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In front of a jury composed by :

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Abstract

Many of the most important open problems in statistical mechanics are related with systems out of thermal equilibrium, which do not possess any a priori known probability distribution, such as the Boltzmann-Gibbs distribution in equilibrium. In this work we use field theory methods to study some systems out of thermal equilibrium. To do so, we first introduce a field theory representation for the systems of interest, as well as the specific formalism to be used throughout, the so-called non perturbative renormalization group (NPRG). This formalism has emerged in the last years as a very efficient way to deal with strongly correlated systems, and has been applied with success to problems both in and out of equilibrium.

Before treating the actual systems of interest, we develop some new tools and methods within the NPRG context, and test them in a simple scalar field theory, belonging to the Ising universality class. By means of these new methods, we are able to obtain results for both the momentum-dependent scaling function of the $d = 3$ Ising model, and the probability distribution function of its order parameter, both without having to fix any free parameter.

Also, in order to tackle in an efficient way the physics of out of equilibrium systems, we study in detail some formal aspects of their passage to a field theory representation, as well as the equivalences between different possible ways to perform this passage.

After these preliminaries, we concentrate in out of equilibrium active-to-absorbing phase transitions in reaction-diffusion systems, and in particular in the subclass known as branching and annihilating random walks. We then, for the first time, understood how to implement the local potential approximation of the NPRG while being fully functional in the fields, for one of these systems.

In parallel, we use the NPRG to find an exact solution to any vertex in a simple reaction-diffusion system, known as pure annihilation. Armed with this, we analyze some properties of branching and annihilating random walks at low branching rates, by means of an expansion in the branching rate around pure annihilation. This perturbative expansion, which is performed around a non-trivial model, allows us to find some striking exact results for some of the most

important universality classes in these systems.

Resumé

Un grand nombre de problèmes ouverts parmi les plus importants en mécanique statistique sont liés aux systèmes hors de l'équilibre thermique, qui ne possèdent pas de distribution de probabilité connue a priori, telle que la distribution de Boltzmann-Gibbs valide à l'équilibre. Dans ce travail, nous utilisons des méthodes de théorie de champs pour étudier certains systèmes hors d'équilibre thermique. Pour ce faire, nous introduisons d'abord une représentation de type théorie de champs pour les systèmes qui nous intéressent, ainsi que le formalisme spécifique utilisé partout dans ce travail, le groupe de renormalisation non perturbatif (NPRG). Ce formalisme a émergé dans les dernières années comme un moyen très efficace pour faire face à des systèmes fortement corrélés, et il a été appliqué avec succès aux problèmes dans et hors de l'équilibre thermique.

Avant de traiter les systèmes qui nous intéressent, nous développons de nouveaux outils et méthodes dans le cadre du NPRG, et nous les testons dans le cas relativement simple d'une théorie de champ scalaire, appartenant à la classe d'universalité d'Ising. Par le biais de ces nouvelles méthodes, nous sommes en mesure d'obtenir des résultats à la fois pour la fonction d'échelle du modèle d'Ising en d = 3, comme pour la fonction de distribution de probabilité de son paramètre d'ordre, sans avoir à fixer aucun paramètre libre.

En outre, afin de faire face de manière efficace la physique des systèmes hors d'équilibre, nous étudions en détail certains aspects formels de leur passage à une représentation de type théorie des champs, ainsi que les équivalences entre les différentes voies possibles pour mettre en oeuvre ce passage.

Après ces préliminaires, nous nous concentrons sur les transitions de phase hors d'équilibre dans des systèmes de réaction-diffusion, et en particulier dans la sous-classe connue sous le nom de marches aléatoires avec branchement et annihilation (BARW). Nous avons ensuite, pour la première fois, compris comment mettre en oeuvre l'approximation du potentiel local de le NPRG tout en étant entièrement fonctionnel dans les champs, pour un de ces systèmes.

En parallèle, nous utilisons le NPRG pour trouver une solution exacte pour un des cas les plus simples de système de réaction-diffusion, connu comme

l'annihilation pure. Armés de cette solution, nous analysons certaines propriétés des systèmes BARW a bas taux de branchement, en utilisant un développement autour de l'annihilation pure. Ce développement perturbatif, qui est réalisé autour d'un modèle non trivial, nous permet de trouver des résultats exacts pour certaines des plus importantes classes d'universalité de ces systèmes.

Resumen

Muchos de los problemas más importantes en mecánica estadística están relacionados con sistemas fuera de equilibrio termodinámico, sistemas que no poseen una distribución de probabilidad conocida a priori, como en el caso de la distribución de Boltzmann-Gibbs en equilibrio. En este trabajo hemos utilizado métodos de teoría de campos para estudiar algunos sistemas fuera de equilibrio termodinámico. Para esto primero introducimos una representación de tipo teoría de campos para el sistema de interés, así como el formalismo específico usado en el trabajo, el Grupo de Renormalizacion No Perturbativo (NPRG). Este formalismo surgió en los últimos tiempos como un método altamente efectivo para lidiar con sistemas fuertemente correlacionados, y ha sido aplicado con éxito tanto a sistemas en equilibrio termodinámico como a sistemas fuera del mismo.

Antes de tratar los sistemas fuera de equilibrio de interés, hemos desarrollamos nuevas herramientas y métodos en el contexto NPRG, y los hemos puesto a prueba en el caso relativamente sencillo de una teoría de campos escalares, pertenecientes a la clase de universalidad del modelo de Ising. A través de estos nuevos métodos, somos capaces de obtener resultados novedosos tanto para la función de scaling dependiente del impulso del modelo de Ising en $d = 3$, que puede ser comparada con resultados experimentales, así como para la distribución de probabilidad del parámetro de orden para este mismo sistema. Ambos resultados fueron obtenidos sin tener que fijar ningún parámetro libre.

Además, con el fin de abordar de manera eficaz la física de los sistemas fuera de equilibrio, hemos estudiado en detalle algunos aspectos formales de su pasaje a una representación de teoría de campos, así como las equivalencias entre las diferentes formas posibles de realizar este pasaje.

Después de estos preliminares, nos concentramos en las transiciones de fase en sistemas de reacción-difusión fuera de equilibrio termodinámico, y en particular en la subclase conocida como Branching and Annihilating Random Walks (BARW). Por primera vez para este tipo de sistemas entendimos cómo implementar la aproximación de potencial local del NPRG manteniendo toda

la dependencia funcional en los campos.

En paralelo, hemos utilizado el NPRG para encontrar una solución exacta para cualquier función de correlación de un sistema sencillo de reacción-difusión sin branching, conocido como aniquilación pura. Partiendo de ésta solución es posible analizar algunas propiedades de BARWs a bajas tasas de branching, por medio de un desarrollo en la tasa de branching alrededor de la aniquilación pura. Este desarrollo perturbativo, que se realiza alrededor de un modelo no-trivial, nos permitió encontrar resultados exactos para algunas de las clases de universalidad más importantes de estos sistemas.

Para Julia y para mi familia
por estar

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Federico Benitez
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In all things of nature there is something of the marvelous.
Aristotle

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Chapitre 1

Strongly correlated systems and phase transitions

Without doubt, many of the challenges for twenty-first century physics reside in the study of strongly correlated systems. These range from low energy properties of quantum chromodynamics to the study of turbulent liquids, passing through the behaviour of disordered and glassy systems, critical phase transitions, plasma physics, quantum criticality, self organization and high temperature superconductivity, among others (see for example [208, 164, 57, 121, 142, 161, 55, 21, 100, 109, 120, 153, 30, 197, 136, 145, 53]). These systems are characterized by the presence of strong spacial or temporal correlations between their microscopic components, which give rise to complex emergent phenomena at macroscopic scales. Usual methods in physics, often based on a perturbative approach – where interactions within the system are considered as a small perturbation of an interaction-less, or otherwise simple, reference model – tend to yield results that are not even qualitatively correct for describing such macroscopic behaviour.

In this work we are mainly interested in the study of strongly correlated systems within statistical mechanics. This has the advantage of presenting the main difficulties of studying this kind of problems, but within a fairly controlled context. That is to say, statistical mechanical problems are usually conceptually simple, and the complexities of strongly correlated behaviour can be treated in an isolated way. Statistical mechanical problems, though admittedly sometimes abstract, can often be seen as toy models with diverse applications, both within Physics and also in other fields (e.g. Biology, Chemistry, Computer Science, etc.).

Strongly correlated systems have been studied within equilibrium statistical mechanics with some success, and many ideas have emerged from this context. Our ambition here, though – and the area where most effort is put forward

nowadays by the community – is to be able to gain knowledge in statistical systems out of thermal equilibrium. For these systems the probability distribution of possible configurations is not known a priori, as is the case in the equilibrium context, with the Boltzmann-Gibbs distribution. Needless to say, out of equilibrium models have a much wider range of applicability - both within and also beyond physics - than their equilibrium counterparts, but at the cost of a much increased level of complexity. In fact, most of these systems are studied in a case-by-case basis, exploiting particular properties of each model, often with very ingenuous methods, based on their detailed analysis. In this work, however, we would like to develop general tools for tackling these problems.

Of particular interest to us in this work is the study of critical phase transitions, both in and out of thermal equilibrium. Phase transition phenomena are at the basis of much of our current understanding of strongly correlated systems. Near a critical point, the correlation length within the system diverges, there is loss of a natural scale, and scale-free collective behaviour emerges, which, despite the underlying complexity, often allows for a great simplification of the analysis. Indeed, critical phase transitions can be classified in universality classes, depending only in very general aspects of the system, such as space dimensionality and the presence of symmetries, and not in the microscopic details of each model. In the case of out of equilibrium systems suffering a critical phase transition, however, this classification is far from being complete, and a definitive alphabet of possible universality classes is still lacking.

Universality can be seen as a consequence of the general phenomena of separation of scales for these complex systems. That is, the existence of emergent behaviour at space and time scales larger than the microscopic scale of the system components, whose detailed dynamics can or can not be completely known. The microscopic dynamics affects the meso- and macroscopic behaviour, but in many interesting cases does so only through a handful of so-called relevant parameters, so that there is an overall simplification in complexity while studying these systems.

Since the pioneering works of Wilson, Renormalization Group (RG) methods are the weapon of choice for dealing with the studies of phase transitions and strongly correlated systems. This is to be expected, as RG deals ultimately with the study of the behaviour of a system when viewed at a different space or time scales. This makes RG methods ideal to handle scale-free situations such as critical phase transitions, and in general to deal with any system showing the aforementioned property of separation of scales.

Field Theory is the natural habitat for RG techniques. Although not the only possibility - one can think of Kadanoff [119] direct space RG, for example - it is arguably the setting where RG ideas are most easily understood, and the main setting to be used throughout this work. In order to be able to do that, it is

necessary to find field theory representations for the systems of interest. There are standard ways to do so, both for equilibrium and for out of equilibrium systems, and we review these in detail later on. Once in possession of a field theory describing the problem, a whole arsenal of standard methods can be used, and in particular methods specifically designed for the study of strongly correlated systems.

In the last decades, many out of equilibrium systems have been studied by using standard perturbative RG techniques [52, 189, 84, 202]. However, the presence of strong correlations and in some cases large couplings greatly difficult the task. In fact, it can even be argued that the collective effects emerging from strong correlations would not allow us to see these systems as small perturbations of interaction-less systems. It is clear that most of these problems demand us to go beyond classical perturbative methods.

In this work, we do so by means of what is known as the Non Perturbative Renormalization Group (NPRG) [201, 18, 63, 90], which is basically a modern reformulation of Wilson's original ideas, without recourse to the machinery of perturbative field theories. The central tool of the NPRG is an exact flow equation, the Wetterich equation, which allows us to study in a controlled yet non-perturbative way the behaviour of a given system at different length and time scales. Of course, this exact equation must be complemented with approximations in any practical calculation, but one of the main advantages of the NPRG is that it allows us to devise new approximation schemes, which have already shown to be very effective when studying strongly correlated systems.

This work is organized as follows. In Chapter 2 we present the specific equilibrium and out of equilibrium systems to be studied, and in Chapter 3 we show how to arrive at a field theory representation for these out of equilibrium systems of interest. While doing so, we find some formal properties not usually discussed for these representations.

In Chapter 4 we introduce the main method used in this work, the NPRG. We do so in the simpler equilibrium context, where we also take the opportunity to present some new results and developments, which we hope will some day be generalized to more complex out of equilibrium problems.

Finally, we use NPRG techniques to tackle the out of equilibrium problems of interest. First, in Chapter 5 we show how to adapt the NPRG techniques to the out of equilibrium formalism. We then go on to perform the first full field dependent study of a simple out of equilibrium system belonging to the Directed Percolation universality class, arguably the most important universality class for out of equilibrium problems. Finally, in Chapter 6 we present some exact results for reaction-diffusion systems, obtained for the first time by using these methods.

Chapitre 2

In and out of equilibrium

In this chapter we present the specific problems under study in this work. They were chosen as simple representatives of systems showing the themes introduced in the preceding chapter : strong correlations, collective behaviour, universality and separation of scales. We consider systems both at and out of thermal equilibrium. The former are very useful to test the accuracy of our methods and approximations, whereas the latter are much less well known, and will be the main focus of this work.

First, in section 2.1, we briefly introduce Ising-like and related systems. The interested reader is encouraged to look for more specific introductions to this important universality class, such as can be found in [91, 132, 131]. The equilibrium phase transitions occurring in these systems have been very much studied before, using a large array of methods, and results for many physical quantities of interest are known with a high degree of accuracy. These systems are then very useful as testing grounds for new methods or approximations, as those in use hereafter.

Then, in section 2.2, we introduce the main class of out of equilibrium systems to be studied in this work, the so-called reaction diffusion systems, and the phase transitions that can occur within these systems, as well as some formalism necessary to study them. Later on we develop the ways to represent these systems as field theories, in order to make possible the application of RG methods.

Finally, we present two possible formalism to describe reaction-diffusion systems, the master equation, and the Langevin equation approaches. Both are of special interest, given that they allow for the construction of a field theory representation for reaction-diffusion systems. The construction of these field theories is presented in the following chapter.

2.1. Ising-like systems

The Ising Model is quite possibly the single most important model showing strong correlated behaviour in equilibrium statistical mechanics. It was initially devised as a model for ferromagnetic materials, but due to universality, this model and its generalizations are useful to describe the critical properties of a large number of systems. As is well known, for dimensions grater than 1 the model presents a continuous phase transition, between an ordered low-temperature state with spontaneous magnetization, and a disordered high temperature state.

The basic degrees of freedom of the model are the so-called classical spin variables $S_{\mathbf{r}}$, which can be seen as vectors of modulus 1 which can either point in an up or a down direction, corresponding respectively to two possible values $+1$ and -1. These spins are located in a regular lattice structure, and are coupled in such a way that they tend to align. In terms of these variables, the Hamiltonian of the model can be written as [1]

$$H = -\beta J \sum_{\langle \mathbf{x},\mathbf{x}' \rangle} S_{\mathbf{x}} S_{\mathbf{x}'} + \sum_{\mathbf{x}} h_{\mathbf{x}} S_{\mathbf{x}} \qquad S_{\mathbf{x}} = \pm 1 \tag{2.1}$$

where the symbol $\langle \mathbf{x},\mathbf{x}' \rangle$ stands for nearest lattice neighbors, β is the inverse temperature, J is the strength of the coupling between neighboring spins, and $h_{\mathbf{x}}$ is a site-dependent external magnetic field. This Hamiltonian possesses a Z_2 symmetry, being invariant under the exchange $S_{\mathbf{x}} \to -S_{\mathbf{x}}$, $h_{\mathbf{x}} \to -h_{\mathbf{x}}$.

An exact solution is easily found [132] in the case $d = 1$, showing no phase transition at all, and the existence of long range order only in the limiting zero temperature case $\beta = \infty$. The two dimensional model in absence of an external field has been famously solved by [159]. Also, high precision results exist for the model in dimension 3, by means of Monte Carlo, high temperature expansions, and high order perturbative field theory methods. On top of that, the universal properties of the model in dimensions 4 and higher are well described at the mean field level. Thus, the Ising model presents itself as a very useful comparison tool, for the development of new schemes to deal with strongly correlated systems. This explains why it continues to be actively investigated, more than a century after being created.

Notice also that even if many properties of Ising systems are already very well known, there remain important quantities which are of difficult access with the available standard tools. As an example, the momentum dependence of the two point correlation function of the model assumes the form (see sec-

1. As is usually done, we include the factor $\beta = 1/(K_b T)$ in the definition of the Hamiltonian and the external magnetic field.

tion 6.83 below)

$$G^{(2)}_{\pm}(p) = \chi g_{\pm}(p\xi) \tag{2.2}$$

with $g_{\pm}(x)$ a universal scaling function of its argument ($\pm$ standing for above or below the critical point respectively), χ is the susceptibility and ξ the correlation length. This momentum-dependent function can be measured experimentally for the physically relevant $d = 3$ case [58], but is hard to obtain by Monte Carlo calculations (except for a narrow momenta regime), and impossible to obtain by perturbative field theory methods. In fact, up to now the best theoretical insight on its form came from an ad-hoc phenomenological ansatz, the Bray ansatz. Below, we show how a new approximation scheme within the NPRG allows for a precise calculation of this function. In any case, there are still things to be understood from the Ising model.

In order to study the Ising model by renormalization group methods, it is generally convenient to rewrite it in terms of a field theory. This can be done in an exact way, by performing a Hubbard-Stratonovich transformation. We now briefly recall how to do this. Consider then the modified Hamiltonian, for the case of no external magnetic field, $h = 0$

$$\begin{aligned} H_{\mu} &= -\beta J \sum_{\langle \mathbf{x},\mathbf{x}'\rangle} S_{\mathbf{x}} S_{\mathbf{x}'} - \beta\mu J \sum_{\mathbf{x}} S_{\mathbf{x}} S_{\mathbf{x}} \\ &= -\frac{1}{2} \sum_{\mathbf{x},\mathbf{x}'} S_{\mathbf{x}} M_{\mathbf{x},\mathbf{x}'} S_{\mathbf{x}'} \end{aligned} \tag{2.3}$$

the μ term modifies the Ising Hamiltonian by a trivial constant term equal to $-\beta\mu JN$ (with N the total number of spins), but is needed in order for the matrix $M_{\mathbf{x},\mathbf{x}'}$ to be invertible. The form of this matrix depends on the specific underlying lattice considered. Here we restrict ourselves to a hypercubic lattice, in which case the matrix $M_{\mathbf{x},\mathbf{x}'}$ is diagonal in Fourier space, with eigenvalues [132]

$$\lambda_{\mu}(\mathbf{q}) = 2\beta\Big(J \sum_{a=1}^{d} \cos q_a + \mu\Big) \tag{2.4}$$

As stated before, then, the matrix $M_{\mathbf{r},\mathbf{r}'}$ is positive, and thus invertible, for $\mu > Jd$. We can then use a Hubbard-Stratonovich transformation, in order to rewrite the Ising model as a lattice field theory, whose partition function reads

$$\begin{aligned} Z_{\mu} &\propto \sum_{\{S_{\mathbf{x}}\}} \int_{-\infty}^{\infty} \prod_{\mathbf{x}} d\varphi_{\mathbf{x}} \exp\Big(-\frac{1}{2} \sum_{\mathbf{x},\mathbf{x}'} \varphi_{\mathbf{x}} M^{-1}_{\mathbf{x},\mathbf{x}'} \varphi_{\mathbf{x}'} + \sum_{\mathbf{x}} \varphi_{\mathbf{x}} S_{\mathbf{x}}\Big) \\ &\propto \int_{-\infty}^{\infty} \prod_{\mathbf{x}} d\varphi_{\mathbf{x}} \exp\Big(-\frac{1}{2} \sum_{\mathbf{x},\mathbf{x}'} \varphi_{\mathbf{x}} M^{-1}_{\mathbf{x},\mathbf{x}'} \varphi_{\mathbf{x}'} + \sum_{\mathbf{x}} \log\cosh \varphi_{\mathbf{x}}\Big) \end{aligned} \tag{2.5}$$

This lattice field theory exactly encodes all the microscopic properties of the Ising model. However, for the purposes of studying its critical regime, it is often convenient to simplify this in two ways. First, a continuum space limit can be taken, expanding the dispersion relation (2.4) for the slow **q** modes. In this case we end up with a continuum field theory, and the measure over the field $\varphi(x)$ would be promoted to a functional measure. Secondly, the potential-like term $\log\cosh\varphi(x)$, can be expanded in powers of the fields, keeping only the most relevant terms in the RG sense. After performing these approximations, we end up with the scalar φ^4 scalar field theory

$$Z = \int \mathscr{D}\varphi(x) e^{-H_{GL}[\varphi]} \tag{2.6}$$

with what is known as the Guinzburg-Landau Hamiltonian

$$H_{GL}[\varphi] = \int d^d x \left[\frac{1}{2}\big(\nabla\varphi\big)^2 + \frac{r_0}{2}\varphi^2 + \frac{u}{4!}\varphi^4 \right] \tag{2.7}$$

this field theory will reappear below. It is generally convenient to add a source term to the theory, linearly coupled to the field $\varphi(x)$. Notice though that this external field is different - although ultimately related to - the physical external magnetic field $h_{\mathbf{x}}$.

Notice that we could have started directly from a Landau type of effective action like Eq. (2.7), and that would suffice for the study of universal properties of the Ising class, such as critical exponents. However, we may be interested in describing also some non-universal properties, such as critical temperatures. While this is usually not possible withing the perturbative RG approach, we shall see that the methods used here, the NPRG equations, also allow for the study of non-universal quantities. Later on we also show how to perform a direct RG study of the Ising model, without recourse to a field theory formalism. This can be achieved by means of a natural generalization of the non perturbative renormalization group formalism, devised to address systems defined on a lattice. See section 4.3.

A trivial, yet important, generalization of this system is given by the so-called $O(N)$ scalar field theories. In these, the classical spin variables can be visualized as arrows in an internal N-dimensional configuration space. This leads to a $O(N)$ symmetric Guinzburg-Landau type of Hamiltonian field theory, in terms of N component scalar field variables

$$H[\phi] = \int d^d x \left[\frac{1}{2}\sum_i \big(\nabla\varphi_i\big)^2 + \frac{r_0}{2}\sum_i \varphi_i^2 + \frac{u}{4!}\big(\sum_i \varphi_i^2\big)^2 \right] \tag{2.8}$$

This class of systems are useful to model the critical properties of a large quantity of physically interesting systems and not only within statistical mechanics. Indeed, for example, the critical exponents which describe the behaviour

of the final point high temperature electroweak phase transition coincide with those of the Ising model [179], in an impressive show of the power of universality ideas. Another example lies in the study of the critical properties of the chiral phase transition at high temperatures and densities in QCD, which can be analyzed by using the $O(4)$ model presented here [165, 203, 177, 19, 176].

So far we have centered our attention in highly correlated systems at thermal equilibrium, of which arguably a lot is already known. Let us now advance to define the systems which interest us the most in this work, out of equilibrium reaction-diffusion processes.

2.2. Reaction-diffusion systems

Much of this work circles around reaction-diffusion systems. These represent one of the simplest class of genuinely out of equilibrium problems. In them, there is, generally speaking, no detailed balance and thus no approach to equilibrium, and fluctuations govern their behaviour in often dramatic ways [91, 194, 86, 105, 189], so that mean field results are generally way off the observed properties of these systems.

Even though there is not equilibrium state, these systems usually show a long time stationary state. We will be dealing exclusively with this stationary behaviour, which is of course simpler to study than the full time dependence of observables. In fact, within the methods used in this work, the technology needed to perform such a time-dependent study is still lacking. However, what interest us the most here is the description of critical behaviour in some of these systems, and most notably of phase transitions between different stationary states.

Reaction diffusion processes can be defined as systems of particles which diffuse freely by following Brownian motions (this can be generalized to ballistic motion, or Lévy-flight dynamics [116, 196]), and which suffer certain reactions, which can be spontaneous reactions (one-body, such as $A \to B$) or mutual reactions (such as $2A + B \to C$).

Reaction-diffusion systems are then defined in terms of the reactions rates of the system. A simple example would be the system defined by the reactions

$$2A \xrightarrow{\lambda} \emptyset \qquad A \xrightarrow{\sigma} 2A \tag{2.9}$$

on top of diffusion with diffusion constant D. Reaction-diffusion systems such as this, with only one particle species and presenting this type of branching and annihilation reactions are often called Branching and Annihilating Random Walks (BARW), and play a central role in this work.

Reaction-diffusion systems were initially introduced as models of chemical reactions, but have shown later on to be useful for the study of many phenomena involving propagation under constraints, such as epidemics of a disease in a population, bacterial growth or car traffic [105], among others.

These complex systems show in many cases out of equilibrium phase transitions between different stationary states. One very common type of transitions are what are called absorbing phase transitions, in which the system can end up in an active state, where particles continue having reactions sustaining a stable macroscopic state, or either in what is called an absorbing state, where dynamics is frozen, and can often be identified with a state with no particles and no reactions. Systems which suffer such type of phase transition are out of equilibrium, as the existence of an absorbing state is by its very nature incompatible with detailed balance, as we shall see below.

For example the system (2.9) presents an absorbing phase transition depending on the values of the branching and annihilation rates, σ and λ respectively, with the absorbing state being given by the empty state, where no particles are left in the system.

Out of equilibrium systems, as we have said before, show a much richer variety of behaviour when compared to its counterparts at or even close to equilibrium. It is possible, nonetheless, to classify many of these phase transitions within a small number of universality classes. This task has mostly been made possible by the introduction, as in equilibrium, of a description of these systems through a field theoretical formalism, which is the path we are also going to follow.

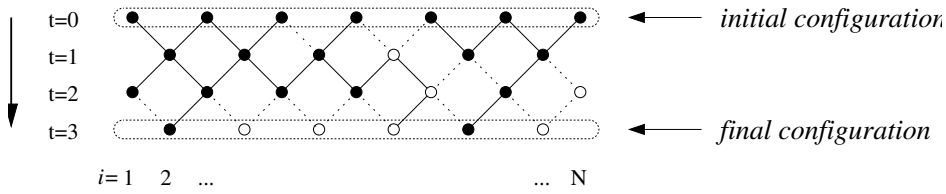

FIGURE 2.1 – Diagrammatic representation of bond directed percolation, one of the systems belonging to the DP universality class. Bonds are created in the preferred (down) direction with probability p. A phase transition can occur depending on the value of p, see Fig. 2.2. Figure taken from [107].

Directed Percolation (DP) is arguably the most important such universality class in out of equilibrium phase transitions. In its original formulation [183], it is a percolation process having a preferred direction of propagation. A schematic representation of a DP system can be seen in Fig 2.1, where DP is represented

as a system consisting of a set of vertices which can be joined by lines with a given probability p, with the additional constraint that any such line must always advance in the preferred direction. This preferred direction can be identified with the time coordinate, or maybe to a height axis in the presence of a gravitational field. In the infinite volume limit there is a continuous phase transition between an active state, with a cluster percolating all along the preferred direction, and an absorbing phase, where no such percolating cluster exists, and therefore propagation along the preferred direction stops at a given finite distance from the origin. See Fig. 2.2.

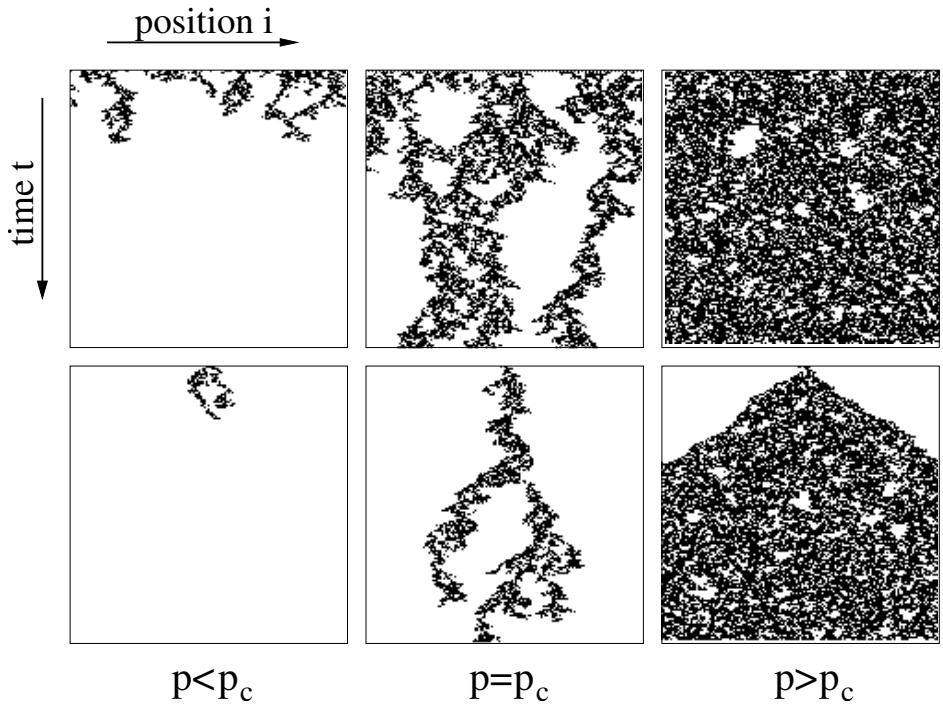

FIGURE 2.2 – Temporal behaviour of Directed Percolation, from a uniformly seeded lattice (top) or from a single seed (botom). The system is, from left to right, in the absorbing phase, at the critical point, and in the active phase. Figure taken from [107].

Following a conjecture put forward by Janssen [113] and Grassberger [95], any absorbing phase transition characterized by a single real order parameter should be in the DP universality class, unless some additional symmetry or quenched disorder is present in the system. The robustness of the DP universality class has been tested by measuring its critical exponents in numerical simulations performed on many different systems, and may be understood in

terms of the simplicity and irreducibility of the dynamic field theory which describes it [52], as we shall see below.

