now and fill its adjacency matrix with $A_{i,i+1} = 1$ for all i where-from it automatically also holds that $A_{i-1,i} = 1$. All other entries are 0. All vertices have degree $k = 2$. We can thus write our previous result as $\Delta T_n/\Delta t = D\left(A_{nm} - \delta_{nm}k\right)T_m = DL_{nm}T_m$. In the continuous case the diffusion equation is $\frac{\partial T}{\partial t} = D\nabla^2 T$. We hence see that the matrix L_{ij} corresponds to the Laplacian in this case.

The spatial analogy should not be taken too far, as it would become rather unaesthetic if we had a weighted graph with lengths in Euclidean space as its weights (it might work if they were inverse weights, but that's not how one would usually think about them). We are best advised not to approach such problems with complex networks, as better tools are at hand, such as the field-theoretical approach in ordinary Euclidean space developed in the rest of this dissertation.. However, we are free to invent a new generalised type of diffusion that does not obey Euclidean space logic and interprets weights in its own way if they are present. After all, we can easily talk about an Internet search robot "diffusing" through the Internet even though it has very little to do with ordinary spatial diffusion.

4.3.3 Reaction-diffusion processes on complex networks

Since this is a relatively new field in which results are still being debated and where they are constantly being updated, I will take the historical perspective in describing its developments.

Reaction-diffusion systems on a complex network, in particular a scale-free network, was first studied by Gallos and Argyrakis [80], although studies of the geometric properties of the spatial distribution of leftover particles in the $A+B \to 0$ reaction, that also described the behaviour of the reactants on a fractal substrate [81] and a related article [82] might be considered predecessors. Gallos and Argyrakis discovered through numerical simulations that particle densities for the reactions $A+A \to 0$ and $A+B \to 0$ on complex networks decay with an exponent $t^{-\alpha}$, where $\alpha > 1$, therefore faster than in ordinary space. It was argued that this is due to the segregation of particles not occurring. Instead, clusters of reactants form around the hubs of the network.

Catanzaro et al. [83] then devised a systematic approach to mean-field calculations on through the consideration of the $A + A \to 0$ process on uncorrelated complex networks.

Uncorrelated here means that in the underlying network ensemble of the random graph, the degrees of different vertices are not correlated, i.e. are independent random variables. They consider both homogeneous networks where they recover the Euclidean result, $a \sim t^{-1}$, while in the case of scale-free graphs the result is shown to depend on the degree distribution. Using exact manipulation of the probability mass function, the asymptotic form of the density of an *infinite* network is shown to have the form $a \sim t^{-\alpha(\gamma)} (\ln t)^{-\beta(\gamma)}$, where α and β satisfy:

$$\begin{aligned} \alpha(\gamma) &= \begin{cases} 1/(\gamma - 2) & 2 < \gamma < 3 \\ 1 & \gamma \geq 3 \end{cases} \\ \beta(\gamma) &= \begin{cases} 0 & 2 < \gamma < 3 \\ 1 & \gamma = 3 \\ 0 & \gamma > 3 \end{cases} \end{aligned} \tag{76}$$

where γ is the exponent of the degree distribution $n \sim k^{-\gamma}$. They also consider finite-size effects and show that due to them, asymptotically the result will be that of a homogeneous network, i.e. $a \sim t^{-1}$ with an amplitude proportional to $N^{3-\gamma}$, where N is the number of points. This is the mean field behaviour, and supposedly it *always* arises in finite scale-free networks. This seems to shed bad light on the prospects of using the Doi-Peliti formalism on complex networks. There are a few remedies, though. First that it does not seem to be entirely true [84] and second, that there are still infinite graphs. We did not deal with bounding our Euclidean space either.

This was followed up by [85] in their study on the $A + B \to 0$ reaction, where they demonstrated that for any set of annihilating species, the asymptotic decays on scale-free networks are independent of each other and with the same α exponent as established

in [83]. In [86] the authors then argued that the properties of complex networks imply that a large amount of pattern formation, which in the $A + B \rightarrow 0$ reaction would correspond to segregation, can increase the rate of reaction in stark contradiction to the regular Euclidean case. They illustrated this on the case of evolving species under competing evolutionary pressures, nicely exemplifying the main area where these results are applied, mathematical biology.

So far only fermionic interactions had been covered. Baronchelli et al.[87] developed a bosonic formalism. They found that using either the bosonic or fermionic formalism hasn't been does not alter the time evolution and critical properties of single-species reactions, but that it does, perhaps surprisingly, shift the distribution of particles over classes of vertices with a given degree.