The BARW system defined by equation (2.9) is one such representative of the DP universality class. Indeed, the active-to-absorbing phase transitions which takes place in the system has been shown to be described in its universal characteristics by the same exponents as DP. This is in line with the Janssen-Grassberger conjecture, as the transition is characterized by the mean density of particles : a single real order parameter. For a diagrammatic sketch of the explicit relation between the system (2.9) and DP see Fig. 2.3.

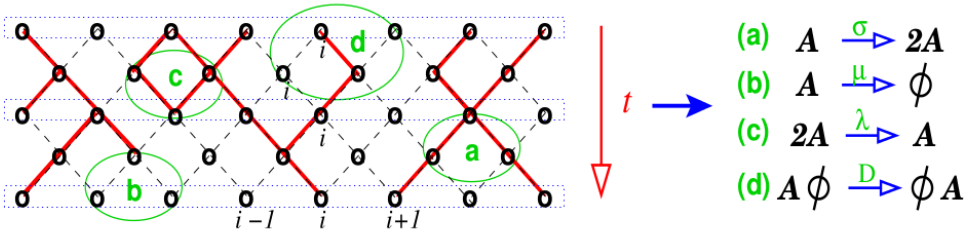

FIGURE 2.3 – Diagrammatic representation of the relation between BARW-DP and Directed Percolation. Figure taken from [50].

It turns out that the DP universality class has already been studied by field-theoretical methods in the context of particle physics, some decades ago [54]. Indeed, the field theory we use in this work to study the system (2.9) can be easily related with what is known as Reggeon field theory, an effective theory describing the soft part of the strong interaction dynamics at high energies. Also, there has been some recent experimental characterization of the DP universality class in turbulent liquid crystals [187].

An example of an additional symmetry which prevents the system to fall into the DP universality class is given by the Parity Conserving (more properly called Generalized Voter) universality class [108], which, in terms of reaction-diffusion processes, comprises systems where the parity of the number of interacting particles of a single species A is conserved. PC/GV systems have been shown to belong to a universality class different from DP. In this work we are interested in some properties of these two important universality classes, of which more will be said below.

In this work we mostly consider the simplest possible reaction diffusion systems. We shall concentrate on three important systems, which are defined re-

spectively by the reactions

$$2A \xrightarrow{\lambda} \emptyset \qquad \text{PA} \tag{2.10}$$

$$2A \xrightarrow{\lambda} \emptyset \qquad A \xrightarrow{\sigma} 2A \qquad \text{BARW} - \text{DP} \tag{2.11}$$

$$2A \xrightarrow{\lambda} \emptyset \qquad A \xrightarrow{\sigma} 3A \qquad \text{BARW} - \text{PC} \tag{2.12}$$

along with diffusion with constant D. The first system, given by (2.10), consist in annihilation by pairs of particles, and trivially does not present a phase transition. The long time stationary state is invariably the absorbing state with no particles (or at most one particle, which has no relevance in a coarse-grained approach). The decay to this state, as well as the response of the system to perturbations when in the stationary state, are non trivial, and are useful in the following. We call this system PA, standing for Pure Annihilation.

We have already defined the system (2.11), which is the simplest BARW system presenting a phase transition, which belongs to the DP universality class. In this work we identify this system as BARW-DP. Later we will be interested by its universal as well as some of its non-universal properties.

Finally, the reaction diffusion system (2.12) is the simplest BARW system belonging to the PC/GV universality class, as can be seen by observing that its reactions conserve the parity of the number of particles. We call this system BARW-PC.

A mean field type of approximation can be easily found for all these reaction-diffusion systems, by treating the density of particles as constant throughout space, thus ignoring the effects of diffusion (in fact, assuming an infinity diffusion rate). This yields the usual rate equations, describing well-mixed chemical reactions. For example, for the system defined by Eq. (2.9) we would have the mean field (rate) equation

$$\frac{\partial \rho_A(t)}{\partial t} = \sigma \rho_A(t) - 2\lambda \rho_A^2(t) \tag{2.13}$$

where ρ_A is the mean density of A particles. This expression is easily justified from a mean field point of view : the density increases with σ proportionally to the existing density, and decreases with the annihilation rate λ times the square of the density, given that two particles must encounter in order to mutually annihilate. Given that we are interested in the long time stationary state, we can look for the stationary solutions of Eq (2.13), which are

$$\rho_A = \frac{\sigma}{2\lambda} \quad \text{and} \quad \rho_A = 0 \tag{2.14}$$

If we now study the stability of these two solutions, it is easy to see that the solution $\rho_A = 0$ is unstable, as any small density will take the system to the finite

density stationary solution. This implies that at the mean field level no phase transition is seen. Now, if one simulates this system by using Monte Carlo methods or related techniques, a phase transition is easily found, at variance with these mean field results. This is in stark contrast with equilibrium phase transitions, where mean field results generally give a good indication of the presence of a phase transition, at least for high enough dimensionality d. Spatial fluctuations are here responsible for the very existence of the phase transition, so that their effect is much more violent than in equilibrium.

Due to universality, it is in general enough to consider only the simplest reactions characterizing a reaction-diffusion system. Other reactions are naturally generated when considering coarse-grained versions of the process at hand, at larger space an time scales. For example, the reaction $A \xrightarrow{\mu} \emptyset$ is not present in the definition of the BARW system (2.9), but it will effectively be generated as a combination of the σ and λ reactions. More complex reactions will also be generated, and thus it is not necessary to consider them when studying universal properties of these systems. This may seem strange at a first look, but the fact is that the low order reactions turn out being the most relevant in the RG sense. Also, the methods used in this work allow, as we shall see, to treat reactions of arbitrarily high orders.

There is conjectured to exist another important universality class in BARW systems, known as the Pair Contact Process with Diffusion (PCPD) universality class. In terms of BARW, this universality class would appear because of the additional constraint that no spontaneous reactions occur in the system, that is, only reactions with at least two reactants, such as $2A \to 3A$ or $2A \to \emptyset$ are considered. This constraint would suffice to take the system away from the DP universality class. The characterization of PCPD is in many regards still an open problem, but we will not be dealing with it in this work. Interested readers can see a recent approach to this system within the methods used in this work in [97].

All these three problems have been extensively studied in the literature, using Monte Carlo [157], as well as field theory methods, within the perturbative [52, 189] and also the non perturbative renormalization group [45, 44, 46, 48], our method of choice in this work.

In what respects BARW-DP, the perturbative expansion around a reactionless reference system (around a Gaussian fixed point in the RG nomenclature) allows for finding a phase transition for spatial dimensions $d \leq 2$, improving mean field results. This was a reasonable turn of events, as one expects fluctuations to have a greater incidence in lower dimensionalities. Later it has been shown, though, using both Monte Carlo and non perturbative RG techniques, that a phase transition exists for all spatial dimensions d. This phase transition

occurs, for $d > 2$, only if the annihilation rate λ is greater than a threshold value λ_{th}. This can explain why a perturbative expansion around a reaction-less system cannot see the phase transition. The full phase diagram was described for the first time in [44], see Fig. 2.4. We will get back to this problem below.

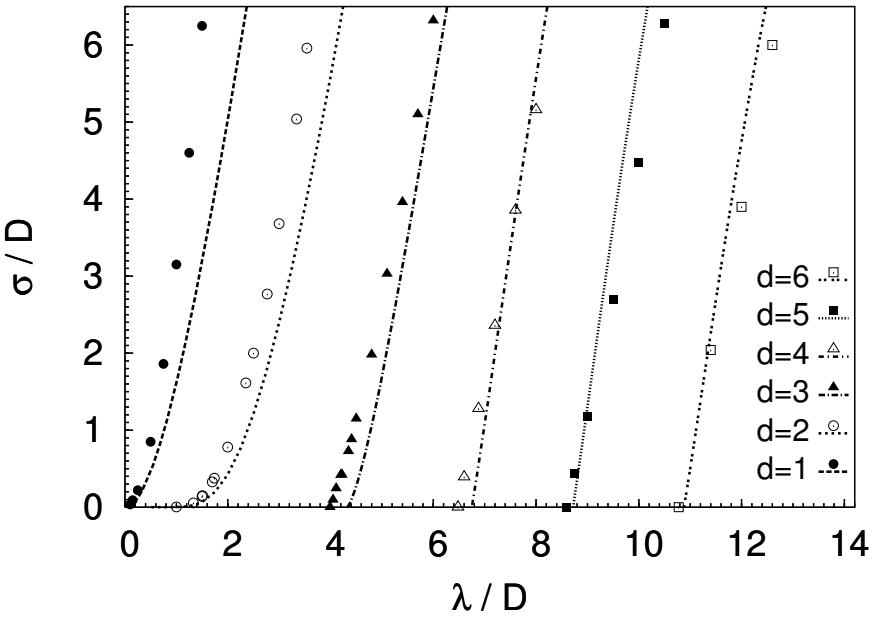

FIGURE 2.4 – Phase diagrams of BARW-DP in dimensions 1 to 6. Lines present NPRG results, symbols follow from numerical simulations. For each dimension, the active phase lies on the left of the transition line, the absorbing phase on the right. Notice in particular the existence of a threshold value λ_{th} for the existence of an absorbing phase in $d > 2$. Results taken from [44].

As for BARW-PC, mean field results again predict the absence of a phase transition, with the system always ending up in an active state. Monte Carlo simulations show however the presence of a phase transition in $d = 1$, where fluctuations are the strongest, belonging to a universality class different from DP. Within perturbative RG, an (upper) critical dimension $d_c > 1$ is found, so that the branching is always dominant for $d > d_c$, there is no absorbing phase, and hence no phase transition. Conversely, for $d < d_c$ the PA behaviour can become dominant, and an absorbing phase exists at small branching σ, whereas at larger σ the system is in its active phase. At 1-loop order, this critical dimension is $d_c^{(1)} = 4/3$, whereas at 2-loops $d_c^{(2)} \simeq 1.1$ is found [52]. NPRG studies, within a low order approximation, are consistent with this scenario and with the 1-loop result [52] for d_c. We discuss this matter in further detail later on.

Moving forward in complexity, we can also consider the case of multiple species reaction-diffusion systems. These have many applications to fields like chemistry and biology, and show a very rich behaviour which has not been much studied using field theory methods (for exceptions see e.g. [195, 190]). Up to now most of the studies rely on mean field and related techniques, as well as of course a great amount of Monte Carlo simulations [157].

In the two species case, there is one system that has been much studied within perturbative RG and has been the object of certain controversy. Following the nomenclature in the literature we call this process the diffusive epidemic process (DEP) [195, 158, 61, 138, 67], it is defined by the reactions

$$A + B \xrightarrow{k} B + B, \qquad B \xrightarrow{1/\tau} A \tag{2.15}$$

where the species A and B diffuse independently, with diffusion constants D_A and D_B respectively. The process can be seen as the spreading of an epidemy, with healthy A individuals becoming sick by contagion of B individuals, with some infection rate k, and sick B individuals recovering spontaneously at a rate $1/\tau$.

A similar process, but with equal diffusion rate $D_A = D_B$ was first introduced in [130] to model the effect of pollution on a biological population. There, it was shown that below a critical population density a continuous absorbing phase transition occurs, which does not belong to the DP universality class, but instead to a new class (usually called KSS), with different critical exponents, calculated to first order in an ϵ-expansion. The generalized model with $D_A \neq D_B$ was analyzed in [195] via field theoretical methods. For the case $D_A < D_B$ the authors predicted a continuous transition of yet a new (WHO) universality class (different from DP and KSS). In the case $D_A > D_B$, a fluctuation-induced first order transition was suggested, and this possibility was made plausible by using analytical and numerical analysis for $d = 2$ in [195]. However, these conclusions have been contested both by newer numerical simulations [85, 138, 67] and by the use of symmetry arguments in the field theory for DEP in [117, 62]. A simple generalization of the non-perturbative RG techniques presented in this work would surely improve our knowledge of this system, but we are not performing this detailed study here.

Another interesting system, also a two particle species, is the diffusive Lotka-Volterra model, a generalization of the predator-prey Lotka-Volterra equation, itself a famous mean field model in ecology and population dynamics [27]. This system has been recently studied by means of perturbative RG techniques, showing DP behaviour close to the predator extinction critical point [190]. Other systems have been the focus of interest in recent literature, such as the three species paper-scissors-rock model, which has been seen in simulations to show

steady states with very complex spatial fluctuations [125, 178, 151]. The study of these kind of systems represent an obvious area of growth for the methods discussed in this work.

2.3. Two useful approaches

In this work we choose two principal tools for studying reaction-diffusion systems : by using the master equation, and by a more phenomenological Langevin equation representation. Even though there are other possible approaches for tackling out of equilibrium problems, such as Fokker-Planck equations [194, 86], or the Poisson representation [86], each with its own strengths, here we are specially interested in being able to obtain a field theory version of the system under study. For reaction-diffusion systems, standard methods exist for doing this within both of the formalism to be presented here.

The main advantage of the master equation formalism is that it allows for a complete translation of the microscopic fluctuation in a way which allows them to be later encoded in an exact way as a field theory. On the other hand, a Langevin equation can often be used in cases where it is impossible to construct a field theory starting from the master equation, such as in the case of the celebrated KPZ equation. Langevin equation can thus be seen as a more generic approach, with the downside that stochastic fluctuation are generally represented in this formalism in an ad-hoc, phenomenological way. Later on we discuss in detail the relations between the two approaches when they can both be applied, as is the case in reaction-diffusion systems.

2.3.1. Master equation for reaction-diffusion

As we shall see below, it is useful for our purposes to express reaction-diffusion processes using the master equation formalism [194, 86]. Within this formalism we can construct a field theory for reaction-diffusion systems which exactly represents its stochastic fluctuations.

A master equation describes how the probability $P(\alpha)$ for the system of being in one of its possible configurations α changes with time. This rate of change is given by the difference of a gain term, stemming from transitions $\beta \to \alpha$ from a different state β to the state α, and a losing term, stemming from transitions from the state α to different states γ of the system. Thus, generically, the master equation is written

$$\frac{dP(\alpha,t)}{dt} = \sum_{\beta} R_{\beta\to\alpha} P(\beta,t) - \sum_{\gamma} R_{\alpha\to\gamma} P(\alpha,t) \tag{2.16}$$

where, for stationary processes, the transition rates $R_{\alpha\to\beta}$ are independent of time. For reaction-diffusion systems defined on a lattice, different states of the system can be identified by the occupation numbers of lattice sites. That is, the state of the system at time t can be determined from the set of numbers $\{n_i^A\} = (n_1^A, n_2^A, \ldots, n_N^A)$, $\{n_i^B\} = (n_1^B, n_2^B, \ldots, n_N^B)$, ..., representing the number of particles of each species in each lattice site. A master equation can in this case be written as a sum over different lattice sites. For simplicity, let us begin by studying PA, Eq (2.10), with single species diffusion and only one reaction to care for. Generalizations will be trivial later on. We can write in this case

$$\frac{dP(\{n_i\},t)}{dt} = \sum_i \left[\frac{\partial P^{(i)}(\{n_i\},t)}{\partial t}\Big|_{2A\to\emptyset} + \frac{\partial P^{(i)}(\{n_j\},t)}{\partial t}\Big|_{\text{Diff}} \right] \tag{2.17}$$

where notation $P^{(i)}(\{n_j\},t)$ stand as a shorthand for terms in which a reaction takes place in the i lattice site.

Due to the annihilation reaction, the probability of having n_i particles on site i changes, given that any two particles present in the site can disappear with probability rate λ. Conversely, this probability can also increase, given that it is also possible that two particles are annihilated from a state with n_i+2 particles in site i. The resulting contribution to the master equation reads

$$\frac{\partial P^{(i)}(\{n_j\},t)}{\partial t}\Big|_{2A\to\emptyset} = \lambda\Big[(n_i+2)(n_i+1)P(\ldots,n_i+2,\ldots,t) - n_i(n_i-1)P(\ldots,n_i,\ldots,t)\Big] \tag{2.18}$$

(following custom, we have absorbed a factor 2 into the definition of λ). A similar expression can be generalized for any possible reaction.

Diffusion is special in this formalism in that it involves terms which mix different lattice sites. Indeed, due to diffusion, the probability of having n_i particles in site i can decrease if any of these particles hops to a nearest neighbor site j, and can increase if a particle hops from any of these neighboring site to site i. Thus

$$\frac{\partial P^{(i)}(\{n_j\},t)}{\partial t}\Big|_{\text{Diff}} = D\sum_{j\in\langle i,j\rangle}\Big[n_j P(\ldots,n_i-1,n_j+1,\ldots,t) - n_i P(\ldots,n_i+1,n_j-1,\ldots,t)\Big] \tag{2.19}$$

This equation can in principle be generalized to other types of diffusion (next-to-nearest neighbors, for example) but one does not expect that to change the universal properties of the system. Different dynamics for the particles, such as ballistic motion or Lévy flights can also be considered, and do change the universal properties of the system. Here we do not deal with such possibilities, but our methods could easily be generalized to study them.

The master equation formalism requires an initial condition for the probabilities of different states of the system. In the case at hand, if we consider that

the particles were initially deposited at random on a lattice, we would be dealing with a Poissonian initial distribution. Each site would then have n_i particles with probability $e^{-\bar{n}_0}\bar{n}_0^{n_i}/n_i!$, where $\bar{n}_0$ represents the mean occupation number. If each site is filled independently we then have

$$P(\{n_i\},0) = e^{-N\bar{n}_0}\prod_i \frac{\bar{n}_0^{n_i}}{n_i!} \tag{2.20}$$

The formalism can be generalized to other reactions and to many particle species in a straightforward way, by adding terms in the master equation corresponding to each reaction at each lattice site, and by using multiple occupation numbers, one for each particle species. Reactions between different species mix different occupation numbers at each site, as for example in

$$\left.\frac{\partial P^{(i)}(\{n_j\},\{m_j\},t)}{\partial t}\right|_{A+B\xrightarrow{\mu}2B} = \mu\Big[(n_i+1)(m_i-1)P(\ldots,n_i+1\ldots,\ldots m_i-1\ldots,t) - n_i m_i P^{(i)}(\{n_j\},\{m_j\},t)\Big] \tag{2.21}$$

Importantly, the master equation formalism can be used to prove some general properties of reaction-diffusion systems. In particular, it allows us to decide if a given system violates the detailed balance condition, thus being out-of-equilibrium in a strong sense [194, 86, 207]. For this, let us see what constraints are imposed by detailed balance in this formalism.

Any model which can be described by using a Master Equation has the ergodic property if any state can be reached from any other state in a finite number of steps. In this work we deal with non-ergodic systems, but in all cases equipped with Markovian dynamics. The master equation can be visualized in a way that is convenient for determining the ergodicity of a given system, by representing the different possible states α of the system as points, joined together by arrows standing for the transition rates $R_{\alpha\to\beta}$. If the model at hand is ergodic, it is possible to find a (oriented) path between any two states of the system. See Fig 2.5.

If the probability rates are time-independent, the master equation has always a stationary solution $P^*_\alpha = \lim_{t\to\infty} P_\alpha(t)$, independent of the initial conditions and in general depending on the probability rates $R_{\alpha\to\beta}$. In order to see this, it is convenient to rewrite the master equation in a matricial form. Assuming for simplicity a discrete set of possible states, we can represent probabilities as a vector $\mathbf{P} = (P_1, P_2, \ldots, P_\alpha, \ldots)$, which allows us to write down the master equation as a matrix equation

$$\frac{d\mathbf{P}}{dt} = \hat{R}\mathbf{P} \tag{2.22}$$

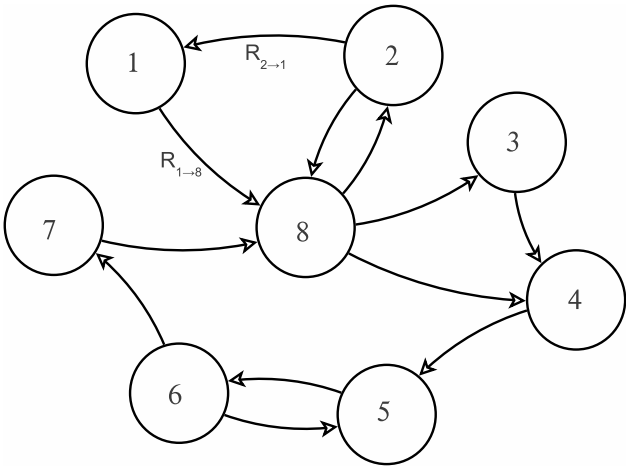

FIGURE 2.5 – Diagrammatic representation of a master equation. States are represented by numbered circles, and transition rates by arrows. This system is ergodic, in that it is possible to arrive to any state to any other in a finite number of steps.

with

$$\hat{R} = \begin{pmatrix} -\sum_\beta R_{1\to\beta} & R_{2\to1} & \cdots & R_{\beta\to1} & \cdots \\ R_{1\to2} & -\sum_\beta R_{2\to\beta} & R_{3\to2} & \cdots & \cdots \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ R_{1\to\alpha} & R_{2\to\alpha} & \cdots & -\sum_\beta R_{\alpha\to\beta} & \cdots \\ \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix} \tag{2.23}$$

In general, the $\hat{R}$ matrix is non-symmetric, and has therefore different right- and left-eigenvectors. In fact, is easy to see that it has a trivial left-eigenvector $\mathbf{1} = (1,1,\ldots,1,\ldots)$, with eigenvalue 0. This is due to the conservation of probability. As eigenvalues are shared between left- and right eigenvectors, this implies there exists a right-eigenvector $\mathbf{P}^*$ which also has an eigenvalue 0, that is, a stationary probability state.

In this stationary state the net probability current is zero, so that

$$\sum_{\beta\neq\alpha} R_{\beta\to\alpha}P^*_\beta - R_{\alpha\to\beta}P^*_\alpha = 0 \tag{2.24}$$

If we want the stationary probability distribution to be the usual Boltzman-Gibbs equilibrium probability distribution, thus forcing the system to relax to equilibrium in the $t\to\infty$ limit, we must impose some constraints to the rates $R_{\alpha\to\beta}$. A well established procedure is to chose rates which satisfy the so-called

detailed balance condition

$$R_{\beta\to\alpha}P_{\beta}^{eq} - R_{\alpha\to\beta}P_{\alpha}^{eq} = 0 \tag{2.25}$$

for each pair of states α, β. This is of course a sufficient but not necessary condition. More generally, detailed balance can be seen as an intrinsic property of the dynamics, requiring no information about any specific steady-state distribution. The Kolmogorov criterion [194], relies on considering closed loops in the space of states, e.g. $\alpha \to \beta \to \gamma \to \ldots \to \zeta \to \alpha$. Going back to the example in Fig. 2.5, the closed loops there are $2 \to 8 \to 2$,$2 \to 1 \to 8 \to 2$, $8 \to 3 \to 4 \to \ldots \to 7 \to 8$, $8 \to 4 \to \ldots \to 7 \to 8$, $5 \to 6 \to 5$, as well as closed paths with repeated visits to some states. Generally, then, for each such loop we can define the product of the associated rates in the forward direction $\prod[\mathscr{L}] = R_{\alpha\to\beta}R_{\beta\to\gamma}\ldots R_{\zeta\to\alpha}$, as well as in the reverse direction $\prod[\mathscr{L}^{rev}] = R_{\beta\to\alpha}R_{\gamma\to\beta}\ldots R_{\alpha\to\zeta}$. In terms of these products, the dynamics is said to satisfy a generalized form of detailed balance (sometimes called semi-detailed balance), and therefore to be close to equilibrium, if

$$\prod[\mathscr{L}] = \prod[\mathscr{L}^{rev}] \tag{2.26}$$

for all loops. This imposes a weaker, but much harder to verify, constraint to arrive to equilibrium.

It is now trivial to see that no such equilibrium probability is reached in the case of active-to-absorbing phase transitions, where the existence of an absorbing state, from which one can enter but can never get out, clearly excludes detailed balance. See as an example Fig. 2.6.

2.3.2. Langevin equation approach

As we shall see below, another possible way to obtain a field theory to describe a given out of equilibrium system, is to start from its Langevin equation representation [194, 86]. The basic idea behind this has to do with the property of separation of scales, as is most evidently exemplified in the original context of the Langevin equation, Brownian motion. In that system, the motion is generated by the collisions of molecules of microscopic sizes with the diffusing macroscopic object, with characteristic collision timescales orders of magnitude smaller than the timescale set by the macroscopic degrees of freedom. These microscopic scales, together with the sheer number of microscopic degrees of freedom, make a direct study of the system molecules + diffusing particle impossible. Thus, it is in general desirable, and also justified, to forgo the microscopic degrees of freedom altogether and substitute them for a suitable random (generally white and uncorrelated) noise term.

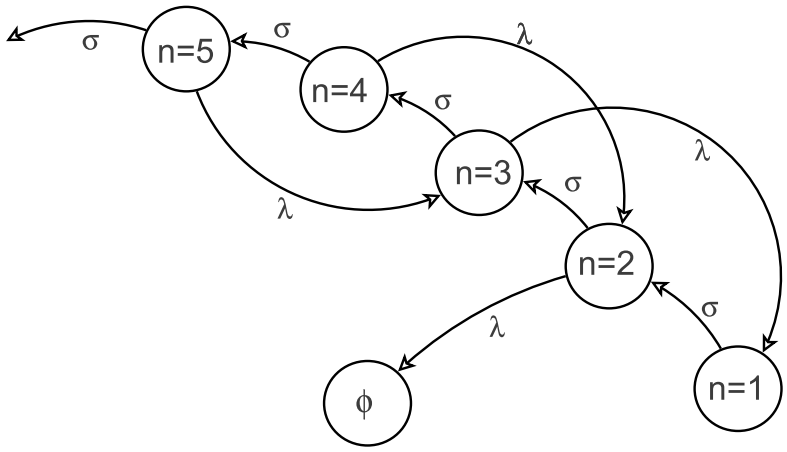

FIGURE 2.6 – Master equation for single site BARW-DP process $2A \to \emptyset$, $A \to 2A$. We clearly see that detailed balance is excluded. Adding diffusion would only increase the complexity of the diagrammatics.

In the case of reaction-diffusion systems, if one is interested in large scale properties, such as the collective behaviour near a phase transition, one may choose to treat particle fluctuations at a microscopic space and time scale as a random noise term applied to a mesoscopic mean local density $\rho(\mathbf{x})$. This would of course constitute an approximation of the full dynamics of the reaction-diffusion process, at variance with the master equation representation, where microscopic fluctuations are treated exactly. The easiest way to construct such an approximation is to start form a mean field approximation defined for the local density, so that instead of completely neglecting the effects of diffusion we would have a mesoscopic mean field description. For the case of BARW-DP, we would change Eq. (2.13) for

$$\frac{\partial \rho_A(\mathbf{x},t)}{\partial t} = D\nabla^2 \rho_A(\mathbf{x},t) + \sigma \rho_A(\mathbf{x},t) - \lambda \rho_A^2(\mathbf{x},t) \tag{2.27}$$

where the form for the diffusion term is given following the usual derivation [194, 86]. A Langevin equation can then be constructed by arguing that microscopic fluctuations affect this local behaviour by means of an additional noise term, so that

$$\frac{\partial \rho_A(\mathbf{x},t)}{\partial t} = D\nabla^2 \rho_A(\mathbf{x},t) + \sigma \rho_A(\mathbf{x}t) - \lambda \rho_A^2(\mathbf{x},t) + \eta(\mathbf{x},t) \tag{2.28}$$

where $\eta(\mathbf{x},t)$ is a random noise uncorrelated in time and space, which we can take as having zero mean.

$$\langle \eta(\mathbf{x},t) \rangle = 0 \qquad \langle \eta(\mathbf{x},t)\eta(\mathbf{x}',t') \rangle = N\delta(t-t')\delta^{(d)}(\mathbf{x}-\mathbf{x}') \tag{2.29}$$

Now, the probability distribution of the noise depends on the microscopic details of the fluctuations. At this point we are more or less in the blind, having neglected the microscopic degrees of freedom, we have no canonical way to obtain the characteristics of the noise probability distribution. We are then forced to use intuition and physical arguments. In this regard, as we shall see later, we generally only consider Gaussian noise, so that no higher order moments of η are needed. Overall, the situation is in many ways analogous to what happens in the study of equilibrium critical phase transitions by using the Landau approach.

In the case of absorbing phase transitions, the noise correlator N has to comply with an additional constraint. This follows from the fact that we know that the system presents an absorbing state, in which no fluctuation exist. Thus, the noise correlator should be zero in this absorbing state, and we can take it as proportional to (some power of) the local density $\rho_A(\mathbf{x}, t)$

$$\langle \eta(\mathbf{x}, t)\eta(\mathbf{x}', t')\rangle = \rho_A^p(\mathbf{x}, t)\delta(t-t')\delta^{(d)}(\mathbf{x}-\mathbf{x}') \tag{2.30}$$

Perhaps the simplest possibility is to take $p = 1$, and this is the usual choice for BARW. We can then rewrite the Langevin equation (2.28) as

$$\frac{\partial \rho_A(\mathbf{x}, t)}{\partial t} = D\nabla^2\rho_A(\mathbf{x}, t) + \sigma\rho_A(\mathbf{x}, t) - \lambda\rho_A^2(\mathbf{x}, t) + \sqrt{\rho_A}\eta(\mathbf{x}, t) \tag{2.31}$$

with

$$\langle \eta(\mathbf{x}, t)\rangle = 0 \qquad \langle \eta(\mathbf{x}, t)\eta(\mathbf{x}', t')\rangle = \delta(t-t')\delta^{(d)}(\mathbf{x}-\mathbf{x}') \tag{2.32}$$

The multiplicative nature of the noise encodes the additional complexity of reaction-diffusion and other out of equilibrium systems, when compared to systems relaxing to equilibrium, where the noise is in general additive. In particular, this multiplicative form for the noise term makes the continuous time limit subtle [194], as we shall see later on.

Notice that there exist also systems where a Langevin equation is the only possible description, or which are defined in terms of a Langevin equation. This is the case of the celebrated KPZ equation [121] describing interface growth

$$\frac{\partial h(\mathbf{x}, t)}{\partial t} = \nu\nabla^2 h(\mathbf{x}, t) + \frac{\lambda}{2}\left(\nabla h(\mathbf{x}, t)\right)^2 + \eta(\mathbf{x}, t) \tag{2.33}$$

In this equation, $h(\mathbf{x}, t)$ is a single valued height profile depending on the d-dimensional substrate coordinate $\mathbf{x}$ and on time t. The term $\eta(\mathbf{x}, t)$ represents an uncorrelated white noise with zero mean $\langle \eta(\mathbf{x}, t)\rangle = 0$ and strength D,

$$\left\langle \eta(\mathbf{x}, t)\eta(\mathbf{x}', t')\right\rangle = 2D\delta^d(\mathbf{x}-\mathbf{x}')\,\delta(t-t'), \tag{2.34}$$

which accounts for the randomness in the growing mechanism. Notice that the noise term does not depend on the h field. However, a transformation is usually performed in this system in order to eliminate the nonlinear term in (2.33), the well-known Cole-Hopf transformation [202, 56]

$$\phi(\mathbf{x}, t) = e^{\frac{\lambda}{2\nu} h(x,t)} \tag{2.35}$$

and absorbing a factor of ν into t leads to the following equations in terms of $\phi(\mathbf{x}, t)$:

$$\frac{\partial}{\partial t}\phi(\mathbf{x}, t) = \nabla^2\phi(\mathbf{x}, t) + \frac{\lambda}{2\nu^2}\eta(\mathbf{x}, t)W(\mathbf{x}, t) \tag{2.36}$$

$$\overline{\eta(\mathbf{x}, t)\eta(\mathbf{x}', t')} = 2\nu D\delta^d(\mathbf{x}-\mathbf{x}')\delta(t-t') \tag{2.37}$$

this equation has the same general structure that the Langevin equations for reaction-diffusion systems, such as Eq. (2.31). In particular it has multiplicative noise. It is in fact very similar to the Langevin equation for the PA system defined above. This similarity can be exploited, and work in this sense is underway.

2.4. Comments

In this chapter we have presented the strongly correlated systems, both in and out of equilibrium, which are studied in this work. In the equilibrium case, we are going to restrain ourselves to the study of the Ising model (together with a small foray into $O(N)$ models), which serves as a useful benchmark of new methods and approximation schemes, as will be shown below. Out of equilibrium we deal with reaction-diffusion systems, which present some of the simplest examples of absorbing phase transitions.

We have introduced two possible ways to describe out of equilibrium systems, the master equation and the Langevin equation approaches. As it turns out, both of these representations allow for a description of the system in terms of a field theory, which is essential for using RG techniques in what follows. However, as is detailed in the next chapter, the master equation formalism, while having a less-general range of applicability, is the only one that enables us to retain all the microscopic information regarding the fluctuations of the system. Relation between the two resulting field theory formalisms will be discussed further below.

Chapitre 3

Field theory for out of equilibrium systems

Renormalization group techniques are the analytical method of choice when studying phase transitions. This is naturally so, given that what these methods study is how the behaviour of a system evolves under changes of scale. As mentioned before, universal emergent properties of systems undergoing a critical phase transitions occur in space-time scales orders of magnitude larger than typical microscopic interaction scales for their constituents. These properties can often be seen as independent of the microscopic details underlying the theory, which can then be recast in a different way to be more efficiently studied.

In order to apply RG techniques it proves convenient to re-express the system at hand as a field theory, which is the natural ground for many of these methods. We have seen before field theory representations for Ising-like systems, and here we show standard constructions in order to arrive to field theoretical representations of out of equilibrium systems. Other possible RG approaches exist of course in the literature, but are most of the time restricted to specific systems or otherwise special cases [105, 8].

3.1. Dynamical response functional formalism

Having presented the out of equilibrium statistical systems to be considered in this work, here we show one possible way to arrive to a field theory representation for studying them, starting from a Langevin equation representation, as explained in the preceding chapter. In general, these systems can always be described, albeit in an approximate way, by a suitable Langevin equation, which, as explained before, exploits the existence of separation of (space and time) scales, and consists in a stochastic differential equation for the macroscopic

modes of interest, while the microscopic rapid fluctuations are encoded as a random noise term. This noise term in general involves an approximation of the microscopic degrees of freedom, of which only the relevant macroscopic effects are sought to be considered.

A Langevin representation can be used for a larger class of out of equilibrium systems than those which can be described by the Doi-Peliti formalism detailed below, stemming from the master equation. This is seen explicitly for example in the case of the famous KPZ equation [121], that can be studied using the NPRG methods used in this work [42, 43], and which is by definition a Langevin equation, so that the formalism described in this section must be used in order to re-express the problem as a field theory.

In the case of reaction diffusion systems, a Langevin formulation can be conceived for the local density field $\rho(\mathbf{x}, t)$ of particles, where this field is defined at a mesoscopic coarse-grained space and time scale, while fluctuations at smaller, microscopic, scales would be encoded in the noise term, whose characteristics must be derived from a priori physical arguments. As an example of this, remember that, in the case of absorbing phase transitions, the noise amplitude had to vanish when the local density tends to zero, in order to make sure that there are no fluctuations around the absorbing state.

We now proceed to reformulate a stochastic process described by a Langevin equation in terms of a path integral representation. In order to do so, we make use of an auxiliary field, the so-called response field, introduced by Martin-Siggia-Rose [139]. This response field allows for the construction of a dynamical response functional field theory, first formulated independently by Janssen [114] and De Dominicis [60].

We can represent a generic Lagevin equation in the form

$$\partial_t \phi(\mathbf{x}, t) = F[\phi](\mathbf{x}, t) + N[\phi]\eta(\mathbf{x}, t) \tag{3.1}$$

The operator $F[\phi]$ contains all the deterministic forces acting over the field ϕ and $N[\phi]$ is generically an operator. In this work we assume that the noise function $\eta(\mathbf{x}, t)$ has zero mean and is uncorrelated in time and space (white noise). This is needed for the dynamical response functional formalism, and can be seen as a consequence of the Markovian hypothesis. Moreover, we assume the noise to be Gaussian correlated, as higher order cumulants can be shown in many cases to be irrelevant in the RG sense [189].

$$\langle \eta(\mathbf{x}, t) \rangle = 0 \quad \text{and} \quad \langle \eta(\mathbf{x}, t)\eta(\mathbf{x}', t') \rangle = \delta(t - t')\delta^{(d)}(\mathbf{x} - \mathbf{x}') \tag{3.2}$$

where the angled brackets denote the statistical average over the fast microscopic degrees of freedom, and the strength of the noise is already encoded in the functional $N[\phi]$. General arguments such as separation of scales and

Markovian dynamics ensure that equations (3.1) and (3.2) are useful for describing a vast array of different physical systems.

Within the Langevin formalism, the mean value over the noise of a physical observable can be written as a sum over the different realizations of the noise $\eta(\mathbf{x}, t)$

$$\langle O[\phi]\rangle = \frac{\int \mathscr{D}\eta\, O[\phi_\eta] P[\eta]}{\int \mathscr{D}\eta\, P[\eta]} \tag{3.3}$$

where $P[\eta]$ is the probability distribution functional for the noise, and the field $\phi_\eta(\mathbf{x}, t)$ is the solution of equation (3.1). This is not a very comfortable way of working out mean values, as the constrain over the field ϕ_η is in general very difficult to control. We would prefer having a path integral over all possible values of the field ϕ. We can rewrite Eq. (3.3) by using a Dirac delta functional, in order to see this constraint more explicitly

$$\langle O[\phi]\rangle \propto \int \mathscr{D}\eta\mathscr{D}\phi\, \mathscr{J}[\phi] O[\phi] P[\eta] \prod_{\mathbf{x},t} \delta\Big(\partial_t\phi(\mathbf{x}, t) - F[\phi](\mathbf{x}, t) - N[\phi]\eta(\mathbf{x}, t)\Big) \tag{3.4}$$

in this expression we have introduced a Jacobian term

$$\mathscr{J}[\phi] = \left|\det\left(\partial_t + \frac{\delta F[\phi]}{\delta\phi} - \frac{\delta\eta}{\delta\phi}\right)\right| \tag{3.5}$$

Here we set this Jacobian term to unity, thus ignoring it. As we shall see below, this amounts to choosing the Itô discretization prescription when going to the continuum limit in the time dependence [194, 86]. In particular, this implies that the Heaviside function in time must be evaluated to zero at $t = 0$, $\Theta(t = 0) = 0$. A more detailed discussion of the Itô prescription is given in chapter 5.2 below, when considering the details of non perturbative RG techniques when studying these systems.

Now, we can re-express Eq. (3.3) by using an auxiliary ("response") field $\tilde{\phi}(\mathbf{x}, t)$, as well as the integral representation of the Dirac δ-function at each space-time point

$$\begin{aligned}\langle O[\phi]\rangle \propto \int \mathscr{D}\eta\mathscr{D}\phi\mathscr{D}[i\tilde{\phi}]\, O[\phi] P[\eta] \\ \times \exp\Big(-\int d^d x\, dt\, \tilde{\phi}(\mathbf{x}, t)\Big(\partial_t\phi(\mathbf{x}, t) - F[\phi](\mathbf{x}, t) - N[\phi]\eta(\mathbf{x}, t)\Big)\Big)\end{aligned} \tag{3.6}$$

Given our assumptions, the noise probability distribution can be written as a Gaussian distribution

$$P[\eta] \propto \exp\left(-\frac{1}{4}\int d^d x\, dt\, \eta(\mathbf{x}, t)\eta(\mathbf{x}, t)\right) \tag{3.7}$$

Combining this expression with Eq. (3.6), we obtain a path integral over three independent fields, ϕ, $\tilde{\phi}$ and η

$$\langle O[\phi]\rangle \propto \int \mathscr{D}\phi\mathscr{D}[i\tilde{\phi}]\, O[\phi] e^{-\int d^d x\, dt\, \tilde{\phi}(\mathbf{x},t)\left(\partial_t\phi(\mathbf{x},t)-F[\phi](\mathbf{x},t)\right)} \times \int \mathscr{D}\eta\, e^{\int d^d x\, dt\, \tilde{\phi}(\mathbf{x},t) N[\phi]\eta(\mathbf{x},t)-\frac{1}{4}\eta(\mathbf{x},t)\eta(\mathbf{x},t)} \tag{3.8}$$

The functional integral over the noise appears then as a simple Gaussian integral, which yields

$$\int \mathscr{D}\eta\, e^{\int d^d x\, dt\, \tilde{\phi}(\mathbf{x},t) N[\phi]\eta(\mathbf{x},t)-\frac{1}{4}\eta^2(\mathbf{x},t)} \propto e^{(N^\dagger[\phi]\tilde{\phi})^2} \tag{3.9}$$

We can then express the probability distribution of the field ϕ as a path integral of the form

$$P[\phi] \propto \int \mathscr{D}[i\tilde{\phi}]\, e^{-S[\tilde{\phi},\phi]} \tag{3.10}$$

where the statistical weight $S[\tilde{\phi},\phi]$ is the dynamical response functional of Janssen-De Domenicis [114, 60]

$$S[\tilde{\phi},\phi] = \int d^d x\, dt \left(\tilde{\phi}(\mathbf{x},t)\left[\partial_t\phi(\mathbf{x},t) - F[\phi](\mathbf{x},t)\right] - (N^\dagger[\phi]\tilde{\phi}(\mathbf{x},t))^2\right) \tag{3.11}$$

Notice that in this path integral representation the microscopic fluctuations are wholly contained in the term quadratic in the response field $\tilde{\phi}$. The dynamical response function $G(\mathbf{x},\mathbf{x}',t,t')$, can be expressed as the correlation between the physical field ϕ and the response field $\tilde{\phi}$. Indeed, $G(\mathbf{x},\mathbf{x}',t,t')$ is defined as the derivative

$$G(\mathbf{x},\mathbf{x}',t,t') = \frac{\delta\langle\phi(\mathbf{x},t)\rangle}{\delta J(\mathbf{x}',t)}\Big|_{J=0} \tag{3.12}$$

with respect to an external source $J(\mathbf{x}',t)$ for the field ϕ, evaluated at $J \to 0$. But if we would have added a source term $J(\mathbf{x}',t)$ in the Langevin Eq. (3.1), this term would be converted in our formalism into a linear contribution $\tilde{\phi}J$ to the response functional $S[\tilde{\phi},\phi]$. That is,

$$\partial_t\phi(\mathbf{x},t) = F[\phi](\mathbf{x},t) + N[\phi]\eta(\mathbf{x},t) + J(\mathbf{x},t) \tag{3.13}$$

implies

$$S_J[\tilde{\phi},\phi] = S[\tilde{\phi},\phi] + \int d^d x\, dt\, J(\mathbf{x},t)\tilde{\phi}(\mathbf{x},t) \tag{3.14}$$

Thus, we have

$$\begin{aligned} G(\mathbf{x}-\mathbf{x}',t-t') &= \frac{\delta\int\mathscr{D}\phi\,\phi(\mathbf{x},t)P_J[\phi])}{\delta J(\mathbf{x}',t)}\Big|_{J=0} \\ &= \int\mathscr{D}\phi\,\phi(\mathbf{x},t)\tilde{\phi}(\mathbf{x}',t')P_{J=0}[\phi] \\ &= \langle\phi(\mathbf{x},t)\tilde{\phi}(\mathbf{x}',t')\rangle \end{aligned} \tag{3.15}$$

the announced result.

Notice that we can in principle also integrate out over the $\tilde{\phi}$ field in the path integral (3.10). This would lead to a theory depending only on the physical field ϕ. However, in many cases, including BARW-DP, this new theory would be non-local in nature, which very much difficults its study.

3.2. Doi-Peliti formalism

In the particular case of reaction-diffusion systems, a specific and in principle exact method exists for the mapping of the dynamics of the system onto a field theory. The method was developed in [68, 173], and uses as input the master equation for the system. In this section we develop this Doi-Peliti formalism, which will prove to be central in this work.

First, a quantum-theory like operator formalism can be constructed for the reaction-diffusion system at hand. With this, a coherent state representation can be found, which allows, via a continuum-time limit, to arrive to a field theory exactly encoding all the information of the stochastic fluctuations. We go step by step in this derivation.

3.2.1. Creation and annihilation operators

In order to simplify the presentation we stick for the time being to the study of one of the simplest possible reactions, pure annihilation, $2A \to \emptyset$. Furthermore, let us start with the single site problem ; we add diffusion later on. The master equation for single site pure annihilation with rate λ reads (see the preceding chapter)

$$\left.\frac{dP(t,n)}{dt}\right|_{2A\to\emptyset} = \lambda\Big((n+2)(n+1)P(t,n+2) - n(n-1)P(t,n)\Big) \tag{3.16}$$

where $P(n,t)$ stands for the probability of having n particles at time t. Now, as shown in [68], there exists a very convenient way of re-expressing this equation in terms of creation and annihilation operators in a (non-quantum) Fock space. This is constructed as follows. The possible states of the system are given by the number n of particles. We then associate to the set of all possible values of n an orthonormal basis in a Hilbert space, and to the state of the system (as given by the probability $P(n,t)$ of being in a given state $|n\rangle$) a vector in this space. Using Dirac notation :

$$|\psi(t)\rangle = \sum_n P(n,t)|n\rangle \tag{3.17}$$

with

$$\langle n \mid m\rangle = n!\delta_{nm} \tag{3.18}$$

These definitions allow us to re-write the master equation in the form

$$\frac{d\,|\psi(t)\rangle}{d\,t} = -\hat{H}|\psi(t)\rangle \tag{3.19}$$

which is very reminiscent of the Schrödinger equation in imaginary time, with $\hat{H}$ a (non-hermitian) operator encoding the probability rates of the system. The formal solution of (3.19) reads

$$|\psi(t)\rangle = e^{-\hat{H}t}|\psi(0)\rangle \tag{3.20}$$

with $|\psi(0)\rangle$ encoding the initial state of the system.

$$|\psi(0)\rangle = \sum_n P(n,0)|n\rangle \tag{3.21}$$

We can also associate an operator to any physical observable O depending only on the occupation numbers. Any such observable is a function of the number of particles n. If O takes the value $O(n)$ when there are n particles on site, we define the action of the operator associated to O as

$$\hat{O}|n\rangle = O(n)|n\rangle \tag{3.22}$$

Now, in order to obtain mean values of operators within this formalism we cannot just use the standard quantum mechanical matrix element, since this would involve two factors of the probabilities $P(n,t)$. It is then useful to define a special projection state $\langle\cdot|$

$$\langle\cdot| = \sum_n \langle n| \tag{3.23}$$

With this, we can write a mean value of an operator as

$$\langle\hat{O}\rangle(t) = \sum_n O(n)P(t,n) = \sum_n \langle n|\, O(n)P(t,n)|n\rangle = \langle\cdot|\,\hat{O}|\psi(t)\rangle = \langle\cdot|\,\hat{O}e^{-Ht}|\psi(0)\rangle \tag{3.24}$$

Due to conservation of probability, the projection state obeys the relations

$$\langle\cdot\mid\psi(t)\rangle = \sum_n P(t,n) = 1, \qquad \langle\cdot|\,\hat{H} = 0 \tag{3.25}$$

where the last relation stems from derivation of the first equation with respect to time.

Having the analogous of a Fock space, it is natural to introduce creation and annihilation operators. In the context of reaction diffusion systems it is useful to introduce them by means of the relations

$$\begin{aligned} a|n\rangle &= n|n-1\rangle & \langle n|\,a &= \langle n+1|\,(n+1) \\ a^\dagger|n\rangle &= |n+1\rangle & \langle n|\,a^\dagger &= \langle n-1| \end{aligned} \tag{3.26}$$

notice that a and $a^\dagger$ have a different normalization as in the quantum case. The usefulness of this admittedly non-standard convention can be seen by rewriting the master equation in terms of these creation and annihilation operators. In the specific case of single-site PA, it is easy to find

$$\frac{d|\psi(t)\rangle}{dt} = \lambda\Big(a^2 - (a^\dagger)^2 a^2\Big)|\psi(t)\rangle = -\hat{H}^{PA-1S}(a, a^\dagger)|\psi(t)\rangle \tag{3.27}$$

as can be seen by substituting the definition (3.17) of the ket $|\psi(t)\rangle$. This construction would not be possible in terms of creation and annihilation operators obeying the usual normalization properties. The usual commutation relations between a and $a^\dagger$ operators are nonetheless preserved, as well as their hermitian conjugacy, as can be seen by directly applying the commutators to any arbitrary state ψ written in the number basis.

$$[a^\dagger, a] = 1, \qquad [a, a] = 0, \qquad [a^\dagger, a^\dagger] = 0 \tag{3.28}$$

Notice that the projection bra is an eigenvector of the creation operator

$$\langle\cdot|\, a^\dagger = \langle\cdot| \tag{3.29}$$

this allows for the simplification of the functional dependence on $a^\dagger$ of observables, when one is interested in mean values. In order to see how this works, one must first perform the normal ordering of the chosen operator, with all creations operators to the left of all annihilation operators. The normal ordering can always be achieved by using the commutation relations (3.29) above. The operator resulting from the application of (3.28) to $\hat{O}(a, a^\dagger)$ in order to put it in normal order will be called $\hat{O}(a, a^\dagger)_N$. We then have

$$\langle\hat{O}(a, a^\dagger)\rangle = \langle\hat{O}(a, a^\dagger)_N\rangle = \langle\cdot|\, \hat{O}(a, a^\dagger)_N|\psi(t)\rangle = \langle\hat{O}(a)\rangle \tag{3.30}$$

with $\hat{O}(a) \equiv \hat{O}(a, a^\dagger = 1)_N$. This allows for a re-writing of the problem just in terms of the creation operator a. Such a procedure proves to be useful later on.

A lattice and diffusion can be easily added to this formalism, by taking into account different lattice sites. We define the vector basis $|n_i\rangle$, with i a lattice site index, and also extend the definition of the creation and annihilation operators for all sites, with

$$[a_i, a_j^\dagger] = [a_i, a_j] = [a_i^\dagger, a_j^\dagger] = 0 \tag{3.31}$$

if site i is different from site j. Diffusion can be written as a reaction which mixes neighboring sites $\langle i, j\rangle$

$$\frac{d|\psi(t)\rangle}{dt}\Big|_D = D\sum_{\langle i,j\rangle}\Big(a_i^\dagger a_j - a_j^\dagger a_i\Big)|\psi(t)\rangle \tag{3.32}$$

We can then write the full Hamiltonian for the PA system in the Doi-Peliti formalism (compare with Eqs. (2.18) and (2.19) before)

$$\hat{H}^{PA}(a,a^\dagger) = D\sum_{\langle i,j\rangle}\left(a_i^\dagger - a_j^\dagger\right)\left(a_i - a_j\right) - \lambda\sum_i\left(a_i^2 - (a_i^\dagger)^2 a_i^2\right) \tag{3.33}$$

Within this Fock space formalism, we can show some general identities which will be of use later on. The first one is

$$e^{za^\dagger a}O(a^\dagger,a)e^{-za^\dagger a} = O(e^z a^\dagger, e^{-z}a) \tag{3.34}$$

with z an arbitrary complex number and $O(a^\dagger,a)$ is an operator in normal order. As we shall see later, we can use this equation to rescale the creation and annihilation operators, while preserving their algebra. The second identity reads

$$e^{ya^\dagger + za}O(a^\dagger,a)e^{-ya^\dagger - za} = O(a^\dagger + z, a - y) \tag{3.35}$$

which is useful in order to shift the operators. We mainly use this last relation under the form

$$e^a O(a^\dagger,a) = O(a^\dagger + 1, a)e^a \tag{3.36}$$

To prove these identities it is sufficient to calculate their matrix element between two arbitrary number states $\langle m|$ and $|n\rangle$, by expressing observable functions in terms of its series expansion in creation and annihilation operators.

$$O(a^\dagger,a) = \sum_{\alpha\beta} O_{\alpha\beta}(a^\dagger)^\alpha a^\beta \tag{3.37}$$

For the l.h.s. of Eq. (3.34), we can write the matrix element between number states as

$$\begin{aligned}
\langle m|\, e^{za^\dagger a}O(a^\dagger,a)e^{-za^\dagger a}|n\rangle &= \langle m|\, e^{zm}\sum_{\alpha\beta} O_{\alpha\beta}(a^\dagger)^\alpha a^\beta e^{-zn}|n\rangle \\
&= \sum_{\alpha\beta} e^{z(m-n)}C_\beta O_{\alpha\beta}\delta_{m-n,\alpha-\beta} \\
&= \langle m|\sum_{\alpha\beta} e^{z(\alpha-\beta)}O_{\alpha\beta}(a^\dagger)^\alpha a^\beta|n\rangle \\
&= \langle m|\, O(e^z a^\dagger, e^{-z}a)|n\rangle
\end{aligned} \tag{3.38}$$

which is the desired result, with $C_\beta = n(n-1)(n-2)\ldots(n-\beta)$. An analogous calculation yields identities (3.35) and (3.36).

3.2.2. Coherent states

Many problems can be studied within the Doi formalism as presented so far [105, 8]. We are here nonetheless mostly interested in having a field theory reformulation of the reaction-diffusion system at hand. In order to arrive to such a goal, we introduce a special basis of states, the coherent states, which are used to construct a path integral representation.

Again, we start by studying a single site. The coherent states can be constructed using the creation operator. They are formally related to the semi-classical representation of states in quantum optics. A coherent state is labeled by a complex number ϕ

$$|\phi\rangle = \mathcal{N} e^{\phi a^\dagger} |0\rangle \tag{3.39}$$

Equivalently, we could have defined

$$|\phi\rangle = \mathcal{N} \sum_n \frac{\phi^n}{n!} |n\rangle \tag{3.40}$$

and also

$$\langle\phi| = \mathcal{N} \sum_n \frac{(\phi^*)^n}{n!} \langle n| \tag{3.41}$$

In all these expressions, the normalization factor $\mathcal{N}$ was introduced in order to ensure the useful property $\langle\phi \mid \phi\rangle = 1$. This imposes $\mathcal{N} = \exp\left(-|\phi|^2/2\right)$. Then, the action of the annihilation operator on a coherent sate is simply

$$a|\phi\rangle = \mathcal{N} \sum_{n=1}^{\infty} \phi \frac{\phi^{n-1}}{(n-1)!} |n-1\rangle = \phi|\phi\rangle \tag{3.42}$$

so that the coherent state $|\phi\rangle$ is an eigenstate of the annihilation operator a, with eigenvalue ϕ.

The coherent states form an overcomplete basis of the Fock space of the theory. To see this, we first obtain a closure relation for the coherent states. To do this, we start with the closure relation in the number basis

$$\hat{1} = \sum_n \frac{1}{n!} |n\rangle\langle n| = \sum_{n,m} \frac{1}{n!} |n\rangle\langle m| \, \delta_{nm} \tag{3.43}$$

A technical step is needed here. We can rewrite the Kronecker delta in an integral form using

$$\delta_{nm} = \frac{1}{\pi\, n!} \int d^2\phi \, e^{-|\phi|^2} \phi^m (\phi^*)^n \quad \text{where} \quad d^2\phi = d(\mathrm{Re}(\phi))\, d(\mathrm{Im}(\phi)) \tag{3.44}$$

With this, we can now re-express the closure relation (3.43)

$$1 = \int \frac{d^2\phi}{\pi} |\phi\rangle\langle\phi| \tag{3.45}$$

This expression generalizes straightforwardly to multiple lattice sites, according to

$$1 = \int \prod_i \Big(\frac{d^2\phi_i}{\pi} \Big) |\{\phi_i\}\rangle\langle\{\phi_i\}| \tag{3.46}$$

where $\{\phi_i\} = (\phi_1, \phi_2, \ldots)$ denotes a set of coherent state eigenvalues, one for each annihilation operator a_j, and the ket $|\{\phi\}\rangle = |\phi_1\rangle \otimes |\phi_2\rangle \otimes \ldots$ is defined using the tensor product.

Coherent states in different sites of the lattice are orthogonal. We deduce the inner product between any two coherent states to be

$$\langle\{\phi_i\} \mid \{\varphi_k\}\rangle = \prod_i \langle\phi_i \mid \varphi_i\rangle = \prod_i \exp\Big(-\frac{|\phi_i|^2}{2} - \frac{|\varphi_i|^2}{2} + \phi_i^* \varphi_i \Big) \tag{3.47}$$

Notice that in this representation the projection state $|\cdot\rangle$ is proportional to the dual coherent state with all eigenvalues $\phi_i = 1$, which we call for brevity $\langle 1|$. Notice also that, for uniform, random initial conditions the particle distribution is a Poissonian on each site i, i.e.,

$$|\psi(0)\rangle = \prod_i \Big(\frac{\bar{n}_0^{n_i}}{n_i!} e^{-\bar{n}_0} \Big) (a_i^\dagger)^{n_i} |0\rangle \tag{3.48}$$

with $\bar{n}_0$ the average number of particles per site. In this case then the initial state $|\phi(0)\rangle$ is proportional to the coherent state $|\bar{n}_0\rangle$ with all $\phi_i = \bar{n}_0$.

Using the coherent states we can arrive to the desired field theory formulation of the out of equilibrium problem. First, the (stochastic) temporal evolution is divided into N slices of size $\Delta t = t/N$ by using the Trotter's formula [208]

$$|\psi(t)\rangle = \exp\big(\hat{H}t\big)\,|\psi(0)\rangle = \lim_{N\to\infty} \big(\hat{1} + \hat{H}\Delta t\big)^N |\psi(0)\rangle \tag{3.49}$$

Then, we can insert between each two slices a complete basis of coherent states with eigenvalues $\{\phi_{i,\tau}\} = (\phi_{1,\tau}, \phi_{2,\tau}, \ldots)$. In this notation, τ indexes the time slice, while i is the lattice index. The expression (3.24) for the stochastic mean value of an observable can then be rewritten as

$$\langle O(t)\rangle = \mathcal{Z}^{-1} \lim_{N\to\infty} \int \prod_{\tau=0}^{N} \Big[d^2\{\phi_{i,\tau}\} \langle\{\phi_{i,\tau}\}|\, \hat{1} + \Delta t \hat{H} |\{\phi_{i,\tau-1}\}\rangle \Big] \\ \times\, d^2\{\phi_{i,0}\} \langle\cdot|\, \hat{O} |\{\phi_{i,N}\}\rangle \langle\{\phi_{i,0}\} \mid \psi(0)\rangle \tag{3.50}$$

where $\mathcal{Z}$ is a normalization factor and

$$d^2\{\phi_{i,\tau}\} = \prod_i d\phi_{i,\tau}\, d\phi_{i,\tau}^* \equiv \prod_i d\big(\mathrm{Re}\phi_{i,\tau}\big)\, d\big(\mathrm{Im}\phi_{i,\tau}\big) \tag{3.51}$$

We now proceed to analyze the various contributions.