Yun, Kahng and Kim [88] argued that if the network is not a synthetic random scale-free graph but rather a proper fractal network, the exponents 76, implied by [85] to be the same for $A + B \rightarrow 0$, are incorrect. Rather one should take the result implied by [81, 82] into account, which states:

$$a \sim t^{d/d_s} \tag{77}$$

where d_s is the spectral dimension of the fractal structure, related to the fractal dimension and random walk dimension, which both have rigorous definitions. For fractal scale-free networks with $n \sim k^{-\gamma}$, the spectral dimensions are [80, 88]:

$$d_s = \begin{cases} \frac{2(\gamma-1)}{2\gamma-3} & 2 < \gamma < 3 \\ 4/3 & \gamma > 3 \end{cases} \tag{78}$$

For non-fractal scale-free networks previous results still apply.

Kwon, Choi and Kim extended the analysis to weighted scalefree networks in the sense

described at the end of section 4.3.1. They established that the processes $A + A \to 0$ are again identical in the thermodynamic limit and that there are three independent regimes, identified by two crossover values of the network parameter θ in which the density decays with different exponents or exponentially. They also show that the kinetics of a weighted scale free network can be mapped onto an unweighted scale free network with $\gamma' = (\theta + \gamma) / (\theta + 1)$, an important result for our preceding discussion of diffusion; the weights don't really matter as we can always find a map to an unweighted network. That is however proven only for "naturally" weighted networks with a parameter θ.

The authors of [89] opposed previous claims that segregation, whatever its effects may be, is caused by the fractal structure of the network and that the diffusion-annihilation processes dynamics are fully determined by the weight and degree distribution and that the knowledge of further details is unnecessary, by providing a counterexample to both. There has also been a very basic study of percolation [90] on complex networks.

It is perhaps somewhat discouraging that I haven't been able to come across a single paper that would apply the Doi-Peliti formalism, or attempt demonstrating its incompatibility with complex networks, although many of them seem to be on the way. As we've seen, having local diffusion rules governed by weights in the adjacency matrix should not be a problem, as we can map the dynamics to an unweighted network, at least for the natural weights. It would however be nice to take a continuum limit. It is hard to see how this would work right now, as the dimensionality is effectively different in the vicinity of each point, but perhaps there could be a way to obtain a coarse grained action in a fractally-dimensioned space. In that case one could also make sense of epsilon expansions for non-physical dimensions and additionally study many regimes where ϵ is genuinely small. But of course it might not be possible. The investigation of diffusion on networks is however fascinating in itself.

4.4 Lévy flights

While field-theoretical techniques are very suited to demonstrating universality and to certain specific problems, it is more than obvious that numerical results are not its strong point._The ϵ expansions, that are usually the final output of RG calculations in RD processes, often behave extremely badly. In the critical dimension they are replaced by logarithmic corrections to exponents and amplitudes, whereas there are usually very few physical (e.g. integer) dimensions below the critical dimension. The critical dimensions of most simple systems are 2 or less, due to the aforementioned reentrance properties of random walks in different dimensions. If $d_c = 2$, the highest dimension, besides the critical, *in principle* accessible to our calculations is 1, but ϵ there equals 1, so the series converges very poorly. In fact we can only thank Nature that she provided us with the occasional series whose radius of convergence is ≥ 1 so that we can sum it up at all. A question arises: Can we calculate any results in $d = 1$ efficiently using the Doi-Peliti formalism? We could if there was either a system whose critical dimension, that need not be integer, was slightly above 1, s.t. that the ϵ parameter in which we performed our expansion would actually be small and the resulting series would converge. But traditional diffusion limited systems don't seem to be of that type. For example, in $kA \to lA$ reactions we have $d_c = 2/(k-1)$ which equals $d_c = 2,\ 1,\ 2/3,\ 1/2,\ \ldots$ for $k = 2,\ 3,\ 4,\ 5,\ \ldots$ respectively. After $d_c = 1$ for $k = 3$, which again isn't analysed in terms of an ϵ expansion, as $\epsilon = 0$, all critical dimensions are smaller than 1 and we can only calculate universal quantities in $d = 0$._This is not entirely useless, as there exist non-trivial problems in 0 dimensions [91], but we would usually like to do more. For DP and other processes we can get higher critical dimensions, but they are still mostly integer and hence subject to these same problems.