Let us first consider the term between square brackets. We define

$$H_{i,\tau} = \frac{\langle\{\phi_{i,\tau}\}|\,\hat{H}|\{\phi_{i,\tau-1}\}\rangle}{\langle\{\phi_{i,\tau}\}\mid\{\phi_{i,\tau-1}\}\rangle} \tag{3.52}$$

This function is obtained in a straightforward way by normal ordering $\hat{H}$ and acting with $a_i^\dagger$ to the left and a_i to the right, such that all creation or annihilation operators become respectively replaced with the coherent state eigenvalues ϕ_i^* or ϕ_i. As for the denominator in the r.h.s. of (3.52), it can be factorized

$$\langle\{\phi_{i,\tau}\}\mid\{\phi_{i,\tau-1}\}\rangle = \prod_i \langle\phi_{i,\tau}\mid\phi_{i,\tau-1}\rangle \tag{3.53}$$

where, for each lattice site we have, according to Eq. (3.47)

$$\begin{aligned}\langle\phi_{i,\tau}\mid\phi_{i,\tau-1}\rangle &= \exp\left(-\frac{|\phi_{i,\tau}|^2}{2} - \frac{|\phi_{i,\tau-1}|^2}{2} + \phi_{i,\tau}^*\phi_{i,\tau-1}\right)\\ &= \exp\left(\frac{|\phi_{i,\tau}|^2}{2} - \frac{|\phi_{i,\tau-1}|^2}{2}\right)\exp\left(-\phi_{i,\tau}^*[\phi_{i,\tau}-\phi_{i,\tau-1}]\right)\end{aligned} \tag{3.54}$$

When stringing together different time slices, the first exponential term is going to cancel out, except for the initial and final times. In the case of the final time we also have to take into account the action of the projection operator. We have

$$\langle\cdot\mid\phi_{i,N}\rangle\exp\left(\frac{|\phi_{i,\tau}|^2}{2}\right) \propto \langle 1\mid\phi_{i,N}\rangle\exp\left(\frac{|\phi_{i,\tau}|^2}{2}\right) \propto \exp\left(\phi_{i,N}\right) \tag{3.55}$$

whereas for the initial time we find

$$\begin{aligned}\langle\phi_{i,N}\mid\psi(0)\rangle\exp\left(\frac{|\phi_{i,0}|^2}{2}\right) &\propto \langle\phi_{i,N}\mid\bar{n}_0\rangle\exp\left(\frac{|\phi_{i,0}|^2}{2}\right)\\ &\propto \exp\left(-|\phi_{i,0}|^2+\phi_{i,0}^*\bar{n}_0\right)\end{aligned} \tag{3.56}$$

The final time also enters in the evaluation of the expression $\langle\cdot|\,\hat{O}|\{\phi_{i,N}\}\rangle$. There, we can always use the normal ordered operator $\hat{O}(\{\phi_{i,N}\})$ so that

$$\langle\cdot|\,\hat{O}|\{\phi_{i,N}\}\rangle = \langle\cdot\mid\{\phi_{i,N}\}\rangle O(\{\phi_{i,N}\}) \tag{3.57}$$

where the latter function is obtained from $\hat{O}$ through the replacement $a_i \to \phi_{i,N}$.

Putting all these pieces together, the mean value (3.50) can be rewritten

$$\begin{aligned}\langle O(t)\rangle = \mathcal{Z}^{-1}\lim_{N\to\infty}\int\prod_{\tau=0}^{N} d^2\{\phi_{i,\tau}\}O(\{\phi_{i,\tau}\})\left[1+\Delta t H_{i,\tau}\right]^N\\ \exp\left(\sum_i\left[-\sum_{\tau=1}^{N}\phi_{i,\tau}^*\left(\phi_{i,\tau}-\phi_{i,\tau-1}\right)+\phi_{i,N}+\bar{n}_0\phi_{i,0}^*-|\phi_{i,0}|^2\right]\right)\end{aligned} \tag{3.58}$$

Let us now determine the $H_{i,\tau}$ term for PA. As the Hamiltonian (3.33) is already normal ordered, the expression for $H_{i,\tau}$ follows simply from (3.33) by substituting all operators $a_i^\dagger$ and a_i for its eigenvalues $\phi_{i,\tau}^*$ and $\phi_{i,\tau-1}$ (following the definition (3.52))

$$H_{i,\tau}^{PA} = D\sum_{\langle i,j\rangle}\left(\phi_{i,\tau}^* - \phi_{j,\tau}^*\right)\left(\phi_{i,\tau-1} - \phi_{j,\tau-1}\right) - \lambda\sum_i\left(\phi_{i,\tau-1}^2 - (\phi_{i,\tau}^*)^2\phi_{i,\tau-1}^2\right) \quad (3.59)$$

Now we can analyze the continuous time limit $N\to\infty$, $\Delta t\to 0$. In this limit, the discrete set of values taken by the variables $\phi_{i,\tau}$ for $\tau = \{0,\ldots,N\}$ gets promoted to a continuous set of values $\phi_i(t)$, for t running between 0 and t_f. The discrete difference between two contiguous temporal values tends then to the time derivative

$$\phi_{i,\tau} - \phi_{i,\tau-1} = \Delta t\frac{\partial\phi_i}{\partial t}(t_\tau) + \mathcal{O}(\Delta t^2) \quad (3.60)$$

keeping terms up to first order in Δt, in coherence with the Trotter's formula. In the continuum time limit we then have

$$-\sum_{\tau=1}^{N}\phi_{i,\tau}^*\left(\phi_{i,\tau} - \phi_{i,\tau-1}\right) \simeq -\Delta t\sum_{\tau=1}^{N}\phi_{i,\tau}^*\frac{\partial\phi_i}{\partial t}(t_\tau) \xrightarrow{N\to\infty} \int_0^{t_f} dt\,\phi_i^*(t)\partial_t\phi_i(t) \quad (3.61)$$

Turning our attention back to $H_{i,\tau}$, we see that ϕ^* and ϕ are in principle evaluated at slightly different time slices τ and $\tau-1$. However, the error introduced by evaluating them at the same value τ is of order Δt^2, and we choose to evaluate both functions in the same instant τ. Doing so has no consequences if no time derivatives are present, like in the case of interaction potential-like terms, but subtleties do arise, related to the Itô prescription to be discussed below.

We again use Trotter's formula, in order to reconstruct the exponential term

$$\lim_{N\to\infty}\prod_{\tau=0}^{N}\left[1+\Delta t H_{i,\tau}\right] = \exp\left(\sum_\tau \Delta t H_{i,\tau}\right) \xrightarrow{\Delta t\to 0} \exp\left(\int_0^{t_f} dt\,H(t)\right) \quad (3.62)$$

Finally, the product over all values of τ of the integration measures in (3.51) is promoted to a functional measure over t for continuous time

$$d^2\{\phi_{i,\tau}\} = \prod_i d\phi_{i,\tau}\phi_{i,\tau}^* \xrightarrow{N\to\infty} \prod_i\int \mathcal{D}\phi_i(t)\mathcal{D}\phi_i^*(t) \quad (3.63)$$

Putting all the pieces together, we obtain the continuum limit of (3.50). This yields an exact representation of the mean value of any observable on the lattice as a functional integral over two fields, ϕ and ϕ^*. Notice that these two complex

conjugate fields are usually considered as independent fields, by performing the change of variables,

$$\{\mathrm{Re}(\phi), \mathrm{Im}(\phi)\} \to \{\phi, \phi^*\} \tag{3.64}$$

which is a usual procedure in field theory [208]. As we shall see in detail below, this transformation is easy to at all orders in a perturbative expansion, but hides many subtleties from a non-perturbative point of view. We choose from now on a change of notation $\phi^* \to \hat{\phi}$ in order to emphasize this independence. We are then led to write

$$\langle O(t) \rangle = \mathcal{Z}^{-1} \int \prod_i \mathcal{D}\phi_i \mathcal{D}\hat{\phi}_i O(\{\phi_i\}(t)) e^{-S[\hat{\phi}_i, \phi_i, t]} \tag{3.65}$$

with

$$-S[\hat{\phi}_i, \phi_i, t_f] = \sum_i \left(\int_0^{t_f} dt \left(\hat{\phi}_i(t) \partial_t \phi(t) + H(t) \right) - \phi_i(t_f) - \bar{n}_0 \hat{\phi}_i(0) \right) \tag{3.66}$$

where we have renamed the final time t_f for clarity. Notice that we have neglected the initial time term $\hat{\phi}_i(0)\phi_i(0)$, which originally coupled the fields at the same instant $t = 0$. As will be discussed below, this term must be zero in the Itô prescription.

We have thus derived a field theory associated to a microscopic reaction-diffusion system. The action (3.66) is of first order in time, which stems from the diffusive character of the microscopic dynamics, possessing a Galilean space-time symmetry. Notice that no a priori assumption was made about the nature of the stochastic noise in the system (nor either the deterministic part) : stochastic fluctuations are automatically translated into field fluctuations in this formalism.

Optionally, we can also look for a continuum space version of the field theory. This limit of course represents an approximation of the physical reaction-diffusion system if it is defined on a lattice, but it is sufficient in order to study its universal properties. This limit can be found via the substitutions $\sum_i \to a^{-d} \int d^d x$, $\phi_i(t) \to a^d \phi(\mathbf{x}, t)$ and $\hat{\phi}_i(t) \to \hat{\phi}(\mathbf{x}, t)$, with a the lattice spacing. The difference between nearest neighbors in the diffusion term tends in the continuum space limit to a gradient term

$$\sum_{\langle i,j \rangle} (\phi_j^*(t) - \phi_i^*(t))(\phi_j(t) - \phi_i(t)) \to a^2 \nabla^2 \phi(\mathbf{x}, t)$$

(to first nontrivial order). Notice that we have arbitrarily chosen $\phi(\mathbf{x}, t)$ to have the same scaling dimensions as a density. While the continuum limit could

have been been defined differently, this prescription ensures that the bulk contribution to the action vanish for $\hat{\phi} \to 1$, as it must due to probability conservation, given property (3.25) above. It is also useful to rescale the initial time contribution $\bar{n}_0 \to a^d n_0$. After a suitable rescaling of the microscopic rates we can rewrite the continuum spatial limit of Eq. (3.65) as

$$\langle O(t) \rangle = \mathcal{Z}^{-1} \int \prod_i \mathcal{D}\phi_i \mathcal{D}\hat{\phi}_i O(\phi(\mathbf{x}, t)) e^{-S[\hat{\phi}_i, \phi_i, t]} \tag{3.67}$$

We now define the generating functional $\mathcal{Z}[\hat{J}, J]$

$$\mathcal{Z}[\hat{J}, J] = \int \mathcal{D}\phi \mathcal{D}\hat{\phi} e^{-S[\hat{\phi}, \phi, t]} e^{\int_{\mathbf{x},t} \left(J\phi + \hat{J}\hat{\phi} \right)} \tag{3.68}$$

where the addition of the sources $J(\mathbf{x}, t)$ and $\hat{J}(\mathbf{x}, t)$ must be done in a particular way, to be discussed below. The action S reads, in the case of PA

$$S^{PA}[\hat{\phi}, \phi, t_f] = \int d^d x \Big[\int_0^{t_f} dt \left[\hat{\phi} \left(\partial_t - D\nabla^2 \right) \phi - \lambda \left(1 - \hat{\phi}^2 \right) \phi^2 \right] - \phi(t_f) - n_0 \hat{\phi}(0) \Big] \tag{3.69}$$

It is often convenient to perform a shift in the field $\hat{\phi}$, defining

$$\hat{\phi}(\mathbf{x}, t) = 1 + \bar{\phi}(\mathbf{x}, t) \tag{3.70}$$

In addition to modifying the form of H, this has the effect of replacing

$$\int_0^{t_f} dt \, \hat{\phi} \partial_t \phi \to \phi(t_f) - \phi(0) + \int_0^{t_f} dt \, \bar{\phi} \partial_t \phi \tag{3.71}$$

Which cancels the final time term $-\phi(\mathbf{x}, t_f)$ in the action, and introduces a new initial term which can again be neglected within the Itô prescription. After applying this field shift we obtain

$$S^{PA}[\bar{\phi}, \phi, t_f] = \int d^d x \Big[\int_0^{t_f} dt \left[\bar{\phi} \left(\partial_t - D\nabla^2 \right) \phi - \lambda \left(2 + \bar{\phi} \right) \bar{\phi} \phi^2 \right] - n_0 \bar{\phi}(0) \Big] \tag{3.72}$$

Notice that, in principle, this field shift would break the original complex conjugate relation between the fields ϕ and $\hat{\phi}$. This conjugacy property can be very useful to analyze the convergence at large fields of the partition function (3.68). Fortunately, it is easy to prove that integration over the shifted field can be contour deformed when performing the functional integral (3.68), so that we can get back to the original variables inside the path integral, in order to recover the known convergence properties.

Alternatively, as mentioned before, it would have also been possible to perform this shift at the level of the creation and annihilation operators. In terms of these we have (for the case of a single site, following Eq. (3.24))

$$\begin{aligned}\langle\hat{O}\rangle(t) &= \langle\cdot|\,\hat{O}(a)e^{-tH(a^\dagger,a)}|\psi(0)\rangle \\ &= \langle 0|\,e^{a}\hat{O}(a)e^{-tH(a^\dagger,a)}B(a^\dagger)|0\rangle \\ &= \langle 0|\,e^{a}e^{-(t_f-t)H(a^\dagger+1,a)}\hat{O}(a)e^{-tH(a^\dagger+1,a)}B(a^\dagger+1)|0\rangle \end{aligned} \tag{3.73}$$

for any $t_f > t$, with $B(a^\dagger) = \sum_n P(n,0)(a^\dagger)^n = \sum_n \left(\frac{\bar{n}_0^n}{n!}e^{-\bar{n}_0}\right)(a^\dagger)^n$ in the Poissonian case. In the last line of (3.73) we have used the conservation of probability (this relation shows that $t_f > t$ can be chosen at will). We can rewrite this equation using (3.36), to obtain

$$\langle\hat{O}\rangle(t) = \langle 0|\,\hat{O}(a)e^{-tH(a^\dagger+1,a)}B(a^\dagger+1)|0\rangle \tag{3.74}$$

Thus, using this trick it is possible to implement the Doi shift (3.70), while maintaining the fact that the operators are hermitic conjugate. In particular, performing this shift at this stage, the coherent states formalism would lead to a shifted action which is written in terms of fields that are complex conjugate, and no additional manipulations would be required. Notice that, once again, the term coming from the initial condition is also shifted and that the term which corresponds to $\phi(t_f)$ disappears.

3.2.3. Generalization to other reactions

The procedure shown above can be easily generalized to other locally interacting particle systems with relative ease, by following the same steps. If for example we want to add a branching reaction $A \xrightarrow{\sigma} 2A$, it suffices to add to the Hamiltonian the term coming from the master equation that corresponds to this reaction

$$\hat{H}^\sigma = -\sigma\sum_i \left(1-(a_i^\dagger)^2\right)a_i^\dagger a_i \tag{3.75}$$

Generically, for a BARW system involving reactions $A \xrightarrow{\sigma_m} mA$ and $kA \xrightarrow{\lambda_k} \emptyset$ the method described above eventually leads to the action

$$\begin{aligned}S[\hat{\phi},\phi,t_f] = \int d^dx\Big[\int_0^{t_f} dt\Big[\hat{\phi}\left(\partial_t - D\nabla^2\right)\phi - \lambda_k\left(1-\hat{\phi}^k\right)\phi^k \\ + \sigma_m\left(1-\hat{\phi}^m\right)\hat{\phi}\phi\Big] - \phi(t_f) - n_0\hat{\phi}(0)\Big]\end{aligned} \tag{3.76}$$

more general field theories for single species systems can be written in an analogous way.

It is also possible to describe multiple species reaction-diffusion systems [195], which, as we have mentioned, appear naturally in chemistry and biology. At the level of the master equation, multiple species systems require additional sets of occupation numbers. For example, for two species the probability shall be written as $P(\{m\},\{n\},t)$, where $\{m\}$, $\{n\}$ denote respectively the occupation numbers of A and B particles. The second quantized formulation then requires different creation and annihilation operators for each particle species. The state vector would therefore be constructed as

$$|\psi(t)\rangle = \sum_{\{m\},\{n\}} P\big(\{m\},\{n\},t\big) \prod_i (a_i^\dagger)^{m_i} (b_i^\dagger)^{n_i} |0\rangle \tag{3.77}$$

In the case of two species pair annihilation $A+B \to \emptyset$ we would have the Hamiltonian operator

$$\hat{H} = D_A \sum_{\langle i,j\rangle} \left(a_i^\dagger - a_j^\dagger\right)\left(a_i - a_j\right) + D_B \sum_{\langle i,j\rangle} \left(b_i^\dagger - b_j^\dagger\right)\left(b_i - b_j\right) \\ - \lambda \sum_i (1 - a_i^\dagger b_i^\dagger) a_i b_i \tag{3.78}$$

Correspondingly, in the mapping to a field theory we must introduce two sets of coherent states, resulting in four independent fields.

Further generalizations are straightforward. The general results is as follows : for a given reaction, two terms appear in the Doi-Peliti Hamiltonian. The first term is always positive and contains one creation and one annihilation operator for each reactant, normal ordered. For example, for $A+B \to \emptyset$ one obtains $a^\dagger b^\dagger ab$. The second term is always negative, and consists in an annihilation operator for every reactant and a creation operator for every product, normal ordered. For example, for $A+B \to \emptyset$ this contribution would be ab, while for $A+A \to A$ it becomes $a^\dagger a^2$ and for $A+B+C \to 3A$ it would read ${a^\dagger}^3 abc$. With this recipe it is easy to obtain a second quantized version of any reaction diffusion system, from which a field theory version can be obtained by rewriting the Hamiltonian in terms of coherent states corresponding to each species $A, B, C\ldots$ (together with suitable initial and final time terms for each field).

Chapitre 4

Non perturbative renormalization group

Having introduced the field theories of interest, we now move on to introduce the method of choice in this work, the Non Perturbative Renormalization Group. It is based on Wilson's original ideas [204, 205] about the RG, re-expressed in a modern and convenient language. In section 4.1 we derive the basic NPRG equations, as presented for the first time in [201]. These equations contain all the information of a given system, but are of course impossible to solve exactly. The interest of NPRG techniques, then, is to devise new approximation schemes, often impossible within other approaches. Since its conception, much progress has been made in using the technique in a very wide range of physical problems, ranging from quantum gravity [152] to superconductivity [141, 7], frustrated [193] and disordered [192] systems and liquid theory [168, 169] among many others.

In section 4.2 we present what is the most used such approximation scheme within the NPRG, known as the Derivative Expansion. Being based on an expansion over the characteristic momenta of a system, it is very well suited for the study of long distance properties of critical systems. Although technically it lacks a small expansion parameter, the derivative expansion can be systematically improved, and high orders of it have been studied in the case of the Ising universality class, reaching the best field theoretical precision for exponents at order ∇^6 [51].

A new approximation scheme within the NPRG has shown to be a powerful mean to tackle problems when we are not only interested in the low momentum regime, but also in momentum-dependent quantities, such as the full momentum dependence of n-point vertices or scaling functions. This scheme is called the BMW approximation (after Blaizot, Méndez-Galain and Wschebor), and is presented in section 4.5, along with some results obtained for the experi-

mentally measured scaling function of the Ising universality class, presented in section 4.6.

As we shall see, the resulting equations are generally too complex for an analytical treatment, and approximations based on numerical analysis must be undertaken. This represents one of the hardest obstacles for exploiting the NPRG techniques (at least when sophisticated approximations are used), as numerical stability of the often complicated systems of partial differential equations turns too often to be a concern.

Also, a natural generalization of the NPRG technique has been recently developed for the specific study of lattice systems [137]. We introduce this lattice-NPRG formalism in section 4.3, in order to use it in section 4.4 for finding the probability distribution of the order parameter of the Ising model in $d = 3$.

4.1. The NPRG equations

In this section we introduce the basic NPRG formalism in the equilibrium context, leaving for later its generalization in order to deal with out of equilibrium statistical systems. General introductions to the NPRG can be found in [63, 18]. Here we simply give a quick overview, which assumes previous knowledge of more standard perturbative RG techniques [208, 132].

As a canonical system for developing the NPRG ideas, we use Euclidean φ^4 scalar field theory, which shows critical behaviour, with a phase transition belonging to the Ising universality class, as we have discussed before. In the following we mostly use the language of quantum field theory, but the same ideas can be developed from the point of view of statistical mechanics or quantum many-body theory, see for example [90, 18].

Renormalization Group techniques are most useful when there is separation of scales in the system, as is the case in phase transitions, where, near the critical point, the behaviour of the system is characterized by lenghtscales orders of magnitudes larger than the microscopic molecular interaction scales. Intuitively, the RG consists in considering modified, effective versions of the theory at different (length or) momentum scales. By studying the flow of these effective theories as we change the scale considered, we can extract physical information about the system, particularly if it presents separation of modes or scale free behaviour. In the canonical case, one knows the microscopic theory defining the model, and wants to know how fluctuations (statistical or quantum) of these microscopic degrees of freedom change its macroscopic behaviour, one length scale at a time. Let us formalize these ideas.

When written as a field theory, all the physical information of a system is

encoded in the generating functional, which reads generically

$$\mathcal{Z}[J] = \int \mathcal{D}\varphi e^{-S[\varphi]+\int_x J(x)\varphi(x)} \tag{4.1}$$

where x stands for the spatial coordinate, $J(x)$ is a source coupled linearly to the physical field, and, as stated before, we are using the case of a scalar field theory as a showcase of the method. Generalizations to field theories having more complex structure are straightforward, as is shown below for the case of out of equilibrium systems.

Correlation functions are obtained by functional differentiation of the generating functional with respect to the external source $J(x)$

$$\langle\varphi(x_1)\dots\varphi(x_n)\rangle = \frac{1}{\mathcal{Z}[J_0(x)]}\frac{\delta^n\mathcal{Z}[J]}{\delta J(x_1)\dots\delta J(x_n)}\Big|_{J_0(x)} \tag{4.2}$$

for a given value of the external source $J(x) = J_0(x)$. As usual, it is in general more convenient to work with the connected correlation functions, also known as the cumulants of the theory, which, as can be shown [132, 208], are generated by the logarithm of the partition function, the free energy

$$\langle\varphi(x_1)\dots\varphi(x_n)\rangle_c = \frac{\delta^n\log\mathcal{Z}[J]}{\delta J(x_1)\dots\delta J(x_n)}\Big|_{J_0(x)} \tag{4.3}$$

We then define as usual

$$W[J] = \log\mathcal{Z}[J] \tag{4.4}$$

Now, within the NPRG one defines a modified theory in which fluctuations with low momenta are suppressed. The frontier between low and high momenta is a scale k that varies between the microscopic scale Λ (when $k = \Lambda$ all fluctuations are suppressed) and 0 (when $k = 0$ all fluctuations are taken into account). See Fig. 4.1 for a schematic representation of the NPRG procedure. This modification can be done in many ways [18, 141], but here we consider the case where it is achieved by the addition of what is known as a regulator term to the action S. From now on we identify with $k = \Lambda$ the microscopic scale, which we can relate to the inverse lattice spacing of the model $\Lambda \sim 1/a$ in a lattice system, or any other such natural momentum cutoff scale. We then have, for every scale k between Λ and 0, an effective theory given by the partition function

$$\mathcal{Z}_k[J] = \int \mathcal{D}\varphi e^{-S[\varphi]-\Delta S_k[\varphi]+\int_x J(x)\varphi(x)} \tag{4.5}$$

with $\Delta S_k[\varphi]$ the (additive) regulator term. It turns out that this flow of effective theories is most easily studied when it is written in terms of what is known as the effective average action Γ_k. The effective action functional Γ of the theory

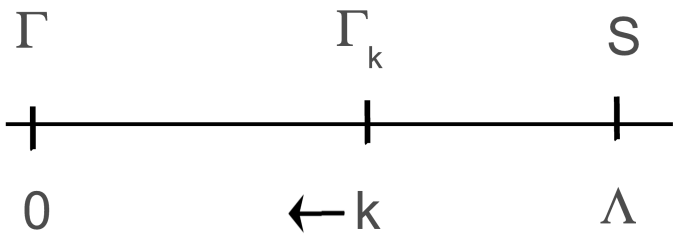

FIGURE 4.1 – Schematic representation of the NPRG flow. At a given momentum scale k one obtains an effective action Γ_k interpolating between the microscopic action S and the full average action Γ. In the standard NPRG procedure the regulator term at $k = \Lambda$ is taken in such a way as to have $\Gamma_{k=\Lambda} = S$, see text.

is a generalization of the Gibbs free energy in statistical mechanics, and stems from the Legendre transform of the usual free energy, so that Γ is a functional of the mean value of φ in presence of sources J.

$$\Gamma[\phi] = \sup_J \Big(\int_x \phi(x) J(x) - W[J] \Big), \qquad \phi(x) = \langle \varphi(x) \rangle_J \tag{4.6}$$

The effective action is the generating functional of the one particle irreducible (1PI) correlation functions of the theory, from which any correlation function can be constructed in a standard way [208]. At a given scale k, an effective average action can be trivially defined as

$$\tilde{\Gamma}_k[\phi_k] = \int_x \phi_k(x) J(x) - W_k[J] \tag{4.7}$$

with

$$\phi_k(x) = \langle \varphi(x) \rangle_J = \frac{\delta W_k[J]}{\delta J} \tag{4.8}$$

In this work we follow the usual convention and consider a slightly modified version of the effective average action, for reasons to be explicited below

$$\Gamma_k[\phi_k] = \Big(\int_x \phi_k(x) J(x) - W_k[J] - \Delta S_k[\phi_k] \tag{4.9}$$

together with (4.8). The effective average action Γ_k performs an average over fluctuations with large characteristic momenta $q > k$, by integrating out these modes. In order to achieve that, the regulator term must comply with certain requisites. Here we consider a regulator term of the form

$$\Delta S_k[\varphi] = \frac{1}{2} \int \frac{d^d q}{(2\pi)^d} \varphi(q) R_k(q) \varphi(-q) \tag{4.10}$$

in momentum space. The cut-off function $R_k(q)$ is used to perform the separation of modes, by adding a mass-like term of order k^2 to the low momentum modes of the field $\phi(q)$, with $q \leq k$, in such a way as to suppress low momentum fluctuations of the system. At the same time, modes with $q > k$ are not significantly modified. As k is changed from the microscopic scale Λ to the the macroscopic scale $k = 0$, Γ_k continuously interpolates between the microscopic action and the full effective action. In order to have this, we must impose the following limits for the cut-off function

$$\begin{aligned} R_k(q) &\to \infty \qquad \text{as} \qquad k \to \Lambda \\ R_k(q) &\to 0 \qquad \text{as} \qquad k \to 0 \end{aligned} \tag{4.11}$$

where this first constraint guarantees that no fluctuation is taken into account at the microscopic scale, thus recovering the usual mean field approximation, $\Gamma_{k=\Lambda} = S$, as we shall show in detail below. The second constraint implies in its turn that $\Gamma_{k=0} = \Gamma$, so that the full theory is recovered. A typical sketch of R_k in momentum space is shown in Fig. 4.2.

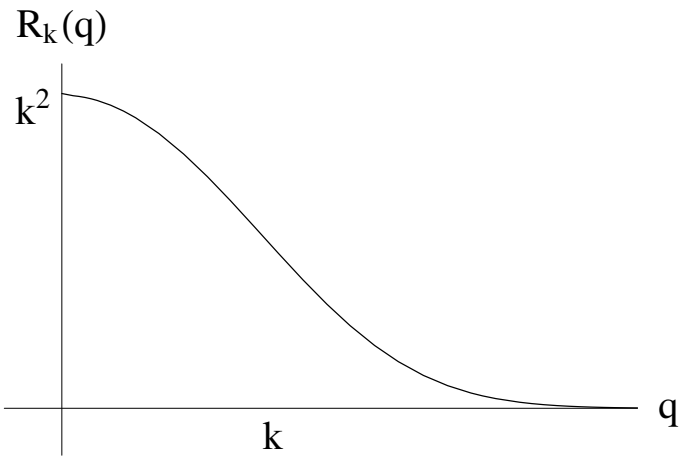

FIGURE 4.2 – Typical form of the cut-off function R_k in the NPRG. It is designed to dampen fluctuations with characteristic momentum $q < k$, by the addition of an artificial mass. At the same time, fluctuations with larger characteristic momentum q are left almost unchanged.

As we change the value of k, we obtain a flow of effective theories. These are non-physical, but if we choose the regulator term to obey properties (4.11), these effective theories share the physics of the system of interest up to the scale k, while modifying the macroscopic physics between k and $k = 0$ (again, see Fig. 4.2). Notice that if the theory shows critical behaviour, as in φ^4 theory, the

partition function has non-analyticities at the critical point. Typically, this regulator term ΔS_k can then be chosen as to rend the theory analytical for all $k \neq 0$, a fact that rests at the basis of most of the approximation techniques within the NPRG.

The NPRG approach consists then in the following

1. Re-write the problem as a field theory, and find its microscopic action S. Generally this implies the use of some kind of coarse-graining argument, although in some cases an exact mapping can be found. In our example, we could be initially interested in the universal aspects of the Ising model, which is known to belong to the same universality class as the φ^4 scalar field theory. This translation into a field theory language is not strictly speaking part of the NPRG formalism, but in many cases it is a hard part of the procedure.
2. The microscopic action is the initial condition for the NPRG flow equations $\Gamma_{k=\Lambda}[\phi] = S[\phi]$ (for a possible alternative see the discussion on the lattice NPRG formalism below).
3. At each momentum scale k the theory is modified by the presence of a regulator term, which suppresses fluctuations with characteristic scales $q > k$. If the theory is fully regularized, this ensures that no non-analyticities exist in momenta in the modified theory. In particular, no authentic scale-free behaviour would be found in the effective theory for $k > 0$.
4. Even though the modified effective theories are non-physical, they are constructed in such a way as to contain the physical information of the system at momentum scales higher than the scale k. They have thus a clear physical meaning, which would not be the case if we worked with the RG flow of effective Hamiltonians, à la Wilson-Polchinski [174]. In both cases the behaviour of the RG flow of theories also yield relevant information about the system. For example, in critical theories one expects the existence of fixed points of the flow (when working with properly rescaled variables, see below) signaling the existence of scale free behaviour when $k \to 0$ [63].

The NPRG flow of effective theories is governed by one equation, known as the Wetterich equation [201]. Here we show a simple derivation for it. The flow of the effective average action Γ_k is given by $\partial_k \Gamma_k$, at a fixed ϕ, that we now compute

$$\partial_k \Gamma_k[\phi] = -\partial_k W_k\Big|_\phi + \int_x \partial_k J(x)\big|_\phi \phi(x) - \frac{1}{2}\int_{x,y} \phi(x)\partial_k R_k(x-y)\phi(y) \qquad (4.12)$$

We then need the derivative of the free energy at fixed ϕ, which can be obtained

using the relation

$$\partial_k W_k\Big|_\phi = \partial_k W_k\Big|_J + \int_y \partial_k J(y)\big|_\phi \frac{\delta W_k}{\delta J(y)} \tag{4.13}$$

which is a functional generalization of a known property in multivariate calculus. It is easy to obtain the first term in (4.13) explicitly by differentiating Eq. (4.5) which leads to

$$\partial_k W_k\Big|_J = -\frac{1}{2}\int_{x,y} \partial_k R_k(x-y)\left[\frac{\delta^2 W_k}{\delta J(y)} + \frac{\delta W_k}{\delta J(x)}\frac{\delta W_k}{\delta J(x)}\right] \tag{4.14}$$

and, going back to Eq. (4.12), and using $\phi(x) = \frac{\delta W_k}{\delta J(x)}$, we obtain

$$\partial_k \Gamma_k = \frac{1}{2}\int_{x,y} \partial_k R_k(x-y)\frac{\delta^2 W_k}{\delta J(x)\delta J(y)} \tag{4.15}$$

In order to obtain the Wetterich equation, which is written only in terms of the effective average action Γ_k and its functional derivatives, we use the equality

$$\begin{aligned}\delta^{(d)}(x-y) = \frac{\delta\phi(x)}{\delta\phi(y)} &= \int_z \frac{\delta\phi(x)}{\delta J(x)\delta J(z)}\frac{\delta J(z)}{\delta\phi(y)} \\ &= \int_z \frac{\delta^2 W_k}{\delta J(x)\delta J(z)}\frac{\delta J(z)}{\delta\phi(y)}\end{aligned} \tag{4.16}$$

Now, using that by definition

$$\frac{\delta\Gamma_k}{\delta\phi(z)} = J(z) - \int_u R_k(z-u)\phi(u) \tag{4.17}$$

we can write

$$\delta^{(d)}(x-y) = \int_z \frac{\delta^2 W_k}{\delta J(x)\delta J(z)}\left[\frac{\delta^2\Gamma_k}{\delta\phi(y)\delta\phi(z)} + R_k(z-y)\right] \tag{4.18}$$

which allows us to finally arrive at the Wetterich equation

$$\partial_k \Gamma_k[\phi] = \frac{1}{2}\int_{x,y} \partial_k R_k(x-y)\left[\Gamma_k^{(2)}[\phi] + R_k\right]^{-1}(x,y) \tag{4.19}$$

This expression is readily generalized for many component fields to [63]

$$\partial_k \Gamma_k[\phi] = \frac{1}{2}\mathrm{tr}\left[\partial_k R_k(x-y)\left[\Gamma_k^{(2)}[\phi] + R_k\right]^{-1}(x,y)\right] \tag{4.20}$$

where tr stands for summation over internal indices and integration over continuous variables, and now R_k and $\left[\Gamma_k^{(2)} + R_k\right]^{-1}$ are matrices in field space.

The initial condition for the Wetterich equation is taken at the microscopic scale Λ, and is provided by the microscopic action

$$\Gamma_{k=\Lambda}[\phi] = S[\varphi = \phi] \tag{4.21}$$

if the cut-off function complies conditions (4.11).

The Wetterich equation is an exact equation, and contains all the physical information of the system, including any non-perturbative or strongly correlated effects which may be present. It is of course a highly non-trivial equation, and in almost any practical application approximations should be performed upon it, in order to extract physical information. These approximations, however, can be of a very different nature from those performed within other methods in the literature. Therein lies the main potentiality of the approach, which, as we shall see below, shows indeed a great capability to generate results difficult to obtain otherwise.

Importantly, if a cut-off function $R_k(q)$ can be found which respects all the symmetries of the theory (that is, all the symmetries present in the microscopic action S and in the functional measure $\mathscr{D}\varphi$), then this equation ensures that the symmetries are preserved in Γ_k for all k, up to the physical case $k = 0$. This can be a very efficient way of dealing with nonperturbative proofs for the existence of symmetries, and we shall see some examples in the following. However, it is not always easy to find a suitable cut-off function which does not break any symmetry of the given theory. It can then be the case that the symmetries are only recovered when $k \to 0$, which can greatly complicate the NPRG treatment for theories with complex symmetries, such as gauge theories [90, 73, 74, 75].

As we will be dealing with translation-invariant systems, we mainly work in Fourier space, where total momentum is conserved and the Wetterich equation reads

$$\partial_k \Gamma_k = \frac{1}{2} \int_q \left[\partial_k R_k(q) \left[\Gamma_k^{(2)}(q, -q) + R_k(q) \right]^{-1} \right] \tag{4.22}$$

where $\int_q$ stands for integration over momenta. This equation has the familiar structure of a 1-loop perturbative result, which can be represented in a diagrammatic way, see Fig. 4.3. In this case, though, the propagator running inside the loop is not the perturbative one, but instead the "dressed" propagator

$$G(q;\phi) = \left[\Gamma_k^{(2)}(q) + R_k(q) \right]^{-1} \tag{4.23}$$

which becomes, in the limit $k \to 0$, the full field dependent propagator of the theory. The 1-loop structure stands in the NPRG case for a functional equation for the effective average action. But this structure allows us, by iteration, to recover the usual perturbative calculations, at any order in the loop expansion for

small couplings. To do so, we can use the bare parameters as inputs in Eq. (4.22) to obtain the 1-loop average action. Substituting this last again into Eq. (4.22) yields the 2-loop average action and so on. But more importantly, this 1-loop structure is useful for designing new approximation schemes, as we shall see below.

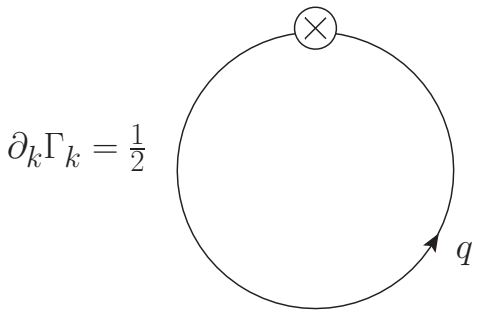

FIGURE 4.3 – Diagrammatic representation of the Wetterich equation (4.22). The circle represents the dressed propagator $G_k(q)$, the cross indicates the insertion of the $\partial_k R_k(q)$ term.

To simplify the expressions for the $\Gamma_k^{(n)}$ the differential operator $\tilde{\partial}_k$ is often used, which by definition only acts on the k dependence of the cut-off term $R_k(q)$. The Wetterich equation can then be written as

$$\partial_k \Gamma_k = \frac{1}{2} \tilde{\partial}_k \int_q \log\left(\left[\Gamma_k^{(2)}(q,-q) + R_k(q)\right)\right] \tag{4.24}$$

The Wetterich equation can be re-expressed as an infinite hierarchy of equations for the vertex functions

$$\tilde{\Gamma}_k^{(n)}(q_1,\ldots,q_n;\phi) = \frac{\delta^n \Gamma_k[\phi]}{\delta\phi(q_1)\ldots\delta\phi(q_n)} \tag{4.25}$$

which in general we evaluate in a uniform field configuration. As is usually done when dealing with translation-invariant systems, we define for convenience the vertex functions to be

$$(2\pi)^d \delta^{(d)}(q_1+\ldots+q_n)\Gamma_k^{(n)}(q_1,\ldots,q_n;\phi) = \left.\frac{\delta^n \Gamma_k[\phi]}{\delta\phi(q_1)\ldots\delta\phi(q_n)}\right|_{\phi(x)=\phi} \tag{4.26}$$

These 1PI vertex functions can be related in a standard way [208] to the n-point correlation functions of the theory. The hierarchy of equations for them [199]

can be found by functional differentiation of Eq. (4.22). Differentiation with respect to $\phi(p)$ yields

$$\begin{aligned}\partial_k \frac{\delta\Gamma_k}{\delta\phi(p)} &= -\frac{1}{2}\int_{q_1} \partial_k R_k(q_1) G_k(q_1,q_2) \frac{\delta\Gamma_k^{(2)}(q_2,q_3)}{\delta\phi(p)} G_k(q_3,-q_1) \\ &= -\frac{1}{2}\int_{q_1} \partial_k R_k(q_1) G_k(q_1,q_2)\Gamma_k^{(3)}(q_2,q_3,p) G_k(q_3,-q_1) \end{aligned} \tag{4.27}$$

where we have omitted dependencies on ϕ in the propagator G_k and the ver-

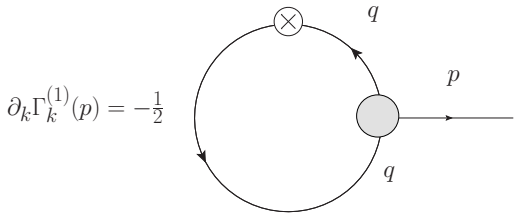

FIGURE 4.4 – Diagrammatic representation of the NPRG flow equation for $\Gamma_k^{(1)}$ at uniform field.

tices $\Gamma_k^{(n)}$ for the sake of brevity. Using standard Feynman diagram conventions, this flow equation can be represented as in Fig. 4.4, with an insertion in one propagator representing the $\partial_k R_k$ term. The diagrams shows the NPRG 1-loop structure when evaluated at uniform field. Proceeding further we can also write an equation for $\Gamma_k^{(2)}$

$$\begin{aligned}\partial_k\Gamma_k^{(2)}(p_1,p_2) = &\int_{\{q_i\}} \partial_k R_k(q_1) \\ &\times G_k(q_1,q_2)\Gamma_k^{(3)}(p_1,q_2,-q_3) G_k(q_3,-q_4)\Gamma_k^{(3)}(p_2,q_4,-q_5) G_k(q_5,-q_1) \\ &-\frac{1}{2}\int_{\{q_i\}} \partial_k R_k(q_1) G_k(q_1,q_2)\Gamma_k^{(4)}(q_2,-q_3,p_1,p_2) G_k(q_3,-q_1)\end{aligned} \tag{4.28}$$

which, evaluated in a uniform field configuration yields

$$\begin{aligned}\partial_k\Gamma_k^{(2)}(p) = &\int_q \partial_k R_k(q) G_k(q)\Gamma_k^{(3)}(p,q,-p-q) G_k(p+q)\Gamma_k^{(3)}(p,q,-p-q) G_k(q) \\ &-\frac{1}{2}\int_q \partial_k R_k(q) G_k(q)\Gamma_k^{(4)}(q,-q,-p,p) G_k(q)\end{aligned} \tag{4.29}$$

where propagators have only one argument due to momentum conservation. Again, this equation can be represented in a diagrammatic way as a dressed 1-loop 1PI equation, as shown in Fig. 4.5. By functional derivation we can then

obtain equations for any $\Gamma_k^{(n)}$. The operator $\tilde{\partial}_k$ can be used to simplify the diagrammatic representation of the NPRG equations. See Fig. 4.6 for an example.

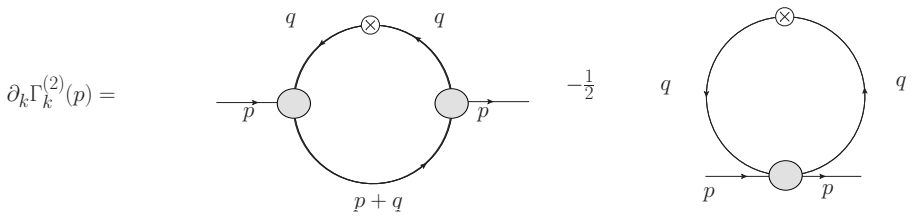

FIGURE 4.5 – Diagrammatic representation of the NPRG flow equation for $\Gamma_k^{(2)}$ at uniform field.

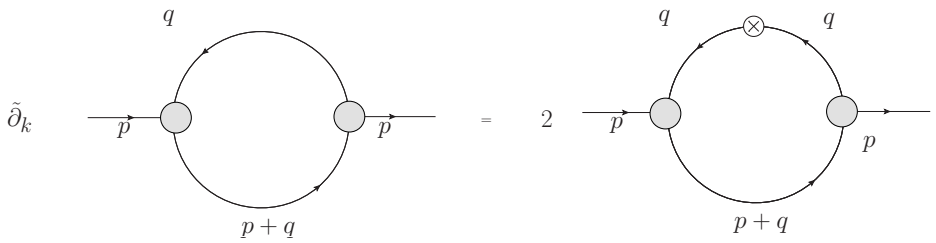

FIGURE 4.6 – Example of the action of the $\tilde{\partial}_k$ operator.

It is clear from the diagrammatic representations that the flow equation for $\partial_k\Gamma_k^{(n)}$ involves $\Gamma_k^{(n+1)}$ and $\Gamma_k^{(n+2)}$, so that we deal with an infinite tower of equations. This hierarchy can be truncated in a more or less sophisticated way, in order to obtain approximate results for low-order vertex functions [199, 73, 74, 75]. We return to this idea when we discuss the BMW approximation later on.

Up to now we have been mostly using the scalar field theory language. In fact, the distinction between theories arises mostly (apart from, obviously, the field content) in the initial condition, the microscopic action. For φ^4 theory, the microscopic action reads

$$S[\varphi] = \int_x \left(\frac{1}{2}\big(\nabla\varphi\big)^2 + \frac{r_0}{2}\varphi^2 + \frac{u}{4!}\varphi^4 \right) \tag{4.30}$$

which has the known Z_2 symmetry $\varphi \to -\varphi$. Notice that in order to work comfortably with this theory, it would be important that the NPRG regulator term does not break this Z_2 symmetry explicitly. This is trivially the case for a mass-like cut-off function R_k such as those we have been discussing, see Eq. (4.10).

In the standard NPRG formalism, one wants the initial condition for the average action, that is, $\Gamma_{k=\Lambda}$ to be given by the microscopic action, or, what is equivalent, to suppress fluctuations of any characteristic scale, and thus to taking a mean field approach. In order to comply with this requisite, we assume, as said before, that $R_{k=\Lambda} \to \infty$. This stems from substituting Eq. (4.17) into the definition of W_k, obtaining

$$e^{-\Gamma_k[\phi]} = \int \mathscr{D}\varphi \exp\left(-S[\varphi] + \int_x \frac{\delta\Gamma_k}{\delta\phi(x)}(\varphi(x)-\phi(x))\right) \times \exp\left(-\frac{1}{2}\int_{x,y}(\varphi(x)-\phi(x))R_k(x-y)(\varphi(y)-\phi(y))\right) \quad (4.31)$$

where the form of the last term is due to our choice, Eq. (4.9), for the definition of the effective average action. If we now choose a function $R_k(q)$ that diverges for all q as $k \to \Lambda$ then, in this limit

$$\exp\left(-\frac{1}{2}\int_{x,y}(\varphi(x)-\phi(x))R_k(x-y)(\varphi(y)-\phi(y))\right) \sim \delta(\varphi-\phi) \quad (4.32)$$

that is, it behaves as a functional Dirac delta. Therefore we have, just as we wanted

$$\Gamma_k[\phi] \xrightarrow{k\to\Lambda} S[\varphi=\phi] \quad (4.33)$$

This, a posteriori, also explains our choice (4.9) for the definition of Γ_k. If the cut-off R_k is such that it does not diverge in the limit $k \to \Lambda$, but is only very large, we have

$$\Gamma_{k=\Lambda}[\phi] \sim S[\varphi=\phi] \quad (4.34)$$

which is usually enough when considering universal quantities, or for large enough Λ in asymptotically free theories (or simply when working up to a given precision).

4.2. Derivative expansion and field truncation

As mentioned before, one of the main advantages of the NPRG formalism is that it allows for the application of new approximation schemes, generally not based on a perturbative expansion. This can be very useful in the study of strongly correlated systems such as critical phase transitions. In this section we discuss two such schemes, which are by now standard NPRG tools : the derivative expansion and the field truncation.

Critical phenomena and phase transitions, by their very nature, depend on the large scale collective behaviour of the microscopic degrees of freedom, and

depend thus on the long distance properties of the system. We can then conceive an approximation scheme which tries to preserve the long distance physics while truncating the short distance or large momentum behaviour. The derivative expansion is exactly such a kind of approximation.

The derivative expansion (DE from now on) is the most widely used approximation scheme within the NPRG [18], and is based on the decoupling of large momentum modes, and on the analyticity of the vertex functions, guaranteed, as we mentioned before, by the presence of the regulator term in the effective average action. It amounts to formulating an ansatz for $\Gamma_k[\phi]$ as an expansion in the space (and eventually time) derivatives of the field, or equivalently in its momentum and frequency dependence. For instance, at order ∂^2 in the equilibrium scalar field theory

$$\Gamma_k[\phi]^{\mathscr{O}(\partial^2)} = \int_x \left[V_k(\phi) + \frac{1}{2} Z_k(\phi)(\nabla\phi)^2 + \mathscr{O}(\nabla^4) \right] \tag{4.35}$$

where the function $V_k(\phi)$, the so-called running effective potential, describes the physics of spatially uniform field configurations. The running effective potential is thus identical to the effective potential in the limit $k \to 0$

$$V_k(\phi) = \frac{1}{\Omega}\Gamma_k[\phi]\Big|_{\phi(x)=\phi} \xrightarrow{k\to 0} V(\phi) \tag{4.36}$$

The field renormalization factor $Z_k(\phi)$ contains information about field configurations which are slowly varying in space, having low characteristic wavenumbers. The functional Wetterich flow equation then reduces at this order to a set of two coupled partial differential equations for the functions $V_k(\phi)$ and $Z_k(\phi)$. Notice that we are expanding in momentum, while at the same time keeping information about all the vertex functions $\Gamma_k^{(n)}$, for arbitrary n.

The lowest order DE approximation is called the Local Potential Approximation (LPA) and amounts to keeping the bare momentum dependence all along the NPRG flow. The LPA ansatz thus reads

$$\Gamma_k[\phi]^{LPA} = \int_x \left[\frac{1}{2}(\nabla\phi)^2 + V_k(\phi) \right] \tag{4.37}$$

At this level of approximation the Wetterich equation (4.22) is projected onto just one partial differential equation for the effective potential. This equation can be readily obtained, and reads [63]

$$\partial_k V_k(\rho) = \frac{1}{2}\int_q \frac{\partial_k R_k(q)}{q^2 + R_k(q) + V_k'(\rho) + 2\rho V_k''(\rho)} \tag{4.38}$$

where

$$\rho = \frac{1}{2}\phi^2 \tag{4.39}$$

is the Z_2 invariant, and $V_k'(\rho)$ and $V_k''(\rho)$ are derivatives of V_k w.r.t. ρ. This equation must be completed with an initial condition for $V_k(\rho)$, which in the case at hand is written as

$$V_\Lambda(\rho) = r_0\rho + \frac{u}{6}\rho^2 \tag{4.40}$$

This relatively simple approximation turns out to be sufficient for describing qualitatively and even quantitatively the critical behaviour of the Ising universality class in $d = 3$ [63]. Notice that, even if it only involves a function evaluated at momentum $p = 0$, the effective potential, the LPA keeps track of all the functional dependence on the fields of this function, a feat which is not possible within the usual perturbative calculations, and which can in principle be used to extract non-universal predictions, such as was the case of the T_c for CO_2 in [181]. This is due to the fact that we are keeping information about all vertex functions $\Gamma^{(n)}$, and not only about the low-order vertices stemming from perturbatively renormalizable coupling constants. Recently, a natural generalization of the LPA has been also used within the lattice NPRG formalism, giving excellent results regarding the critical temperature T_c of the Ising model. We discuss this in more detail below.

For purposes of obtaining a good description of this universality class in all space dimensions (in particular in dimension $d = 2$), higher orders of the DE should be used, using for example the ∂^2 ansatz (4.35). The ∂^2 order of the DE leads in the Ising case to a coupled set of flow equations for $Z_k(\phi)$ and $V_k(\phi)$. The function $Z_k(\phi)$ can be used to obtain the value of the critical exponent η. It is convenient to rewrite this function as

$$Z_k(\phi) = Z_k\zeta_k(\phi) \tag{4.41}$$

with the renormalization condition

$$\zeta_k(\phi_0) = 1 \tag{4.42}$$

where one usually takes ϕ_0 to be the running minimum of the potential $V_k(\phi)$. The usual method then consists in defining a running anomalous dimension

$$\eta_k = -k\partial_k \log Z_k \tag{4.43}$$

Sometimes a third intermediate approximation is used, which amounts to ignoring the field dependency of $Z_k(\phi)$ (that is to say, impose $\zeta_k(\phi) = 1$ for all values of ϕ and k). One ends up with a set of coupled differential equations for the potential $V_k(\phi)$ and a field renormalization constant Z_k. This approximation, which we call LPA' in tis work, offers a certain improvement ever the LPA results.

Notice that, whereas Z_k diverges close to the Ising critical point, η_k approaches a fixed point value η^* near the fixed point governing the phase transition. It has been demonstrated [18, 63, 23] that this fixed point value coincides with the anomalous dimension critical exponent η. Having a good approximation to η turns out to be important in order to improve the accuracy of the results. Indeed, the LPA yields $\eta = 0$ (as is clear from the absence of a field renormalization term Z_k), which is simply too far away from the exact value $\eta = 0.25$ in $d = 2$ to expect it to work in this dimension. The much smaller value of the anomalous dimension in $d = 3$, of the order of $\eta \sim 0.036$, explains why the LPA yields much better results in this dimension.

order	ν	η
∂^0	0.6506	0
∂^2	0.6281	0.044
∂^4	0.632	0.033
∂^6	0.6303	0.0358
7-loops	0.6304(13)	0.0335(25)
Monte-Carlo	0.63002(10)	0.03627(25)

TABLE 4.1 – Critical exponents of the three dimensional Ising model. ∂^0, ∂^2 and ∂^4 correspond to the order of the truncation of the derivative expansion (the NPRG method)[39]. For completeness, we have recalled in the last lines the results obtained both perturbatively [208] and by using Monte-Carlo [103].

Table 4.1 shows the results obtained from different orders of the DE in the Ising universality class, as well as the 7-loop results from [208] for reference. As can be seen, the seriew converges rapidly to the best known results in the literature, besting even 7-loops results when comparing with Monte-Carlo.

The DE ansätze presented here can be easily generalized to treat $O(N)$ models in all dimensions for any value of N (including $N = 0$ or negative values of N [148]), as well as different values of d [198, 18], always yielding competitive results.

The derivative expansion has been pushed to orders as high as six [51] in the study of the ϕ^4 scalar field theory, with results for universal quantities that are among the best that exist in the literature. When considering more complex problems though, it is often convenient to perform a field expansion for the functions intervening in the Γ_k ansatz, such as $V_k(\phi)$ and $Z_k(\phi)$ in Eq. (4.35). The field expansion for a generic function $X_k(\rho)$ of an invariant ρ is written as

its Taylor series around a given configuration ρ_0

$$X_k(\rho) = \sum_{i=0}^{p} x_k^{(i)} (\rho - \rho_0)^i \tag{4.44}$$

to a given order p. The main advantage of the field truncation it that it turns the partial differential equations for the quantities $X_k(\rho)$ in the DE into a set of coupled ordinary differential equations for the couplings $x_k^{(i)}$, which reduces considerably the numerical complexity involved in the solution of the NPRG equations. Most of the time it proves useful to start by a field truncation, even if its convergence properties are in general very difficult or impossible to assess.

A truncation in the field can always be considered, even without recourse to the DE. This has been studied within other approximations method in the NPRG [73, 74, 75, 98], for a wide range of systems.

4.3. Lattice NPRG

In the last years a version of the NPRG has been specifically developed [70, 137] for dealing with lattice systems, without having to necessarily pass through a continuum space formulation. This can be vital for condensed matter applications, as in the study of highly correlated fermion or boson systems and quantum phase transitions, where mean field theories are unable to give a good starting point for the NPRG flow, due to on-site fluctuations. An example is provided by the localization transition between a Mott insulator and a superfluid in lattice boson systems, where the two-pole structure of the local (on-site) propagator is crucial for the very existence of the transition, but is impossible to reproduce starting from the mean field approximation.

The idea behind the lattice formulation of the NPRG is to start from a reference system which already includes on site fluctuations. This initial reference system can be made to correspond to the local limit of decoupled lattice sites, which is in general possible to solve, at least by a simple numerical analysis. In the long distance limit, the lattice NPRG is equivalent to the usual NPRG formalism explained above, yielding identical results for universal quantities.

We consider a lattice field theory defined on a d-dimensional hypercubic lattice

$$H[\varphi] = \frac{1}{2} \sum_{\mathbf{q}} \varphi_{-\mathbf{q}} \varepsilon_0(\mathbf{q}) \varphi_{\mathbf{q}} + \sum_{\mathbf{x}} V_0(\varphi_{\mathbf{x}}) \tag{4.45}$$

where $\{\mathbf{x}\}$ denotes the N sites of the lattice, and ϵ_0 is the dispersion relation of the system, to be explicited below. For the sake of simplicity we again consider the case of a one-component scalar field $\varphi_{\mathbf{x}}$. Its Fourier transform $\varphi_{\mathbf{q}} =$

$N^{-1/2}\sum_{\mathbf{x}} e^{-i\mathbf{q}\cdot\mathbf{x}}\varphi_{\mathbf{x}}$ is the Fourier transformed field, with the momentum $\mathbf{q}$ restricted to be in the first Brillouin zone of the reciprocal lattice.

The potential V_0 is defined as the zero momentum contribution to the Hamiltonian. We also define the quantities $\varepsilon_0^{max} = \text{máx}_{\mathbf{q}}\,\varepsilon_0(\mathbf{q})$ and $\varepsilon_0 = \text{lím}_{\mathbf{q}\to 0}\,\varepsilon_0(\mathbf{q})/\mathbf{q}^2$. Lengths are measured with respect to the lattice spacing.

As in the preceding sections, we implement the NPRG procedure with the addition of a regulator term to the Hamiltonian

$$\Delta H_k[\varphi] = \frac{1}{2}\sum_{\mathbf{q}} \varphi_{-\mathbf{q}} R_k(\mathbf{q})\varphi_{\mathbf{q}} \tag{4.46}$$

In the standard NPRG formalism, the cut-off function is taken to (almost) diverge in the limit $k \to \Lambda$, in order to have an initial condition for the average action which is given by the microscopic action. Here, instead, we choose a form for the regulator term more adapted to the characteristics of a lattice system. We take

$$\begin{aligned} &R_k(\mathbf{q}) \sim 0 && \text{for} && \varepsilon_0(\mathbf{q}) > \varepsilon_0 k^2 \quad \forall \mathbf{q} \\ &R_k(\mathbf{q}) \sim \varepsilon_0 k^2 && \text{for} && \varepsilon_0(\mathbf{q}) < \varepsilon_0 k^2 \quad \forall \mathbf{q} \end{aligned} \tag{4.47}$$

a sketch of the effect of the lattice propagator on the effective dispersion relation can be seen in Fig. 4.7.

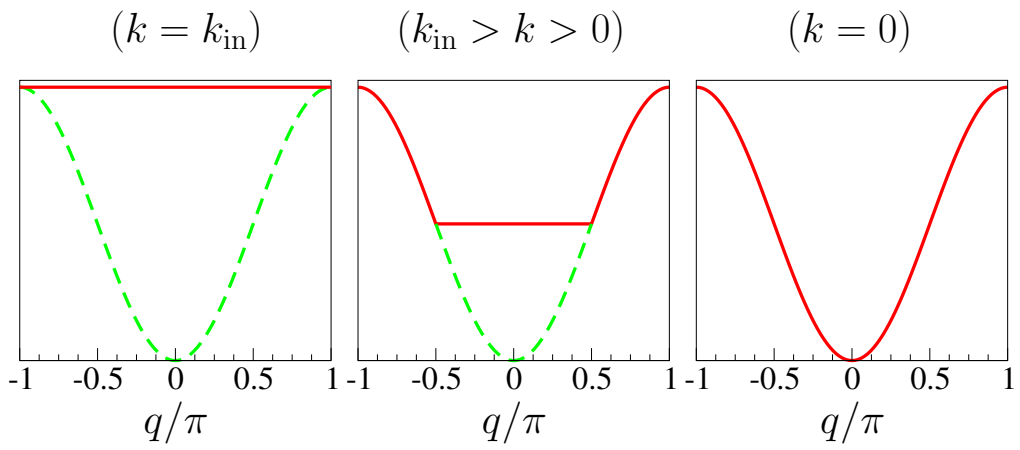

FIGURE 4.7 – Sketch of effective dispersion relation for different values of k in the lattice version of the NPRG in $d = 1$. Figure extracted from [137].

During the initial phase of the standard NPRG flow, when $k \to \infty$, fluctuation are integrated on momentum scales higher than ε_0^{max}, or, correspondingly, in lenghtscales smaller than the lattice spacing. Thus, the first part of the RG

procedure is purely local, since the effective dispersion $\varepsilon_0(\mathbf{q}) + R_k(\mathbf{q}) \sim \varepsilon_0 k^2$ remains dispersionless for all modes. The intersite coupling starts to play a role only for $k < k_{in}$, with k_{in} given by $\varepsilon_0 k_{in}^2 = \varepsilon_0^{max}$. In the lattice NPRG formalism, we bypass the initial stage of the flow up to this scale k_{in}. The initial condition for the average effective action, $\Gamma_{k_{in}}[\phi]$, would thus no longer be given by the microscopic Hamiltonian, but its computation reduces to a single-site problem, which can be seen as the integration of local fluctuations up to the scale k_{in}. In order to ensure these properties, the cut-off function must satisfy that at the initial scale

$$R_{k_{in}} = -\varepsilon_0(\mathbf{q}) + C \tag{4.48}$$

so that the sites are indeed decoupled. One of the most natural choices is to take $C = \varepsilon_0^{max}$, allowing to set up the NPRG procedure in the usual way, that is, modifying the dispersion relation for low energy modes without affecting the high energy modes.