There are however systems where we can tune the critical dimension._These are systems characterised by the so called Lévy flights, which are analogous to Brownian motion,

i.e. ordinary random walk diffusion, but are discontinuous. As Brownian motion is associated with a Wiener stochastic process, so Lévy flights have an underlying Lévy stochastic process. To sketch the differences between the two, consider a discrete time Lévy process in order to prevent unnecessary excursions into rigorous stochastic calculus, càdlàg function spaces, etc. Then the main difference is that in Lévy diffusion, the distribution of jump lengths in a single time step has a much fatter tail than in the corresponding Brownian case. We usually consider a power law tail. This can remind one of scale-free networks discussed in the previous section and indeed, the similar effects have been acknowledged by [83]. We choose a power law with tails heavy enough so that the second moment of the jump length diverges. In general we will thus have a much more thouroughly mixed system than in standard diffusion. Lévy processes are ubiquitous in physical, biological and even financial systems. For a list of phenomena where an understanding of Lévy statistics is indispensable and a comprehensive introduction to the mathematical theory, see [92]. Even when we let the time-step go towards zero, i.e. we take a continuum limit, the discontinuities remain. In mesoscopic systems such as the ones considered in this dissertation, we can take the discontinuities to be unphysical and only effective. The lack of reality makes this point somewhat more subtle in quantum phenomena, but we fortunately don't have to deal with it here.

For our purposes a qualitative exposition based on [94] will suffice: the probability of jumping a length l is proportional to $P \propto l^{-d-\sigma}$, where $\sigma < 2$ characterises the Lévy power law. Due to additional terms in the Langevin equation and/or the diffusion sector of the master equation, the propagator becomes $G_0(\vec{p}, \omega) = (-i\omega + Dp^\sigma)^{-1}$. Since $i\omega \sim t^{-1}$ and Dp^σ appear in a sum, meaning they must have the same dimensions and hence scaling properties, we see that if $p \sim \kappa$, time intervals scales as $t \sim \kappa^{-\sigma}$. Invoking the arguments of dimensionless action again, like in section 3.4, we can read off the dimensions of coupling constants from the Lagrangian. We obtain $[\lambda] = \kappa^{\sigma-d}$, and by considering the relevance of the interaction under RG flow, this immediately implies

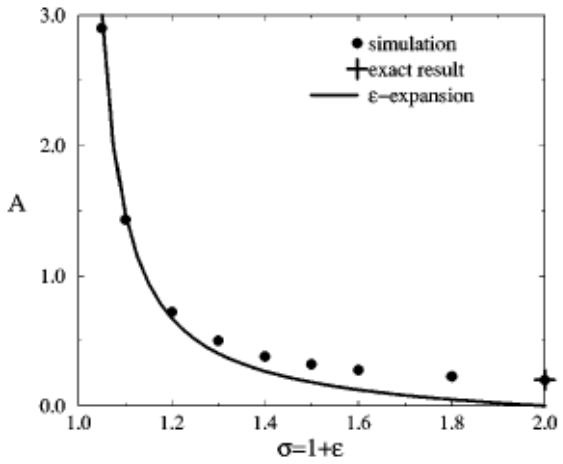

Figure 7: The comparison between a numerical simulation of standard diffusion and the value of an analytic ϵ expansion for a Lévy flight with σ slightly above 1 with the remaining parameters equal. The agreement is approximate at best. Taken from [93].

$d_c = \sigma$. Thus if we are interested in the behaviour in one dimension, we can study the process with anomalous diffusion characterised by a σ slightly larger than 1 and obtain a quickly converging ϵ expansion. This of course is by no means the same process as ordinary diffusion and there is a considerable amount of discrepancy between the two, as is shown in figure 7. Yet it is at least of the same order and potentially smaller as the discrepancy in a usual ϵ expansion with $\epsilon \sim 1$ as in [95]. Additionally, had we tried analysing a process that can actually be described by σ slightly larger than one, there would obviously be no discrepancy, but that partly depends on luck.

The performance of utilising Lévy processes to aid ϵ convergence is described in [93] on the example of a $A + A \to (0, A)$ reaction, finding the performance favourable. These methods have then been used to study the $A + A \to 0$ annihilation with quenched disorder in [96]. Whereas quenched disorder (random irregularities frozen into the lattice) tends to drive a reaction into the sub-diffusive regime (i.e. diffusion playing a smaller

part, which typically leads to an increased overall reaction rate), Lévy flights are superdiffusive. The overall effect of the interplay still depends on the parameters of the disorder and Lévy statistics. The mechanism was also proposed as a viable model of turbulent fluid transport, further acknowledged in [97]. There have also been investigations into vicious walkers, as briefly exposed in section 4.2.2, obeying Lévy statistics [98], indicating that walkers with smaller σ, i.e. longer average jump lengths, have a greater survival probability.