Notice that, by making these choices, the standard and lattice NPRG procedures only differ in the initial condition when no approximation are performed. Both schemes would be equivalent for $k < k_{in}$ if the Wetterich equation (4.22) were solved exactly between the initial scale and k_{in}. Given that the use of approximations is unavoidable, the lattice NPRG appears as better suited for the study of systems originally defined on a lattice, and has the additional advantage of allowing the study of their non universal properties. For example, as shown in [137], lattice NPRG allows for a very accurate determination of the critical temperature T_c for the Ising and XY models in $d = 2$ and $d = 3$, even within a LPA type of approximation.

Being based on the local limit, this procedure is reminiscent of direct space Kadanoff scaling [119], but fluctuations are here integrated out in a different way, with an effective coupling which is long range and oscillating in real space for all $0 < k < k_{in}$.

Interestingly, the lattice NPRG can be applied to classical spin models without having to first derive a field theory. In the case of the Ising model in a d dimensional hypercubic lattice, this is done as follows. The effective partition function for the Ising model reads, in presence of an external field h

$$\begin{aligned}\mathcal{Z}_k[h] &= \sum_{\{S_\mathbf{x}\}} \exp\left(-J \sum_{\langle \mathbf{x},\mathbf{x}'\rangle} S_\mathbf{x} S_{\mathbf{x}'} - \frac{1}{2}\sum_{\mathbf{x},\mathbf{x}'} S_\mathbf{x} R_k(\mathbf{x},\mathbf{x}') S_{\mathbf{x}'} + \sum_\mathbf{x} h_\mathbf{x} S_\mathbf{x} \right) \\ &= \sum_{\{S_\mathbf{x}\}} \exp\left(\sum_\mathbf{q} S_{-\mathbf{q}} \Big[\varepsilon_0(\mathbf{q}) - 2\varepsilon_0 d + R_k(\mathbf{q}) \Big] S_\mathbf{q} + \sum_\mathbf{x} h_\mathbf{x} S_\mathbf{x} \right)\end{aligned} \tag{4.49}$$

where J represents in this context the coupling constant of the model, and we absorb the temperature in the definition of the couplings. For nearest neighbor

interactions

$$\varepsilon_0(\mathbf{q}) = 2\varepsilon_0 \sum_{i=1}^{d} \left(1 - \cos q_i\right) \tag{4.50}$$

as can be checked performing the discrete Fourier transform. The magnetization at site $\mathbf{x}$ is given by

$$m_{\mathbf{x}} = \langle S_{\mathbf{x}} \rangle = \frac{\partial \log \mathcal{Z}_k[h]}{\partial h_{\mathbf{x}}}\Big|_{h=0} \tag{4.51}$$

The standard NPRG formulation cannot be used, as the partition function is not a functional integral over a continuous field. A typical regulator term of the form $\varepsilon_0 k^2 \sum_{\mathbf{q}} S_{-\mathbf{q}} S_{\mathbf{q}} = \varepsilon_0 k^2 \sum_{\mathbf{x}} S_{\mathbf{x}}^2 = N\varepsilon_0 k^2$ would only add a constant term to the Hamiltonian. This is not the case within the lattice NPRG formalism. For analytical convenience we use here the generalization [137] of the popular step regulator first introduced in [135] for the use in lattice NPRG

$$R_k(\mathbf{q}) = (\varepsilon_0 k^2 - \varepsilon_0(\mathbf{q}))\Theta\big(\varepsilon_0 k^2 - \varepsilon_0(\mathbf{q})\big) \tag{4.52}$$

using this regulator, one finds

$$\mathcal{Z}_{k_{in}}[h] = \sum_{\{S_{\mathbf{x}}\}} \exp\left(-2d\varepsilon_0 N + \sum_{\mathbf{x}} h_{\mathbf{x}} S_{\mathbf{x}}\right) = e^{2d\varepsilon_0 N} \prod_{\mathbf{x}} z(h_{\mathbf{x}}) \tag{4.53}$$

with

$$z(h) = \sum_{S=\pm 1} e^{hS} = 2\cosh(h) \tag{4.54}$$

the partition function of a single site in an external field h. Up to an additive constant, we find

$$\Gamma_{k_{in}}[m] = \sum_{\mathbf{x}} V_{k_{in}}(\rho_{\mathbf{x}}) + \frac{1}{2} \sum_{\mathbf{q}} m_{-\mathbf{q}} \varepsilon_0(\mathbf{q}) m_{\mathbf{q}} \tag{4.55}$$

where the initial effective potential is given by [1]

$$V_{k_{in}}(\rho) = \frac{1}{2}\log(1-2\rho) + \sqrt{2\rho}\,\mathrm{atanh}\big(\sqrt{2\rho}\big) - 4d\varepsilon_0\rho \tag{4.56}$$

with $\rho_{\mathbf{x}} = m_{\mathbf{x}}^2/2$

The NPRG flow for the effective potential can be studied using the LPA, just as in the continuous case. The LPA flow equation reads, using the cut-off (4.52)

$$\partial_k V_k(\rho) = \frac{\varepsilon_0 k^2}{\varepsilon_0 k^2 + V_k'(\rho) + 2\rho V_k''(\rho)} \frac{1}{N} \sum_{\mathbf{q}} \Theta(\varepsilon_O k^2 - \varepsilon_0(\mathbf{q})) \tag{4.57}$$

We then have a version of the LPA which conserves information about the lattice. This is very convenient, e.g. to access non-universal properties of the system. We use this formalism later on, when studying the probability distribution of the order parameter of the Ising Model.

1. Here we have used the relationship $\log\cosh\mathrm{atanh}\, x = -\frac{1}{2}\log(1-x^2)$

4.4. Probability distribution of the Ising order parameter

The probability distribution of the order parameter fluctuations, $P(M)$, is a directly measurable scaling function characteristic of a given universality class. It is defined as

$$P(M,T,L) = P\Big(\sum_{\mathbf{x}} S_{\mathbf{x}} = M\Big) \xrightarrow{L\gg a} L^{\beta/\nu} f\Big(ML^{\beta/\nu}, \frac{L}{\xi}\Big) \tag{4.58}$$

Here we calculate not only the critical distribution $P(M,T_c)$ but consider the full family of finite-size scaling functions. Namely, we consider $P(M,a)$, where $a = (L/\xi)^{1/\nu}$. In this way, $a \to 0$ yields the critical distribution ($L/\xi >> 1$), while $a \to \infty$ yields a Gaussian function for the macroscopic variable, even if we are at the critical point. Thus there is a family of critical distribution functions between these two limits, with a smooth crossover of scaling functions which characterize the universality class.

We can study these functions within the NPRG formalism. Following the previous construction, the Hamiltonian (2.1) of the theory is modified by the regulator term, so that we have an effective Hamiltonian at the scale k

$$H_k[\{S_{\mathbf{x}}\}] = H[\{S_{\mathbf{x}}\}] + \Delta H_k[\{S_{\mathbf{x}}\}] \tag{4.59}$$

This effective Hamiltonian allows then to formally define a scale-dependent probability distribution

$$P_k[M_0] = \sum_{\{S_{\mathbf{x}}\}} \delta\Big(\sum_i S_i - M_0\Big) \frac{e^{-\beta H_k}}{Z_k[h=0]} \tag{4.60}$$

using the relation

$$\delta\Big(\sum_i S_{\mathbf{x}} - M_0\Big) = \int_0^1 d\lambda\, e^{2\pi i\lambda\left(\sum_{\mathbf{x}} S_{\mathbf{x}} - M_0\right)} \tag{4.61}$$

we obtain

$$P_k[M_0] = \frac{1}{Z[0]} \int_0^1 d\lambda\, e^{-2\pi i\lambda M_0 + W_k[h=2\pi i\lambda]} \tag{4.62}$$

inserting the definition of the effective average action Γ_k we get, with $M_\lambda = \frac{\partial W_k}{\partial h}$

$$P_k[M_0] = \frac{1}{Z[0]} \int_0^1 d\lambda\, e^{-\Gamma_k[\frac{M_\lambda}{\Omega}] + 2\pi i\lambda\left(M_\lambda - M_0\right) - \Delta H_k[\frac{M_\lambda}{\Omega}]} \tag{4.63}$$

so that, using the saddle point approximation, for N sufficiently large

$$P_k[M_0] \xrightarrow{N\gg 1} \frac{1}{Z[0]} e^{-\Gamma_k[\frac{M_0}{\Omega}] - \Delta H_k[\frac{M_0}{\Omega}]} \tag{4.64}$$

This is the basic relation used in this chapter. The universality of these scaling functions is easily proven by using a scaling argument [29].

The probability distribution scaling functions can be obtained by means of Monte Carlo methods. Here we compare Monte Carlo results for cubic systems of linear size L and periodic boundary conditions, simulated by cluster MC method against those obtained by using the lattice version of the NPRG, at the level of the LPA presented in the previous section. In order to be able to accurately compare our results, is is important to adapt our methods to a finite system size. We thus consider a spin system of linear size L. We rewrite the LPA flow equation for the effective potential but this time in terms of the local magnetization $m = \langle S \rangle$. As mentioned before, we choose here to work with the regulator (4.52)

$$\partial_k V_k(m) = \frac{\varepsilon_0 k^2}{\varepsilon_0 k^2 + V_k''(m)} \frac{1}{L^3} \sum_{\mathbf{q}} \Theta(\varepsilon_O k^2 - \varepsilon_0(\mathbf{q})) \tag{4.65}$$

with $\varepsilon_0 = \beta J$, together with the initial condition

$$V_{k_{in}}(m) = \frac{1}{2}\log(1-m^2) + \phi\,\mathrm{atanh}\big(m\big) - 2d\varepsilon_0 m^2 \tag{4.66}$$

at a scale $k_{in} = \sqrt{4d}$.

Notice that the initial potential $V_{k_{in}}$ is a continuous function and is well defined for all $-1 \le m \le 1$, as it should. In particular we have $V_{k_{in}}(1) = \log 2 - 2d\varepsilon_0$. The second derivative of the potential at this point, which appears in the flow equation (4.65), is however divergent, which ensures that the effective potential does not flow at this limiting point, keeping its value fixed, and serving thus as one boundary condition.

Given the Z_2 symmetry present in the model, the effective potential must be an even function of the magnetization, and it is easy to check that this property is maintained along the NPRG flow. We can thus use as another boundary condition $V_k'(m=0) = 0$ all along the flow.

We have then a completely well-defined EDP problem. Notice though that this is a very hard numerical problem to solve, given that the initial condition is not everywhere derivable, and given that the r.h.s. of the flow equation (4.65) is not a continuous function of k, due to the the underlying discrete nature of the finite lattice problem. This forced us to employ more refined numerical algorithms. In particular we have used [1] an iterated (Newton) fixed precision backwards Euler implicit algorithm to arrive at some preliminary results. As they are too preliminar, the results are going to be presented in detail either in a later version of the manuscript or elsewhere.

An interesting point arises with flow equation (4.65). It is easy to check that the flow stops for $k < 2\pi/L$. Even though this is of course a consequence of

the explicit form of the cut-off function (4.52), it is easy to see that a similar relation would be fulfilled for any other standard cut-off profile. This has important consequences for what follows, and is in many ways an intuitive result of the RG approach.

It is also enlightening to look at the special limit $L \to \infty, a \to 0$. In this case, using the property mentioned in the previous paragraph, we can relate the probability distribution function for the magnetization with what is known as the dimensionless potential

$$V_k(m) = k^d v_k(\tilde{m}) \qquad m = k^{d-2/2}\tilde{m}$$

In fact, near the RG fixed point, this dimensionless potential is known to attain a universal fixed point form as $k \to 0$ [63], which we call v^*. But is easy to check that

$$\Gamma_k = L^d V_k = L^d k^d v_k^* \tag{4.67}$$

as $k \to 0$, and thus, using that the flow stops for $k \sim 1/L$ we can deduce that

$$P(M, T_c, L \to \infty) \propto e^{-v_k^*(M)} \tag{4.68}$$

which gives a physical meaning to the dimensionless potential.

4.5. The BMW approximation

The derivative expansion has proven to be a very powerful technology for the study of critical properties. However, being in essence an expansion in momenta, the DE is ill-suited for studying momentum-dependent quantities. Even though this may not seem as a great disadvantage when studying collective, long distance properties, such as critical exponents, the very structure of the NPRG flow equations demands for a sufficiently accurate description of the momentum structure of vertex functions $\Gamma_k^{(n)}$. On top of that, a good description of momentum dependent quantities has also an intrinsic interest, and is essential to describe many important physical systems such as weakly interacting boson systems [79], strongly correlated fermions [141], and quantum phase transitions [197, 136, 7], as well as some out of equilibrium systems such as the KPZ equation [121].

Recently, a new approximation scheme, which allows for the accurate NPRG study of momentum-dependent quantities, has been introduced by Blaizot, Méndez-Galain and Wschebor (BMW) in [25]. The BMW approximation is reminiscent of earlier attempts by Parola and Reato [168, 169, 170], in the context of the so-called hierarchical reference theory of liquids. During these last years, the BMW approximation has been tested at its leading order in the case

of $O(N)$-symmetric scalar field theories, yielding excellent results for physical quantities in all momentum regimes [26, 12, 13]. Also, a BMW-like type of approximation has been used with great success in the study of the KPZ equation [42, 43].

The BMW scheme is based on the analyticity properties of the NPRG flow stemming from the addition of the regulator term, as well as in general properties of the vertex functions. To introduce this scheme, it is useful to make the distinction between external and internal momenta in the NPRG equations for the $\Gamma_k^{(n)}$ vertices. We call q the internal momentum running inside the loop of the NPRG equations, and p_i the n momenta entering the vertex. See Fig. 4.8 for an example.

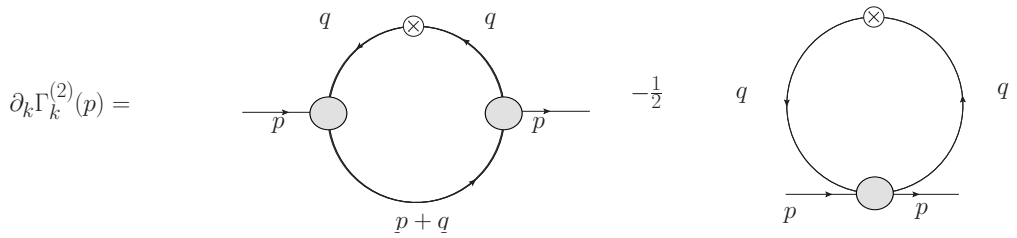

FIGURE 4.8 – NPRG flow equation for the $\Gamma_k^{(2)}$ vertex.

Behind the derivative expansion lies the condition that all momenta, external and internal, must be small compared with the characteristic scales of the problem. These scales can either be physical scales, such as a mass scale m in the system, or the scale k set by the NPRG procedure. Thus, the DE is valid in the limit $p \ll m$ in the massive case, or $p \ll k$ in the critical case without physical mass. This implies that in particular the DE is only valid in the critical case for as long as $k \gg p$. When the limit $k \to 0$ is approached, the DE becomes in the critical case only valid for momentum independent quantities $p \to 0$.

Notice now that the flow equation for any $\Gamma_k^{(n)}$ vertex always contains a derivative of the cut-off function, $\partial_k R_k(q)$, in front of the loop propagators. A typical profile for this function can be seen in Fig 4.9. The presence of this term assures that the loop internal momentum q is effectively cut-off at a scale $q \sim k$, so that the loop integral is approximately only performed for momenta $q \lesssim k$. As k flows to zero this property justifies an expansion in the internal momentum q, an expansion which would not be justified for the external momenta.

In order to see how the BMW approximation works in a concrete example, consider the flow equation for the 2-point vertex for a scalar ϕ^4 field theory. It

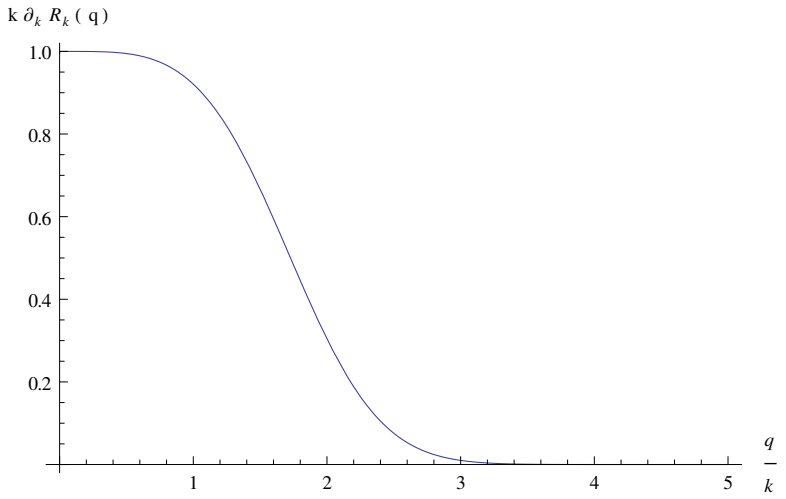

FIGURE 4.9 – Typical profile of the function $k\partial_k R_k(q)$, which appears in the NPRG equations. Example taken from a smooth cut-off function.

reads

$$\partial_k \Gamma_k^{(2)}(p) = \int_q \partial_k R_k(q) G_k(q) \Gamma_k^{(3)}(p,q,-p-q) G_k(p+q) \Gamma_k^{(3)}(p,q,-p-q) G_k(q) - \frac{1}{2}\int_q \partial_k R_k(q) G_k(q) \Gamma_k^{(4)}(q,-q,-p,p) G_k(q) \quad (4.69)$$

A diagrammatic representation of this equation can be seen in Fig 4.8. As argued before, the internal momentum q is capped off by the regulator term $\partial_k R_k(q)$, so that $q \lesssim k$. The BMW approximation starts then by ignoring this q dependence, and can be written, in this case

$$\begin{aligned} &\Gamma_k^{(3)}(p,q,-p-q) \to \Gamma_k^{(3)}(p,-p,0), \\ &\Gamma_k^{(4)}(p,-p,q,-q) \to \Gamma_k^{(4)}(p,-p,0,0) \end{aligned} \quad (4.70)$$

Notice that in the limit $k \ll p$ this is completely justified, given that $q \lesssim k$. In the converse limit, $p \ll k$, this approximation is at least as justified as the DE. Notice also that we are not approximating the momentum dependence of the internal propagators G_k, which would constitute too strong an approximation, when comparing e.g. with the perturbative approach [25].

The BMW approximation uses relation (4.70) to close the hierarchy of NPRG

equations, by using the properties,

$$\Gamma_k^{(3)}(p,-p,0;\phi) = \frac{\partial \Gamma_k^{(2)}(p,-p;\phi)}{\partial \phi}$$
$$\Gamma_k^{(4)}(p,-p,0,0;\phi) = \frac{\partial^2 \Gamma_k^{(2)}(p,-p;\phi)}{\partial \phi^2} \tag{4.71}$$

that are valid because ϕ is a uniform field configuration. This property, together with Eqs. (4.71) allow us to write down a closed integro-differential equation for the 2-point vertex

$$\partial_k \Gamma_k^{(2)}(p) = \left(\partial_\phi \Gamma_k^{(2)}(p)\right)^2 \int_q \partial_k R_k(q)\, G_k(p+q,\phi) G_k^2(q,\phi) - \frac{1}{2}\partial_\phi^2 \Gamma_k^{(2)}(p) \int_q \partial_k R_k(q)\, G_k^2(q,\phi) \tag{4.72}$$

We can generalize this procedure in a straightforward way for higher order vertices. We define the BMW approximation of order s by closing the hierarchy of NPRG equations for the vertex functions at the level of the $\Gamma_k^{(s)}$ vertex. To see how this works, remember that generically the flow of $\Gamma_k^{(s)}$ contains contributions from the $\Gamma_k^{(s+1)}$ and the $\Gamma_k^{(s+1)}$ vertex functions, whose q dependence can be neglected following the previous argument. That is, we can perform the substitutions

$$\Gamma_k^{(s+1)}(p_1,\ldots,p_s-q,q) \to \Gamma_k^{(s+1)}(p_1,\ldots,p_s,0),$$
$$\Gamma_k^{(s+2)}(p_1,\ldots,p_s,q,-q) \to \Gamma_k^{(s+2)}(p_1,\ldots,p_s,0,0) \tag{4.73}$$

Now, we can use the general property (for uniform field configurations)

$$\Gamma_k^{(s+1)}(p_1,\ldots,p_s,0;\phi) = \frac{\partial \Gamma_k^{(s)}(p_1,\ldots,p_s;\phi)}{\partial \phi} \tag{4.74}$$

where we have re-explicited the field dependence. This relation, together with the equivalent relation for $\Gamma^{(s+2)}$, allows for closing the hierarchy of NPRG equations at the level of the $\Gamma_k^{(s)}$ vertex. It is important to see that only the equation for $\Gamma_k^{(s)}$ is approximated : the flow of lower order vertices $\Gamma_k^{(m)}$ with $m < s$ is calculated by using their exact NPRG equations

Notice also that the zero momentum part of the vertex functions can always be expressed as derivatives of the effective potential, e.g. $\Gamma_k^{(2)}(p=0;\phi) = V_k''(\phi)$. This is used in the BMW approximation by calculating in a separate way the flow of the potential V_k (using the exact NPRG equation) and the flow

of the momentum dependent part of the vertex functions, e.g. $\Delta\Gamma_k^{(2)}(p;\phi) = \Gamma_k^{(2)}(p;\phi) - V_k''(\phi)$. this improved the desription of zero momentum physical quantities [26, 11]

The case $s = 0$ can be related to the local potential approximation, the leading order of the DE. Following our recipe, one should neglect the q dependence of the $\Gamma_k^{(2)}$ function in the flow equation for the effective average action Γ_k, the Wetterich equation. That would correspond to the ansatz

$$\Gamma_k^{\{s=0\}} = \int_x V_k(\phi) \tag{4.75}$$

which is somewhat too trivial to yield interesting results. A minor modification in this case would be to preserve the bare momentum dependence of the 2-point function, yielding the usual LPA ansatz

$$\Gamma_k^{LPA} = \int_x \left(\frac{1}{2}\left(\nabla\phi\right)^2 + V_k(\phi)\right) \tag{4.76}$$

which is known to be a reasonably good approximation for studying the critical properties of the Ising universality class, at least in $d = 3$. We could modify in a similar way the $s = 0$ BMW scheme in other theories, in order to make it equivalent to the LPA for every case.

If we want to go beyond the DE then, we must take the BMW approximation to higher order s, the leading order example being $s = 2$. The numerical implementation of the BMW at the $s = 2$ level of approximation was performed in [12, 13] for the case of $O(N)$-symmetric scalar field theories, yielding results in excellent agreement with the literature, in all momenta regimes. As an example, we quote here the results for the critical exponents, in Tables 4.2, 4.3 and 4.4. Even though the BMW approximation is not specifically designed to deal with the low momentum regime, we obtain excellent results for these exponents. Later on we discuss the results for a momentum dependent function, the universal scaling function for the Ising model.

The two-dimensional case, for which exact results exist, provides an even more stringent test of the BMW scheme. We focus here on the Ising model $N = 1$ which exhibits a standard critical behavior in $d = 2$, and the corresponding critical exponents. The perturbative method that work well in $d = 3$ fails here : for instance, the fixed-dimension expansion that provides the best results in $d = 3$ yields, in $d = 2$ and at five loops, $\eta = 0.145(14)$ [167] in contra- diction with the exact value $\eta = \frac{1}{4}$ [2]. We find instead $\eta = 0.254$, $\nu = 1.00$, and $\omega = 1.28$

2. It has been conjectured (see [162] and references therein), and this is confirmed by $1/N$ calculations, that the presence of non-analytic terms in the flow of the φ^4 coupling u could be responsible for the discrepancy between exact and perturbative results in $d = 2$. According to Sokal, no problem should arise when all couplings, including the irrelevant ones, are retained in the RG flow, as done here. This probably explains the quality of our results in $d = 2$.

in excellent agreement with the exact values $\eta = \frac{1}{4}$, $\nu = 1$ and the conjectured value $\omega = \frac{4}{3}$ [208].

TABLE 4.2 – Results for the anomalous dimension η in $d = 3$, compared with results obtained within the DE at order $O(\nabla^2)$, field theory (FT) and Monte Carlo (MC) methods

N	BMW	DE	FT	MC
0	0.034	0.039[198]	0.0272(3)[167]	0.0303(3))[93]
1	0.039	0.0443[39]	0.0318(3) [167]	0.03627(10) [103]
2	0.041	0.049[198]	0.0334(2) [167]	0.0381(2)[37]
3	0.040	0.049[198]	0.0333(3) [167]	0.0375(5)[38]
4	0.038	0.047[198]	0.0350(45) [99]	0.0365(10)[101]
10	0.022	0.028[198]	0.024 [3]	-
100	0.0023	0.0030[198]	0.0027 [150]	-
$\mathcal{O}(1/N)$	$0.23/N$		$0.270/N$ [150]	-

TABLE 4.3 – Results for the critical exponent ν in $d = 3$, compared with results obtained within the DE at order $O(\nabla^2)$, field theory (FT) and Monte Carlo (MC) methods

N	BMW	DE	FT	MC
0	0.589	0.590[198]	0.5886(3) [167]	0.5872(5) [163]
1	0.632	0.6307[39]	0.6306(5) [167]	0.63002(10) [103]
2	0.674	0.666[198]	0.6700(6) [167]	0.6717(1) [37]
3	0.715	0.704[198]	0.7060(7) [167]	0.7112(5)[38]
4	0.754	0.739[198]	0.741(6)[99]	0.749(2)[101]
10	0.889	0.881[198]	0.859 [3]	-
100	0.990	0.990 [198]	0.989[150]	-
$\mathcal{O}(1/N)$	$1-1.034/N$		$1-1.081/N$ [150]	-

Of course, the BMW approximation taken to nontrivial orders is in general numerically more involved that the DE, mostly because we have to take explicitly into account the double dependence - on field and on momentum - of the vertex functions along the flow. Nonetheless, these results for the $O(N)$ model were obtained by using simple numerical methods, such as explicit Euler integration, and Simpson's rule for integration [154].

TABLE 4.4 – Results for the correction to scaling exponent ω in $d = 3$ compared with results obtained within the BMW method, field theory (FT) and Monte Carlo (MC) results

N	BMW	FT	MC
0	0.83	0.794(6) [167]	0.88 [93]
1	0.78	0.788(3) [167]	0.832(6) [103]
2	0.75	0.780(10) [167]	0.785(20) [37]
3	0.73	0.780(20) [167]	0.773 [38]
4	0.72	0.774(20) [99]	0.765 [101]
10	0.80	-	-
100	1.00	-	-

4.6. The scaling function of the Ising universality class

As mentioned before, the main advantage of the BMW scheme over other NPRG approximation methods is its ability to accurately describe momentum-dependent quantities in all temperature or external field regimes. A stringent test of this is given by the study of the universal scaling function of the Ising universality class in $d = 3$, which has been measured experimentally [58].

Near the critical point and for momenta $p \ll u$ one expects the scaling behaviour

$$G^{(2)}_{\pm}(p) = \chi g_{\pm}(p\xi) \tag{4.77}$$

with, by definition, $G^{(2)}$ the density-density (in the case of a fluid) correlation function, $\chi^{-1} = \Gamma^{(2)}(p = 0)$ the compressibility, and

$$\xi = \left(\frac{\partial^2_\phi V_{k=0}(\phi = 0)}{Z_{k=0}} \right)^{-\frac{1}{2}}$$

the correlation length that diverges close to criticality with critical exponent ν. Here $\pm$ refers to the two phases, respectively above and below the critical temperature. The functions $g_{\pm}(x = p\xi)$, with the above normalizations are universal and behave as

$$g^{-1}_{\pm}(x) = 1 + x^2 + O(x^4) \tag{4.78}$$

For small x they are well described by the Ornstein-Zernicke (mean-field) approximation :

$$g_{OZ}(x) = \frac{1}{1 + x^2}. \tag{4.79}$$

The corrections to the Ornstein-Zernicke behavior are usually parameterized at small x by [140]

$$g_{\pm}(x)^{-1} = 1 + x^2 + \sum_{n=2} c^{\pm}_n x^{2n}. \tag{4.80}$$

The above behavior of $g_{\pm}(x)^{-1}$ is a priori valid only for $x \lesssim 1$ but since the coefficients c_n are very small (to give a few examples : $c_2^+ = \text{âĹŠ}3.90(6) \times 10^{\text{âĹŠ}4}$, $c_3^+ = 0.88(1) \times 10^{\text{âĹŠ}5}$, $c_4^+ = \text{âĹŠ}0.4(1) \times 10^{\text{âĹŠ}6}$ [35], $c_2^- = \text{âĹŠ}1.2(6) \times 10^{\text{âĹŠ}2}$ [188]), it turns out that the Ornstein-Zernicke approximation is actually valid over a wide range of x values, as we shall see later.

For large x (that is, $\xi \gg p^{-1}$) the scaling functions show critical behavior with an anomalous power law decay

$$g_{\pm}(x) \sim \frac{C_1^{\pm}}{x^{2-\eta}} \qquad \text{for } x \gg 1 \tag{4.81}$$

which allows for the experimental determination of the exponent η. This expression also allows us to parametrize corrections, as given by Fischer and Langer [78]

$$g_{\pm}(x) = \frac{C_1^{\pm}}{x^{2-\eta}}\left(1 + \frac{C_2^{\pm}}{x^{(1-\alpha)/\nu}} + \frac{C_3^{\pm}}{x^{1/\nu}} + \ldots\right). \tag{4.82}$$

Beside the constants $c_n^{\pm}$ and $C_n^{\pm}$, the constants $S_M^{\pm}$ and $S_Z^{\pm}$, defined by

$$S_M^{\pm} \equiv M_{gap}^2 \xi^2 \tag{4.83}$$

$$S_Z^{\pm} \equiv \chi/(\xi^2 Z_{gap}) \tag{4.84}$$

are also of interest in order to understand the analytical behaviour of the theory. Here M_{gap} (the mass gap of the Minkowskian version of the model) and Z_{gap} are related to the long-distance behavior of the two-point function in direct space :

$$G(\mathbf{r}) \approx \frac{Z_{\text{gap}}}{4\pi|\mathbf{r}|} e^{-M_{\text{gap}}|\mathbf{r}|} \tag{4.85}$$

The critical limits of $S_M^{\pm}$ and $S_Z^{\pm}$ are related to the imaginary zeroes $\pm i x_0$ of $g_{\pm}^{-1}(x)$ closest to the origin by

$$\begin{aligned} S_M^{\pm} &= -x_0^2 \\ S_Z^{\pm} &= \left.\frac{dg^{-1}(x)}{dx^2}\right|_{x=\pm i x_0} \end{aligned} \tag{4.86}$$

We limit from now on to the study of the high temperature phase. As already observed in Ref. [34], the c_n^+ coefficients show the pattern

$$|c_n^+| \ll |c_{n-1}^+| \ll \ldots \ll |c_2^+| \ll 1 \tag{4.87}$$

Therefore, a few terms of the expansion of $g_+(x)$ in powers of x^2 provide an excellent approximation of $g_+(x)$ in a relatively large region around $x = 0$. This is

in agreement with the theoretical expectation that the singularity of $g_+(x)$ nearest to the origin is the three-particle cut [76, 28]. If this is the case, the convergence radius r_+ of the Taylor expansion of $g_+^{-1}(x)$ is $r_+ = 3\sqrt{S_M^+}$. For φ^4 theory, it is known that the difference between the mass gap and ξ^{-1} is very small and replacing one by the other corresponds to an error which is beyond the accuracy of the existing calculations [140] ; taking then $S_M^+ \approx 1$, we should have, at least for large enough values of n

$$c_{n+1}^+ \approx -\frac{1}{9} c_n^+. \tag{4.88}$$

This behavior can be checked explicitly in the large-N limit of the N-vector model [34].

More generally, different approximate results for the universal scaling functions exist in the literature, obtained either by Monte Carlo methods [140], or by the use of an analytical ansatz (called the Bray ansatz [28]), that interpolates between the two know asymptotic regimes (4.80) and (4.81), using ε expansion results. Experimental results from neutron scattering in CO_2 near the critical point also exist [58].

In Bray's interpolation for the high temperature phase one assumes $g_+^{-1}(x)$ to be well defined in the complex x^2 plane, with a branch cut on the negative real x^2 axis, starting at $x^2 = -r_+^2$, where $r_+^2 = 9M_{\text{gap}}^2\xi^2 \equiv 9S_M$, following the expectations mentioned before. With these assumptions, Bray's ansatz in the high temperature phase reads :

$$\begin{aligned} g_+^{-1}(x) = & \quad \frac{2\sin\pi\eta/2}{\pi C_1^+} \\ & \times \int_{r+}^{\infty} du\, F_+(u) \Big[\frac{S_M}{u^2 - S_M} + \frac{x^2}{u^2 + x^2} \Big] \end{aligned} \tag{4.89}$$

where $F_+(u)$ is the spectral function, which satisfies $F_+(+\infty) = 1$, $F_+(u) = 0$ for $u < r_+$, and $F_+(u) \geq 0$ for $u \geq r_+$. On top of this, one must impose $g^{-1}(0) = 1$, which fixes the value for C_1^+.

One must then specify $F_+(u)$. Bray [28] proposed the use of a spectral function with the exact Fischer-Langer asymptotic behavior, of the type

$$F_{+,B}(u) = \frac{P_+(u) - Q_+(u)\cot\frac{1}{2}\pi\eta}{P_+(u)^2 + Q_+(u)^2} \tag{4.90}$$

where

$$\begin{aligned} P_+(u) &= 1 + \frac{C_2^+}{u^\iota}\cos\frac{\pi\zeta}{2} + \frac{C_3^+}{u^{1/\nu}}\cos\frac{\pi}{2\nu} \\ Q_+(u) &= \frac{C_2^+}{u^\iota}\sin\frac{\pi\zeta}{2} + \frac{C_3^+}{u^{1/\nu}}\sin\frac{\pi}{2\nu} \end{aligned} \tag{4.91}$$

with $\zeta \equiv (1-\alpha)/\nu$. This definition contains a certain number of parameters. On top of the critical exponents, which can be entered using either the BMW values or the best available results in the literature, one must also fix S_M^+, C_2^+ and C_3^+. For S_M^+ one can use the best estimate in the literature, given by the high temperature expansion of improved models [36], which yield $S_M^+ \sim 1$. Bray proposed to fix $C_2^+ + C_3^+$ to its 1-loop ε-expansion value $C_2^+ + C_3^+ = -0.9$, and then to determine C_1^+ by requiring $F_{+,B}(r_+) = 0$. These conditions allows for a little parameter tuning, by adjusting the relative weight of the C_2^+ and C_3^+ parameters. When comparing our results with Bray's ansatz, we shall use this freedom. We now turn to the scaling function computed by the BMW method.

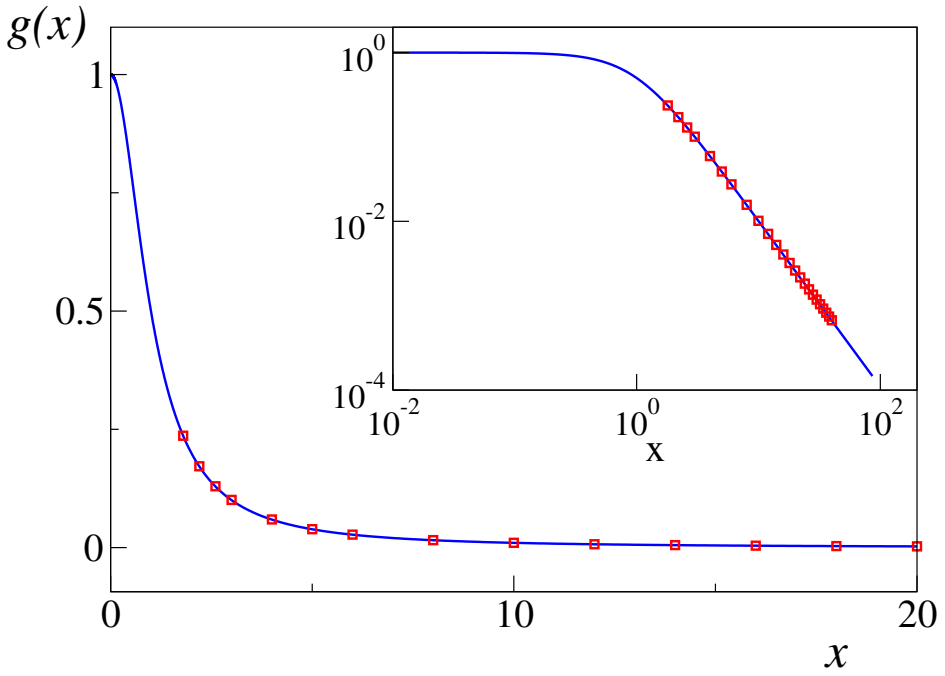

FIGURE 4.10 – The 2-point scaling function $g_+(p\xi)$ as a function of $x = p\xi$ in the high-temperature phase ($d = 3$, $N = 1$). Solid blue line : BMW result. Red squares : Experimental results of [58]. Inset : same data with logarithmic scales.

In terms of the variables used in this work, we find that

$$g_+^{-1}(p\xi) = \frac{\Gamma_k(p\xi)}{\partial_\phi^2 V_k(0)} \tag{4.92}$$

when $k \to 0$. In [13], for purposes of comparison with existing results, we have only computed the high temperature scaling function. We have performed the

calculation for different values of the correlation length (and hence of the reduced temperature). When plotted, one can indeed see perfect data collapse for different values of ξ, which is the first non trivial test of the quality of our results for the scaling function.

In Fig.4.10 we plot the BMW scaling function together with the experimental results from reference [58]. Due to the small values taken by the coefficients c_n and the critical exponent η in $d = 3$, the Ornstein-Zernicke behavior dominates even beyond $p\xi = 1$. In order to measure the deviation from this behavior, one usually makes use of the auxiliary function

$$h(x) = \log\Big[\frac{g(x)}{g_{OZ}(x)}\Big]. \tag{4.93}$$

with g_{OZ} defined in Eq. (4.79). In Fig.4.11 we plot this function together with the experimental results from [58] and the results from the Bray ansatz for two "extreme" choices of the C_2^+ and C_3^+ parameters, which can be read in the figure. One can there see that the BMW approximated result compares well with all these results. In particular, it is in between the results obtained from the two Bray ansätze considered. There are no free parameters in the BMW scheme.

Let us mention that even with large system sizes, the Monte Carlo results suffer from significant systematic errors for $p\xi$ larger than typically 5 to 10. This probably comes from the fact that the universal behavior of the structure factor shows up only when ξ and the separation l between the spins at which we calculate the correlation function are large compared to the lattice spacing and small compared to the lattice size : even for lattice sizes of a few hundreds of lattice spacings this leaves only a small window of useful values of ξ/l [140].

A comment is in order regarding the experimental results of [58]. Figure 4.11 shows a clear deviation between the experimental and both the BMW and Bray's ansatz results, when considering the function $h(x)$. On top of that, one can observe this same deviation when comparing with Monte Carlo data in the x regime where it is most reliable [140]. We thus are inclined to think that deviations are most probably due to the presence of systematic errors in the experimental data in [58].

On top of these results we can also compare results for the values of the coefficients c_2^+ and C_1^+. The results for BMW are $c_2^+ \sim -4.5\times10^{-4}$ to be compared with the IHT best estimate [36] $c_2^+ = -3.90(6)\times10^{-4}$, whereas for C_1^+ BMW yields $C_1^+ = 0.914$, to be compared with the ε-expansion result $C_1^+ = 0.92$.

We conclude this section by noting that (i) the structure factor encompasses much more informations on the universal behavior of a model than the (leading) critical exponents (that are moreover difficult to measure experimentally), (ii) Bray's ansatz, although powerful, depends on two parameters C_2 and C_3 that are poorly determined perturbatively as well as on two critical exponents, (iii)

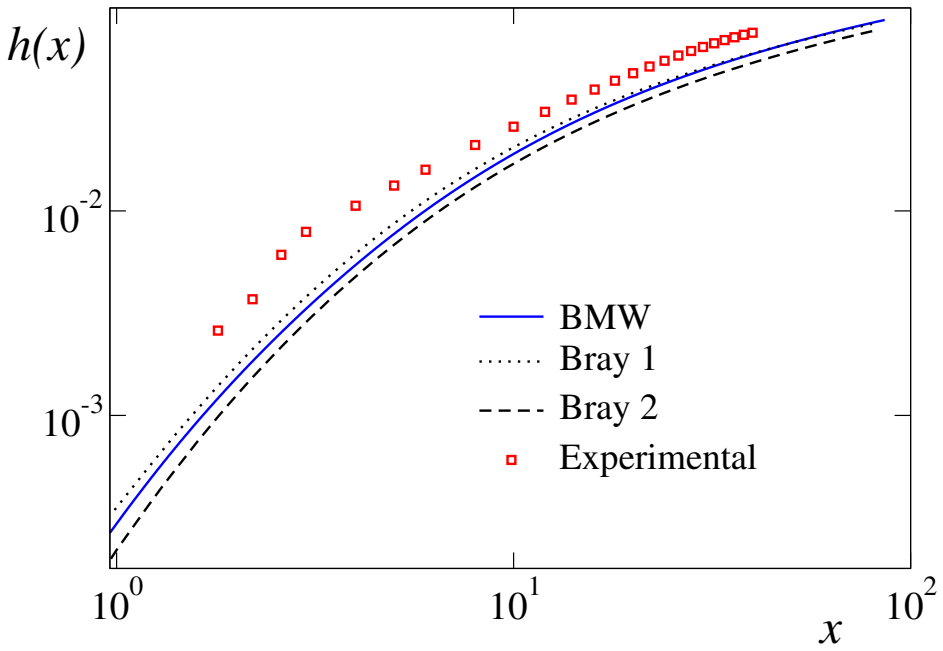

FIGURE 4.11 – Deviation of the scaling function to its trivial Ornstein-Zernicke form, Eq.(4.93). The dotted and dashed lines correspond to two "extreme" choices of the parameters C_2 and C_3 of Bray's ansatz. Dotted line : $C_1 = 0.924$, $C_2 = 1.8$, $C_3 = -2.28$. Dashed line : $C_1 = 0.918$, $C_2 = 2.55$, $C_3 = -3.45$.

the present state of the art of the Monte Carlo simulations is by far insufficient to compute reliably the structure factor in the interesting region of momentum where $p\xi$ is large, (iv) the BMW method leads to a determination of the structure factor that has no free parameter once a choice of regulator has been made (possibly involving an optimization procedure as described in [13]). The results above, summarized in Fig.4.11, suggest that the BMW method leads to an accurate determination of the structure factor in the whole momentum range while the experimental results seem to suffer at small momentum from systematic deviations.

In conclusion, in this example we see that NPRG techniques, by means of the state-of-the-art BMW approximation, allow for an unprecedented level of accuracy - without any fitting parameter - in the calculation of correlation functions at all momentum regimes, and in particular in the difficult case of the study of critical scaling functions.

4.7. Comments

In this chapter we presented the basic NPRG formalism, as well as some of the most important approximation schemes within it, the derivative expansion and the BMW approximation. In particular, we have for the first time exploited the BMW approximation in order to find the momentum dependent scaling function of the $d = 3$ Ising model universality class. The results compare very well with previous results, including experimental results. Also, we have performed a study of the probability distribution by using the recently proposed lattice version of the NPRG equations, at the LPA level. These results constitute new contributions of this work to the NPRG literature in equilibrium systems.

We hope the different applications of NPRG-based approximations presented in this chapter have convinced the reader about the great potentialities of this method for treating strongly correlated systems. Now, after having successfully applied NPRG methods to the Ising and $O(N)$ models, we proceed to what constitutes a higher challenge for the method, its application to out of equilibrium systems.

Chapitre 5

Out of equilibrium NPRG

The NPRG, as introduced in the preceding chapter, has shown to be a powerful mean to study strongly correlated system. However, the presentation so far has dealt with the relatively simple case of equilibrium scalar field theories. Here we present the formalism for out of equilibrium systems, which are the main focus of this work. This implies two main complications with respect to the equilibrium case. First, all the physical information is no longer encoded in a single real field, for, as we have seen before, we have now a response field to also take into account. Secondly, and most importantly, the dynamical properties of the system, and in particular its causality properties, lead to nontrivial constraints on the NPRG flow. This is most readily seen in the context of the so called Itô prescription, related to how the continuous time limit is taken.

We start by deriving the out of equilibrium version of the Wetterich equation. Then, in section 5.2 we show how the subtleties which arise after taking the continuum-time limit for these systems can be dealt with in the NPRG language. The formalism leads then us to write down the LPA flow equation for generic reaction-diffusion systems, in section 5.4. We finish the chapter with a discussion on previous NPRG results for out of equilibrium systems.

5.1. Derivation of the NPRG equations

Here we shall re-derive the NPRG equations in the context of out of equilibrium systems. As we shall see, this represents a rather straightforward generalization of the Wetterich formalism as presented before.

Let us start by building, as in equilibrium, a scale dependent generating functional of the correlation and response functions

$$\mathcal{Z}_k[j,\bar{j}] = \int \mathcal{D}\phi(x)\mathcal{D}\bar{\phi}\, \exp\left(-S[\Phi] - \Delta S_k[\Phi] + \int_x J^t(x)\cdot\Phi(x)\right) \tag{5.1}$$

where, by convention, we have set $x = (\mathbf{x}, t)$, and we have defined the vectors

$$\Phi(x) = \begin{pmatrix} \psi(x) \\ \bar{\psi}(x) \end{pmatrix} \qquad J(x) = \begin{pmatrix} j(x) \\ \bar{j}(x) \end{pmatrix} \tag{5.2}$$

and the regulator term

$$\Delta S_k = \frac{1}{2}\int_{x,x'} \Phi^t(x) \cdot \hat{R}_k(x-x') \cdot \Phi(x') \tag{5.3}$$

where $\hat{R}_k$ is the 2×2 matrix of mass-like cut-off functions suppressing the fluctuations of the slow modes. Its explicit form depends on the particular system at hand, and in particular on its symmetry properties. We will see that below with an example.

We can also define, as in equilibrium, the generating functional of the connected correlation functions $W_k[J] = \log \mathcal{Z}_k[J]$ and its (modified) Legendre transform, the effective average action $\Gamma_k[\Psi]$

$$\Gamma_k[\Psi] = \int_x J^t \cdot \Phi - W_k[J] - \frac{1}{2}\int_{x,x'} \Psi^t(x)\hat{R}_k(x-x')\Psi(x') \tag{5.4}$$

with

$$\Psi = \langle \Phi \rangle_J = \frac{\delta W_k[J]}{\delta J} \tag{5.5}$$

It is convenient to define two notations (a tensorial and a scalar one) for vertex (1PI) correlation functions.

$$\hat{\Gamma}_k^{(n)}[\{x_i\};\Psi] = \frac{\delta^n \Gamma_k[\Psi]}{\delta\Psi(x_1)\ldots\delta\Psi(x_n)} \tag{5.6}$$

and

$$\Gamma_k^{(n,m)}[\{x_i\},\{x'_j\};\Psi] = \frac{\delta^{n+m}\Gamma_k[\Psi]}{\delta\psi(x_1)\ldots\delta\psi(x_n)\delta\bar{\psi}(x_1)\ldots\delta\bar{\psi}(x'_m)} \tag{5.7}$$

where $\{x_i\}$ stands for $(x_1,\ldots,x_n)$ and $\{x'_j\}$ for $(x'_1,\ldots,x'_m)$.

The exact flow of the effective average action is given by Wetterich equation, which in this context reads

$$\partial_k \Gamma_k[\Psi] = \frac{1}{2}\mathrm{tr}\int_{x,x'} \partial_k \hat{R}_k(x-x') \cdot \hat{G}_k[x,x';\Psi] \tag{5.8}$$

with $\hat{G}_k = \left[\hat{\Gamma}_k^{(2)} + \hat{R}_k\right]^{-1}$ the full field-dependent propagator. Observe that Eq. (5.8) presents the same 1-loop structure as in equilibrium.

In summary, then, the NPRG formalism can be easily rewritten for out of equilibrium systems by abandoning the scalar notation and working with both

the density and response fields as components of a vectorial field Ψ. As said before, correlation functions are given by (combinations of) derivatives of Γ_k with respect to the ψ component of the field, whereas response functions also involve derivatives w.r.t. the $\bar{\psi}$ component.

As we have seen, for the case of the out of equilibrium systems studied in this work, the microscopic action has the general form

$$S[\Phi] = S_0[\Phi] + S_{int}[\Phi] = \int_x \bar{\phi}(x)\big(\partial_t - D\nabla^2\big)\phi(x) + \int_x V[\Phi] \tag{5.9}$$

For reaction-diffusion processes, the kinetic part describes diffusion, whereas the potential term $V[\Phi]$ encodes all the reactions between the particles. Notice that as we are interested in stationary properties, in this work we ignore terms in the microscopic action corresponding to the initial time, which would complicate the presentation.

For these systems then, it is easy to see that the dynamical dependence (that is, in Fourier space, the dependence in $\mathbf{q}$ and ω) of the bare propagator (defined as the inverse of the Gaussian part in the action) involves only the product of the fields $\bar{\phi}\phi$ and not for example $\bar{\phi}\bar{\phi}$. Thus, in order to regularize the theory, we only need to add an effective mass of the type $\bar{\phi}\phi$ to the slow modes. The cut-off matrix $\bar{R}_k(q)$, with $q = (\mathbf{q}, \omega)$, then reads

$$\hat{R}_k(q) = \begin{pmatrix} 0 & R_k(q) \\ R_k(q) & 0 \end{pmatrix} \tag{5.10}$$

The cut-off function $R_k(q)$ should satisfy analogous properties to those presented in Eqs. (4.11) above, that is

$$\begin{aligned}
&R_k(q) \sim k^2 && \text{for} && \mathbf{q}^2 \ll k^2 \quad \text{and} \quad |\omega| \ll k \\
&R_k(q) \to 0 && \text{for} && \mathbf{q}^2 \gg k^2 \quad \text{or} \quad |\omega| \gg k \\
&R_k(q) \to 0 && \text{for} && k \to 0 \quad \forall\, q \\
&R_k(q) \to \infty && \text{for} && k \to \Lambda \quad \forall\, q
\end{aligned} \tag{5.11}$$

so that, once again, the regulator term acts as a mass of order $\sim k^2$ for the low momentum and frequency modes, while it does not alter the integration of high momentum modes in the effective average action.

5.2. Causality and Itô prescription within the NPRG

Both the Doi-Peliti and the Janssen-De Dominicis formalisms are derived in discrete time, and subtle ambiguities arise when performing the continuous time limit [194, 86]. This ambiguity implies the choice of a prescription

when going from discrete to continuous time, usually between the so-called Itô or Stratonovich discretization schemes. This problem is independent of the field character of the theory and is present in other formalisms dealing with out of equilibrium systems. This discretization problem is also present in the perturbative RG formalisms, where it is easily dealt with, as the Itô prescription amounts there to the cancellation of tadpole diagrams [52, 189].

Let us start by analyzing what is the origin of these ambiguities. Consider first the Doi-Peliti procedure which uses a coherent state decomposition of the identity, at time slices of size $\Delta t \to 0$, to perform the continuous time limit. Considering for simplicity a single site problem, we can construct an expression for the generating functional

$$\mathcal{Z} = \int \prod_{\tau=0}^{N} d^2\phi_\tau \exp\left(- \sum_{k=1}^{N} \phi_k^*(\phi_k - \phi_{k-1}) + \Delta t \sum_{k=1}^{N} H(\phi_k^*, \phi_{k-1}) \right) \tag{5.12}$$

where we have ignored initial and final time contributions, see section 3.2. As we have seen, in the limit $N \to \infty$, $\Delta t \to 0$, the discrete sums become integrals over time and $\phi_k^*(\phi_k - \phi_{k-1})/\Delta t$ tends to $\phi^* \partial_t \phi$. This continuous time theory becomes ambiguous when considering the propagator of the model, when the inverse of the operator $\partial_t \delta(t - t')$ appears at coinciding times $t = t'$. To remove these ambiguities, we need to go back to the original time discretized version of the model, where all quantities are well defined.

Remember then that, in the Doi-Peliti case, due to the way the coherent states were introduced, the field ϕ^* always appears at a time equal or larger than the time of the ϕ field. We have ignored this in order to arrive at a path integral representation, but in order to not end up with ambiguities, this should be taken into account in a detailed way.

Interestingly, we can see that this time ordering of fields also occurs in the case when the Itô discretization is chosen in field theories derived from Langevin equations.

When deriving a field equation from Langevin dynamics in section 3.1 before, we have consciously neglected a Jacobian term, which has the form

$$\mathcal{J}[\phi] = \left| \det\left(\partial_t \delta(x - x') + \frac{\delta F[\phi(x)]}{\delta \phi(x')} - \frac{\delta N[\phi(x)]}{\delta \phi(x')} \eta \right) \right| \tag{5.13}$$

This Jacobian can be evaluated by using the identity det = exp tr log, and again one must deal with the ill-defined operator $\partial_t \delta(t - t')$. As in the Doi-Peliti case, the ambiguity has to be removed in order to make consistent calculations. Since this ambiguity is related to the continuous time limit, it is useful to first review the discrete time version of the Langevin equation.

A Langevin equation such as (2.31), where the noise term has a field dependence, must always be accompanied by a time-ordering prescription. In the Itô

prescription, all density fields to the r.h.s. of the equation must be evaluated at times strictly earlier than the time at which the equation is considered, that is, the discrete version of Eq. (3.1) in the Itô discretization reads

$$\phi_n - \phi_{n-1} = \Delta t\Big[F(\phi_{n-1}) + N(\phi_{n-1})\eta_{n-1}\Big] \tag{5.14}$$

where n and $n-1$ are time indices. Notice that we are again for simplicity considering a single site problem.

We can construct a field theory in a standard way, now within a discrete time formalism. With the stochastic process (5.14) is associated a transition probability between values of the variable ϕ at consecutive time steps

$$T_{\Delta t}(\phi_n;\phi_{n-1}) = \big(2\pi N^2(\phi_{n-1})\Delta t\big)^{-\frac{1}{2}} \exp\left(-\frac{\big(\phi_n - \phi_{n-1} - \Delta t F(\phi_{n-1})\big)^2}{2N^2(\phi_{n-1})\Delta t}\right) \tag{5.15}$$

This can be rewritten as a Gaussian integral over an auxiliary $\tilde{\phi}$ variable

$$T_{\delta t}(\phi_n - \phi_{n-1}) = \int_{-i\infty}^{i\infty} \frac{d\tilde{\phi}_n}{2\pi i} \exp\big(-\tilde{\phi}_n\big(\phi_n - \phi_{n-1} - \Delta t F(\phi_{n-1})\big) + \Delta t N^2(\phi_{n-1})\tilde{\phi}_n^2\big) \tag{5.16}$$

with $\tilde{\phi}_n$ the conjugate or response variable, associated with the transition from ϕ_{n-1} to ϕ_n. For a Markov chain of N transitions between times 0 and $t_f = N\Delta t$, the total transition probability is given by the product of the transition probabilities corresponding to each timeslice, and we then obtain the generating functional

$$\mathcal{Z} \propto \int \prod_{n=1}^{N} d\phi_n d\tilde{\phi}_n \, e^{-S[\phi,\tilde{\phi}]} \tag{5.17}$$

with

$$S[\phi,\tilde{\phi}] = \Delta t \sum_{n=1}^{N} \tilde{\phi}_n \left(\frac{(\phi_n - \phi_{n-1})}{\Delta t} - F(\phi_{n-1})\right) - N^2(\phi_{n-1})\tilde{\phi}_n^2 \tag{5.18}$$

We see that in this action all the $\tilde{\phi}$ fields appear at a later or equal time than all the ϕ fields, just as was the case for the Doi-Peliti formalism discussed above. Moreover, this precise calculation does not yield a Jacobian term. Therefore, both procedures are implicitly sharing the same time ordering structure, which we identify as equivalent to the Itô prescription.

Let us analyze this in further detail. We consider again the quadratic part of the action S_0, in discrete time

$$S_0[\phi,\tilde{\phi}] = \Delta t \sum_{n=1}^{N} \tilde{\phi}_n \frac{\big(\phi_n - \phi_{n-1}\big)}{\Delta t} + w\tilde{\phi}_n\phi_{n-1} \tag{5.19}$$

with typically $w = \nabla^2 + m^2$. We denote by $\mathcal{Z}_0$ the corresponding generating functional, to which we add a source term

$$\mathcal{Z}_0[j,\tilde{j}] = \frac{1}{2\pi}\int \prod_{n=1}^{N} d\phi_n d(i\tilde{\phi}_n) e^{-S_0[\phi,\tilde{\phi}]+\sum_{n=1}^{N} j_n\phi_n+\tilde{j}_n\tilde{\phi}_n} \tag{5.20}$$

Integrating over $\tilde{\phi}$ in $\mathcal{Z}_0$ produces a product of delta functions which enforces the relation

$$M\cdot {}^t(\phi_0,\ldots,\phi_N) = {}^t(\tilde{j}_0,\ldots,\tilde{j}_N) \tag{5.21}$$

with $M_{ij} = \delta_{i,j} + \nabla^2\delta_{i-1,j}$ in this case. The matrix M is the discrete version of the matrix whose determinant appears in Eq. (5.13) above. It is clear from its form that with the Itô prescription $\det M = 1$. This result can be generalized to any interacting theory, given that interactions terms would appear only as over-diagonal terms in the corresponding M matrix. This proves that in Itô's discretization the Jacobian $\mathcal{J}$ is unity, consistently with what we have said before.

With this matrix M one can compute the free two-point function (propagator)

$$G_{0,kl} = \langle\phi_k\tilde{\phi}_l\rangle_0 = \frac{\delta^2\log\tilde{Z}_0}{\delta j_k\delta\tilde{j}_l} = M^{-1}_{kl} = \Theta(k-l)(-w)^{k-l} \tag{5.22}$$

which vanishes if the field ϕ appears at an earlier time than the field $\tilde{\phi}$, as a signature of causality. Notice that $\langle\phi_k\tilde{\phi}_k\rangle = 1$ whereas $\langle\phi_k\tilde{\phi}_{k+1}\rangle = 0$, which explains why the continuous time limit is delicate.

Thus, if we choose to use the Itô prescription, the Langevin formalism has the same solution to the time-ordering ambiguities as the Doi-Peliti approach, a solution which can be implemented at the level of the propagator of the theory.