There are also many results on Lévy flights generalisations of processes in the DP class. Hinrichsen and Howard [94] calculated the variation of some of the critical exponents with σ. Olla has recently applied this to study a demographic model [99] and identified the regimes where the model is equivalent to a set of Brownian walkers and other demographic models.

4.5 Other applications

There are many areas of research besides the ones listed that I did not have time or space to go into. For example there is the work on persistence by John Cardy [100], which again beautifully employs an operator delta function, much like Wijland did in his hard-core repulsion paper [16], which through the retainment of additional terms in the coherent state integral step leads to an elegant expression for the probability that a particle hasn't visited a particular site yet.. There are numerous studies of the effects of different types of disorder [101, 102, 103, 104] and there is the Pair Contact Process with diffusion. The latter consists of the reactions $A + A \to (0,\, A)$ and $A + A \to (n + 2)\, A$, which qualitatively differs from BARW in that they don't include any processes involving a single reactant. It is an active research area as the renormalizable action of the model diverges under RG flow and because it's universality class is not fully understood yet [8].

5 Conclusion

I have presented a general survey of the area of reaction-diffusion systems with an emphasis on field-theoretical techniques. These are fascinating in themselves from several perspectives, from the elegance of the coherent state path integral representation to the continuous wonder at how a tool with such shaky mathematical foundations manages to predict facts about the world so well. This might be more of a point in *quantum* field theory, as non-equilibrium physics is experimentally not quite on its level yet and is therefore still struggling with more approximate quantities. However, the possibility of extracting information from something as ill defined as an ϵ expansion is definitely something nobody would take for granted before learning field theory. Field theory and especially the renormalisation group associated with it also give us a powerful language to pose and answer problems related to scaling. Our whole non-equilibrium statistical treatment also enables us to present field theory gradually and pedagogically, clearly demonstrating its probabilistic framework without mixing in quantum probability. This also makes it easier to spot and easily appreciate the distinguishing characteristics of quantum probability upon taking up quantum field theory.

We focused mainly on reaction-diffusion processes which is a broad enough area to cover a variety of topics without straying from it. Besides a pedagogical introduction to the technical implementation of field theory and its relation to other statistical tools, we also touched briefly on directed percolation and phase transition in general, multi-species reactions, reaction-diffusion on networks, Lévy flights and have indicated what other areas also fall under reaction-diffusion research.

Directed percolation is important as a universality class and also because it can be used to build realistic models of infection. The simple $A + B \to 0$ embodies the history of RD research and is not yet fully settled, also reminding us of how little we still know about non-equilibrium dynamics. Reaction diffusion on networks is a relatively new area

and while there are currently no publications describing field-theoretical techniques on complex network in circulation, there might one day be. Even so the collection of results points towards it as a field with a lot of possibilities. Lévy flights are another type of process that can be really neatly incorporated into the field-theoretic framework, allow us to regulate the critical dimension and are important for generalisations of diffusive motion that seem to be pervading RD research at the moment.

The possible directions of further research are so vast that one needs strict additional criteria in suggesting a subset of them. Unsolved problems, such as listed at the end of [8], including better understanding and classifying BARW and DP, and even performing merely performing a full RG analysis of the $A + B \to 0$ in the case of unequal densities, have all remained unsolved by today. Nonperturbative renormalisation group ideas [105, 106, 46] might yield some insight here. On the other hand the unrepayed stubbornness with these problems might incite us to focus our resources elsewhere and count on a spurious connection with a new area of physics or at least a new method in an old area arising to elucidate the hard problems left behind. Personally I would also like to see the field of reaction-diffusion processes on complex networks grow somewhat and to have more researchers tinker around with field theory in fractal dimension, and fail, if necessary.

Finally promoting multidisciplinarity seems to be a worthy goal in the area these days, as the main applications of it come from mathematical biology, where e.g. polymer research relies heavily on the paradigm[107], evolution and the related game theory, epidemiology and, in comparison, the somewhat unexotic condensed matter physics. The investigation of reaction-diffusion processes and field-theoretical techniques are bound to remain firm pillars of our increasing our knowledge on statistics far from equilibrium for the foreseeable future and I am sure these methods will undoubtedly be applied to elegant resolutions of exciting new problems, spanning nearly all the sciences.

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