The continuum limit is at the end of the day easily dealt with in the usual perturbative approach to the RG. Indeed, the ambiguity occurs only in tadpole diagrams in which the bare propagator $G_0(t-t') \propto \Theta(t-t')$ starts and ends at the same vertex, so that $\Theta(0)$ is needed. Taking into account that at discrete time the interaction vertices come with the fields shifted in time according to Eq. (5.18), that is, the vertices are of the form $\tilde{\phi}^n_k\phi^m_{k-1}$, we see that the bare vertices actually involve two times separated by the time step Δt. Thus, the propagator appearing in a tadpole (see Fig. 5.1), joining a ϕ field with a $\tilde{\phi}$ field, is in fact of the form $\langle\phi_{k-1}\tilde{\phi}_k\rangle$, which is vanishing when considering a tadpole because of (5.22). That is to say, in the continuum propagator within a tadpole should be read as $\langle\phi(t)\tilde{\phi}(t+\Delta t)\rangle = G_0(t-(t+\Delta t))$, so that $Theta(0)$ should be understood as

$$\Theta(0) = \lim_{\Delta t\to 0}\Theta(-\Delta t) = 0 \tag{5.23}$$

which yields the standard prescription used in perturbation theory : in Itô's discretization, the tadpoles must be set to zero.

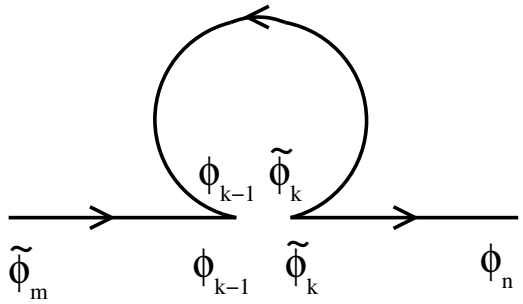

FIGURE 5.1 – Example of a perturbative tadpole diagram. The arrows go from $\tilde{\phi}$ to ϕ, allowing to keep track of causality. In this example, the interaction term in the action is $(\tilde{\phi}\phi)^2$ and the time separation between the $\tilde{\phi}$ and the ϕ fields at the vertex is the time step Δt of Itô discretization. The graph is vanishing because the arrow in the tadpole is going backward in time. Figure taken from [41].

For what follows, it is interesting to notice that one can remove the continuum time ambiguities either by considering that in the vertices the appearances of $\tilde{\phi}$ field are shifted in time with respect to the ϕ fields, or by considering this shift to take place directly in the propagator, as only the product of vertices and propagators enters in the calculation of physical observables. Within this second point of view, the Itô prescription is enforced by shifting the time t' of $\tilde{\phi}(t')$ in $G_0(t-t')$ and replacing $\langle\tilde{\phi}(\mathbf{x}',t')\phi(\mathbf{x},t)\rangle_0$ by

$$\langle\tilde{\phi}(\mathbf{x}',t')\phi(\mathbf{x},t)\rangle_{0,\varepsilon} = \langle\tilde{\phi}(\mathbf{x}',t'+\varepsilon)\phi(\mathbf{x},t)\rangle_0 \tag{5.24}$$

with $\varepsilon \to 0^+$. This can be written equivalently in Fourier space as

$$\langle\tilde{\phi}(\mathbf{q}',\omega')\phi(\omega,q)\rangle_{0,\varepsilon} = e^{-i\epsilon\omega'}\langle\tilde{\phi}(\mathbf{q}',\omega')\phi(\mathbf{q},\omega)\rangle_0 \tag{5.25}$$

which precisely amounts to changing $G_0(t=0)$ in tadpoles for $G_0(t=-\varepsilon)$, as it should according to Eq. (5.23).

Within the NPRG, the Itô prescription is not that easy to implement, and causality properties are more subtly integrated into the formalism. In the NPRG, the flow of a given vertex function involves integrals of products of other vertex functions and of dressed propagators G_k, and give rise to effective vertices which are non-local in time. However, just as in the perturbative case, an ambiguity can only arise when two times coincide, and if the vertex functions $\Gamma_k^{(n,m)}$

are smooth functions of their time argument, one would expect no ambiguities to arise, because the two ends of a propagator $G(t-t')$ joining two legs of $\Gamma_k^{(n,m)}$ are integrated over, so that the value of $G_k(0)$ bears no weight in these integrals. This value would only play a role if the propagator were multiplied by a singular function of time, such as a Dirac function $\delta(t-t')$.

Unfortunately, this is precisely what happens in the derivative expansion (DE), where the vertex functions are, in direct space, expanded as a formal power series of Dirac functions and their derivatives. As in the perturbative case, we can get rid of the ambiguities by shifting in the propagator (the full propagator in this case) G_k the time of the ϕ field by an infinitesimal amount ε. In order to see how this works, one must first prove a general causality property within the NPRG. In discrete time it reads

$$\left\langle \prod_{i=1}^{n} \phi_{k_i} \prod_{j=1}^{m} \tilde{\phi}_{l_i} \right\rangle = 0 \quad \text{if} \quad \exists\, l_j \,\text{such that}\, l_j > k_i, \forall\, k_i \tag{5.26}$$

that is, for any response function to be nonzero, the largest time must be that of a ϕ field. This is trivial from a perturbative point of view, given that any vertex must be perturbatively constructed by using local bare vertices and propagators. With some work we can also show this property to hold within the NPRG for every scale k, if the cutoff function $R_k(q)$ is conveniently chosen [41] (see below).

Indeed, one wants the regulator term coupling ϕ with $\tilde{\phi}$ to preserve causality. An easy way to accomplish this property is for the regulator to be either a time-independent function (actually, independent of frequency) : $R_k(t-t', \mathbf{x}-\mathbf{x}') = \delta(t-t')R_k(\mathbf{x}-\mathbf{x}')$, or else a function proportional to $\Theta(t-t')$. In this work we have chosen to work whenever possible with a frequency independent cutoff function for reasons of simplicity, and also because the frequency-dependent option greatly complicates the numerical analysis of NPRG equations. This choice is allowed as far as there is not a symmetry relating the space and time coordinates in the theory, such as the Galilean symmetry in the study of the Cole-Hopf version of the KPZ equation. Notice also that, even though our choice implies that we are effectively not regularizing the frequency dependence of the theory, this dependence is completely regular in the case of the theories at hand, at least at the leading orders of the DE, and we only need to regularize the momentum dependence in order to obtain well converged results (for example in the presence of UV divergences). Following the previous arguments, it is also convenient to choose a cutoff term with a response field $\tilde{\phi}$ shifted in time, so as to be consistent with Itô prescription

$$\Delta S_k = \int_{t,\mathbf{x},\mathbf{x}'} R_k(\mathbf{x}-\mathbf{x}')\phi(\mathbf{x},t)\tilde{\phi}(\mathbf{x}',t+\varepsilon) \tag{5.27}$$

The proof that Eq. (5.26) is preserved at every scale k is made by induction on the scale. This property is trivially true, for a local microscopic theory, at the scale $k = \Lambda$, as long as, as is the usual case, the regulator term ensures that $\Gamma_\Lambda \sim S$. Then, if Eq. (5.26) holds true at a given scale k^*, it also holds at a scale $k^* - \delta k$, if the variation of the response functions due to the NPRG flow also satisfies this property. This type of non perturbative proof will be used repeatedly in this work.

Now, as we have seen before, the flow of the generating functional of the correlation and response functions reads

$$\partial_k W_k[j,\tilde{j}]\Big|_{k=k^*} = \int_{t,\mathbf{x},\mathbf{x}'} \partial_k R_{k^*}(\mathbf{x}-\mathbf{x}')\langle\phi(\mathbf{x},t)\tilde{\phi}(\mathbf{x}',t+\varepsilon)\rangle_{k^*} \tag{5.28}$$

with the average being taken at the scale k^* of the RG flow. From here we can construct the flow of the connected functions

$$\partial_k \frac{\delta^{n+m} W_k[j,\tilde{j}]}{\delta j_1,\dots\delta\tilde{j}_m}\Big|_{k=k^*} = \int_{t,\mathbf{x},\mathbf{x}'} \partial_k R_{k^*}(\mathbf{x}-\mathbf{x}')\langle\phi_1\dots\tilde{\phi}_m\phi(\mathbf{x},t)\tilde{\phi}(\mathbf{x}',t')\rangle_{k^*} \tag{5.29}$$

where the subindices i stand as a shorthand of $(\mathbf{x_i}, t_i)$ in this context. By hypothesis, the response function appearing on the r.h.s. of Eq. (5.29) is nonvanishing only when its largest time is that of a ϕ field. It cannot be $\phi(\mathbf{x},t)$ since $\tilde{\phi}(\mathbf{x}',t+\varepsilon)$ is posterior and it must be thus one of the other ϕ_i fields. This proves that the contribution of the momentum shell δk to the response function $W_k^{(n,m)}$ is nonvanishing only if its largest time corresponds to one of its ϕ fields. By iterating from the initial condition at $k = \Lambda$ we conclude that the property (5.26) holds for any k.

A similar, converse relation can be written which states that for any correlation function to be nonzero, the smallest time must be that of a $\tilde{\phi}$ field, if at the bare level all interaction monomials have at least one $\tilde{\phi}$ field. Notice that this is not the case for some of the theories we study later on, such as BARW-PC, where the microscopic action contains a term proportional to ϕ^2. The proof of this second causality property is completely analogous to the previous proof.

It is important to note, for our later use, that similar results can be obtained for the 1PI vertex functions $\Gamma^{(n,m)}$, with the difference that the latest time in this case must correspond to a $\tilde{\psi}$ field. This difference arises due to the fact that the 1PI vertices are amputated vertices, so that in order to construct the connected correlation and response function from them, a propagator must be attached to all of its legs. This propagator then attaches a ψ field to an outgoing $\tilde{\psi}$ leg, and conversely a $\tilde{\psi}$ field to an incoming ψ field. See Fig. 5.2 for a graphical example.

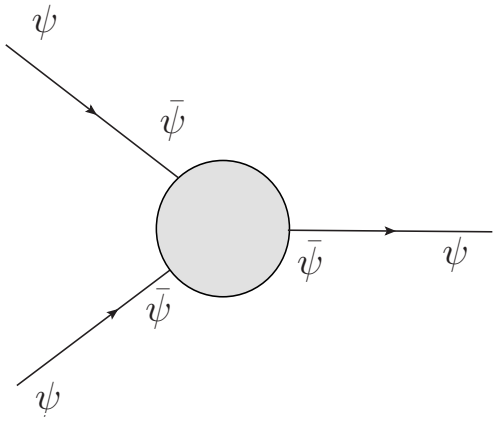

FIGURE 5.2 – Relation between $G^{(2,1)}$ and $\Gamma^{(2,1)}$, showing the ordering of ψ and $\bar{\psi}$ fields.

Relation (5.26) implies in particular that the running propagator $G_k^{(1,1)} = W_k^{(1,1)} = \langle\tilde{\phi}(\mathbf{x}',t')\phi(\mathbf{x},t)\rangle$ remains proportional to $\Theta(t-t')$ for all values of k. Thus, the ambiguity at coinciding times remains identical to that encountered in the perturbative RG scheme. As said before, we can remove this ambiguity in the perturbative case by shifting the time at which the $\tilde{\phi}$ fields are evaluated either at every vertex or directly at the level of the propagator. This second way of doing it allows for the nonperturbative proof we just gave, and thus will be the method of choice when working with the NPRG. The way to keep track of this shift in time in the NPRG is to modify the propagator in the same way as with the bare propagator before, Eq. (5.25). The nonperturbative version of the Itô prescription amounts then to replacing the full propagator for

$$\langle\tilde{\phi}(\mathbf{x}',t')\phi(\mathbf{x},t)\rangle_\varepsilon = \langle\tilde{\phi}(\mathbf{x}',t'+\varepsilon)\phi(\mathbf{x},t) \tag{5.30}$$

which would read in Fourier space

$$\langle\tilde{\phi}(\mathbf{q}',\omega')\phi(\omega,q)\rangle_\varepsilon = e^{-i\epsilon\omega'}\langle\tilde{\phi}(\mathbf{q}',\omega'+\varepsilon)\phi(\mathbf{q},\omega)\rangle \tag{5.31}$$

Notice that when this function is evaluated in a uniform field configuration, it becomes time-translation invariant and thus proportional to $\delta(\omega-\omega')$, in which case $\exp(-i\varepsilon\omega') = \exp(i\epsilon\omega)$.

Given these causality properties, we can also prove a more ambitious result, also related, if perhaps in a more subtle way, to causality. What we show is that, if in the initial conditions for the theory all interaction monomials are proportional to the ψ field (conversely, to the $\tilde{\psi}$ field), then this property is preserved all along the NPRG flow. In other words, no vertex function of the form $\Gamma_k^{(0,n)}$ (conversely $\Gamma_k^{(n,0)}$) is generated. It follows that if the interaction monomials in

$\Gamma_{k=\Lambda}[\Psi]$ were all proportional to the product $\bar{\psi}\psi$, this property is also preserved along the flow.

In order to prove this, it is convenient to work in the setting of the 1PI vertex functions, the natural ground for the NPRG formalism. From there we can construct similar results for the connected correlation functions. The proof makes use of the 1-loop structure of the NPRG flow equations for the $\Gamma_k^{(n,m)}$ vertices, and is most easily understood by using the diagrammatic representation introduced before. Again, we use an induction in the scale for the proof. Let us then assume that $\Gamma_{k^*}^{(0,n)} = 0$ for all n at a given scale k^*, and show how this property is preserved at the scale $k^* - \delta k$.

Consider then the flow of a any $\Gamma_k^{(0,n)}$. This flow is given by a sum of terms which can be represented as 1PI 1-loop diagrams. Each of these terms contains a certain number of vertices attached to the internal loop, and each of them must have, by hypothesis, at least one ψ incoming leg, see Fig. 5.3. The only way in which this diagram can have a nonzero contribution to the flow of $\Gamma_k^{(0,n)}$ is if all such ψ legs in all vertices belong to the internal loop propagator, and are not external legs in the diagram. This in turn implies that the internal loop must be a closed loop of propagators, where each participating vertex has exactly one incoming ψ leg belonging to the loop, as in Fig. 5.3.

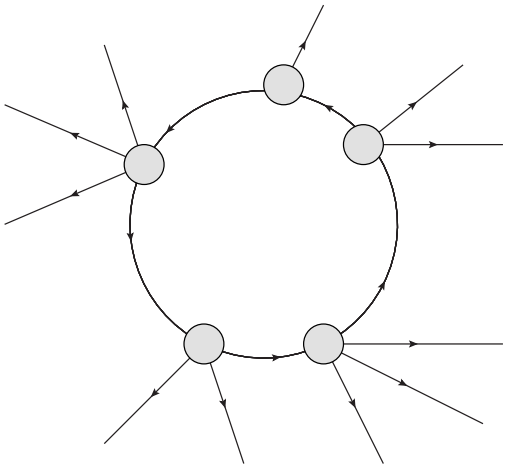

FIGURE 5.3 – A diagram contributing to the flow of $\Gamma^{(0,n)}$ in the NPRG.

Now, given property (5.26) above, we know that for each of the vertices, the time corresponding to the incoming ψ leg must be the smallest time for all the legs in each vertex (see comment above). This leads to a contradiction, as these legs form a closed oriented loop, attached by propagators that are, as we have

seen, always causal. This implies the desired result. It proves to be an important property in what follows.

5.3. Considerations on the source terms

Up to now we have circumvented a fundamental aspect of the NPRG formalism for out of equilibrium systems, which is the explicit form of the source terms used for the definition of the effective average action Γ_k as a Legendre transform. As we shall see in this section, this turns out to have profound consequences when numerically implementing the NPRG. This section presents original work.

Let us start by first considering the partition function $\mathcal{Z}$ of the theory at zero source for a generic out of equilibrium system. Even though the action in these cases is known to be a complex functional of the fields, it is easy to see that the partition function itself is real. This property helps us to define the appropriate J, $\bar{J}$ source terms. It proves convenient to separate the analysis between the MSRDJ context and the Doi-Peliti one, even if in the end we use the same ideas in both formalisms.

5.3.1. MSRJD formalism

In the case of the MSRJD formalism, stemming from a Langevin equation, the "microscopic" action is a functional of a real field ϕ and an imaginary field $\hat{\phi}$. In order to simplify the presentation we work with real fields, by defining $\hat{\phi} = i\tilde{\phi}$, $\tilde{\phi} \in \mathbb{R}$. The action is in general complex, but can be written as a polynomial of ϕ and $\hat{\phi}$ with real coefficients, and thus complies with the additional constraint

$$\left(S[\phi,\tilde{\phi}]\right)^* = S[\phi,-\tilde{\phi}] \tag{5.32}$$

With this, we can verify the reality of the zero-source partition function

$$\begin{aligned}\mathcal{Z}^*[0,0] &= \int \mathcal{D}\phi\mathcal{D}\tilde{\phi}\, e^{-S^*[\phi,\tilde{\phi}]} \\ &= \int \mathcal{D}\phi\mathcal{D}\tilde{\phi}\, e^{-S[\phi,-\tilde{\phi}]} = \mathcal{Z}[0,0]\end{aligned} \tag{5.33}$$

where the last equality stems from the change of variables $\tilde{\phi} \to -\tilde{\phi}$. In fact, a similar argument can be put forward for any correlation function at zero exter-

nal field

$$\begin{aligned}\langle \phi^n (i\tilde{\phi})^m \rangle^*_{J=0,\tilde{J}=0} &= \frac{1}{\mathcal{Z}[0,0]} \int \mathcal{D}\phi \mathcal{D} i\tilde{\phi}\, \phi^n (-i\tilde{\phi})^m e^{-S^*[\phi,\tilde{\phi}]} \\ &= \frac{1}{\mathcal{Z}[0,0]} \int \mathcal{D}\phi \mathcal{D}\tilde{\phi}\, \phi^n (-i\tilde{\phi})^m e^{-S[\phi,-\tilde{\phi}]} = \langle \phi^n (i\tilde{\phi})^m \rangle_{J=0,\tilde{J}=0}\end{aligned} \tag{5.34}$$

again performing the change of variables $\tilde{\phi} \to -\tilde{\phi}$. Notice that, barring non-analyticities, this information is enough to conclude that with an appropriate choice of sources the partition function $\mathcal{Z}[J,\tilde{J}]$ must be real. Now, in order to assure this, it is easy to see that the source terms J, $\tilde{J}$ should be taken as real independent fields, so that J is the source of the ϕ field, and $\tilde{J}$ is the source of the real field $i\tilde{\phi}$.

$$\mathcal{Z}[J,\tilde{J}] = \int \mathcal{D}\phi \mathcal{D}\tilde{\phi} e^{-S[\phi,\tilde{\phi}] + \int_x \left(J\phi + \tilde{J}(i\tilde{\phi}) \right)} \tag{5.35}$$

which is, by the same mechanism as before, a real functional.

In fact, with this choice for the source fields we can prove that $\mathcal{Z}[J,\tilde{J}]$ is not only real but also positive, a property that is important to define the "free energy" functional $W[J,\tilde{J}] = \log \mathcal{Z}[J,\tilde{J}]$. Indeed, within the MSRJD formalism, the most general action functional is at most quadratic in the $\tilde{\phi}$ field and the partition function is written in the form

$$\mathcal{Z}[J,\tilde{J}] = \int \mathcal{D}\phi \mathcal{D}\tilde{\phi} \exp\left(-\int_x \left\{ N[\phi]\tilde{\phi}^2 + i\tilde{\phi} F[\phi] - \tilde{J}\phi - J i\tilde{\phi} \right\} \right) \tag{5.36}$$

Gaussian integration over the real $\tilde{\phi}$ yields

$$\mathcal{Z}[J,\tilde{J}] = \int \mathcal{D}\phi \exp\left(-\frac{1}{4} \int_x N^{-1}[\phi] \left\{ (F[\phi] - J)^2 - \tilde{J}\phi \right\} \right) > 0 \tag{5.37}$$

which proves the desired result, even though, as mentioned before, Eq. (5.37) is not useful for any practical calculation. This also proves that the free energy functional $W[J,\tilde{J}]$ is also real.

These properties allow for the definition of a real average action $\Gamma^L[\psi,\tilde{\psi}]$, by the use of the standard Legendre transform

$$\Gamma^L[\psi,\tilde{\psi}] = \sup_{J,\tilde{J}} \left(\int_x \left(J\psi + \tilde{J}\tilde{\psi} \right) - + W[J,\tilde{J}] \right) \tag{5.38}$$

with

$$\psi(x) = \frac{\delta W}{\delta J(x)} = \langle \phi(x) \rangle_{J,\tilde{J}}, \qquad \tilde{\psi}(x) = \frac{\delta W}{\delta \tilde{J}(x)} = \langle i\tilde{\phi}(x) \rangle_{J,\tilde{J}} \tag{5.39}$$

where every isolated term is real, up to and including the ψ and $\tilde{\psi}$ average fields. This reality is a nice property, given that it would not be easy to generalize the Legendre transform to complex fields.

We have then a real effective action Γ^L which is a functional of two real fields $\psi, \bar{\psi}$. However, this natural choice for the source terms leads to a series of problems when implementing an approximated NPRG flow numerically, most notably because of the appearance of poles in the flow of the effective potential. Worse yet, the initial condition for the flow, written in terms of the average action, is not stable for large $\psi, \tilde{\psi}$ fields if these are real. We re-discuss these matters further below.

In fact, we would like the effective action $\Gamma[\psi, \tilde{\psi}]$ to behave in a way analogous to the bare action $S[\phi, \tilde{\phi}]$ [208]. This would be specially important when considering convergence properties of the effective action at large fields. That is to say, we would like the analogous of property (5.32) for the effective action Γ

$$\left(\Gamma[\psi, \tilde{\psi}]\right)^* = \Gamma[\psi, -\tilde{\psi}] \tag{5.40}$$

which is obviously not the case for Γ^L defined in Eq. (5.38) In order to verify property (5.40) we define a modified effective action, which is in a way an analytic continuation of the real one

$$\Gamma[\psi, \tilde{\psi}] = \Gamma^L[\psi, i\tilde{\psi}] \tag{5.41}$$

this simple redefinition suffices to maintain all the good properties of a Legendre transform, while at the same time obeying the property (5.40).

Using these definitions for the sources and the effective action, we can regularize the theory by adding to the action a term $\Delta S_k[\phi, i\tilde{\phi}]$ that satisfies also Eq. (5.32). Then we can define a running Γ_k in the usual way, and obtain its flow as explained above. An important point to be checked is whether the initial condition for the flow of Γ_k coincides with the bare action S. Let us show that this is indeed the case. We can choose for the regulator term the generic explicit form (cf. discussion on causality in section 5.2 before, where we have seen that the regulator term is not allowed to have terms proportional to $\phi\phi$ in these theories)

$$\Delta S_k = \int_{x,y} \left(R_k^{(1)} \phi(i\tilde{\phi}) + R_k^{(2)} \tilde{\phi}\tilde{\phi} \right) \tag{5.42}$$

so that the auxiliary real "Legendre" effective average action is defined by

$$\Gamma_k^L[\psi, \tilde{\psi}] + W_k[J, \tilde{J}] = \int_x \left(J\psi + \tilde{J}\tilde{\psi} \right) - \int_{x,y} \left(R_k^{(1)} \psi\tilde{\psi} - R_k^{(2)} \tilde{\psi}\tilde{\psi} \right) \tag{5.43}$$

(every function and field in this equation is real) with

$$\begin{aligned}\frac{\delta\Gamma_k^L}{\delta\psi} &= J - \int_x R_k^{(1)}\tilde{\psi} \\ \frac{\delta\Gamma_k^L}{\delta\tilde{\psi}} &= \tilde{J} + \int_x \left(2R_k^{(2)}\tilde{\psi} - R_k^{(1)}\psi\right)\end{aligned} \tag{5.44}$$

This allows us to write down the relation

$$\begin{aligned}e^{-\Gamma_k^L[\psi,\tilde{\psi}]} = \int \mathscr{D}\phi\mathscr{D}\tilde{\phi}\, \exp\Big(-S[\phi,\tilde{\phi}] - i\int_{x,y} R_k^{(1)}\phi\tilde{\phi} - \int_{x,y} R_k^{(2)}\tilde{\phi}\tilde{\phi} + \int_x \left(J\phi + \tilde{J}i\tilde{\phi}\right)\Big) \\ \times \exp\Big(-\int_x \left(J\psi + \tilde{J}\tilde{\psi}\right) + \int_{x,y} R_k^{(1)}\psi\tilde{\psi} - \int_{x,y} R_k^{(2)}\tilde{\psi}\tilde{\psi}\Big)\end{aligned} \tag{5.45}$$

Now we can perform the translation

$$\begin{aligned}\phi &\to \phi + \psi \\ i\tilde{\phi} &\to i\tilde{\phi} + \tilde{\psi}\end{aligned} \tag{5.46}$$

while, up to a contour deformation for the integration over $\tilde{\phi}$, keeping both fields real. Substituting (5.44) for the sources, and after some algebra, we obtain

$$\begin{aligned}e^{-\Gamma_k^L[\psi,\tilde{\psi}]} = \int \mathscr{D}\phi\mathscr{D}\tilde{\phi}\, \exp\Big(-S[\phi+\psi,\tilde{\phi}-i\tilde{\psi}] - i\int_{x,y} R_k^{(1)}\phi\tilde{\phi} \\ - \int_{x,y} R_k^{(2)}\tilde{\phi}\tilde{\phi} + \int_x \frac{\delta\Gamma_k^L}{\delta\psi}\phi + \int_x \frac{\delta\Gamma_k^L}{\delta\tilde{\psi}}i\tilde{\phi}\Big)\end{aligned} \tag{5.47}$$

This is the relation we were looking for. Indeed, if $R_k^{(1)}, R_k^{(2)} \xrightarrow{k\to\Lambda} \infty$, the regulator terms in the functional integral over ϕ and $\tilde{\phi}$ play the role of a functional Dirac delta, and we obtain

$$\Gamma_\Lambda^L[\psi,\tilde{\psi}] = S[\psi,-i\tilde{\psi}] \tag{5.48}$$

which, given our definition (5.41) of the effective average action Γ_k, implies

$$\Gamma_\Lambda[\psi,\tilde{\psi}] = S[\psi,\tilde{\psi}] \tag{5.49}$$

the desired property.

We see that the use of real source terms, together with the definition of Γ_k using an analytic continuation trick, ensures all the good properties we know from the equilibrium case. Even though these constructions may appear at first sight as somewhat artificial, they turn out to be fundamental when actually implementing the out of equilibrium NPRG to study any given system. However, before doing that, let us see how the equivalent formalism works in the case of the Doi-Peliti construction.

5.3.2. Doi-Peliti formalism

In the case of the Doi-Peliti formalism, we work with two complex conjugate fields ϕ and $\bar{\phi}$, which can be parametrized as

$$\phi(x) = \frac{\phi_1(x) + i\phi_2(x)}{\sqrt{2}} \qquad \bar{\phi}(x) = \frac{\phi_1(x) - i\phi_2(x)}{\sqrt{2}} \tag{5.50}$$

while the action written in terms of these variables obeys the relation

$$\big(S[\phi_1, \phi_2]\big)^* = S[\phi_1, -\phi_2] \tag{5.51}$$

The reality of the zero-source partition function $\mathcal{Z}[0,0]$ can be proven in the same ways as in the previous section. Moreover it is easy to argue that $\mathcal{Z}[0,0]$ must be positive, given the way this function is constructed in the Doi-Peliti formalism. Indeed, when we performed the coherent-state decomposition above, we defined

$$\mathcal{Z}[0,0] = \mathcal{Z} = \langle \cdot \mid \psi(t) \rangle = \sum_n P_n(t) = 1 \tag{5.52}$$

If we use real source fields J_1 and J_2 so that

$$\mathcal{Z}[J_1, J_2] = \int \mathscr{D}\phi_1 \mathscr{D}\phi_2 \, e^{-S[\phi_1,\phi_2] + \int_x \left(J_1\phi_1 + J_2 i\phi_2 \right)} \tag{5.53}$$

the reality and positivity properties of $\mathcal{Z}[J_1, J_2]$ rest assured, at least for a small region in the fields. Work is underway to fully prove the positivity of $\mathcal{Z}[J_1, J_2]$ in the Doi-Peliti formalism.

The positivity of $\mathcal{Z}[J_1, J_2]$ allows us again to perform a well-defined Legendre transform to obtain the auxiliary "Legendre" effective action

$$\Gamma^L[\psi_1, \psi_2] + W[J_1, J_2] = \int_x \Big(J_1\psi_1 + J_2\psi_2 \Big) \tag{5.54}$$

with

$$\psi_1 = \frac{\delta W}{\delta J_1} = \langle \phi_1 \rangle_{J_1,J_2} \quad \psi_2 = \frac{\delta W}{\delta J_2} = \langle i\phi_2 \rangle_{J_1,J_2} \tag{5.55}$$

where every isolated term is real, up to and including the ψ_1 and ψ_2 average fields.

Once again, in order to reproduce the complexity properties (5.51) at the level of the effective action we define

$$\Gamma[\psi_1, \psi_2] = \Gamma^L[\psi_1, i\psi_2] \tag{5.56}$$

It is straightforward to show that the effective average action Γ_k defined from this has all the good desired properties with respect to complex conjugation.

Notice that in this case the regulator term is taken diagonal in terms of ϕ_1 and ϕ_2.

$$\Delta S_k[\phi_1,\phi_2] = \int_q R_k(q)(\phi_1^2(q) - \phi_2^2(q)) \tag{5.57}$$

And we have for the initial condition of the NPRG flow.

$$\Gamma_\Lambda[\psi_1,\psi_2] = S[\psi_1,\psi_2] \tag{5.58}$$

this property is proven in the same way as for the scalar field theory before, given the form of the regulator, Eq. (5.57).

With this, we finish the presentation of all the particularities of the NPRG in the setting of out of equilibrium problems. Next we show with an important example how all these elements work together in practice. Later on we will comment how these development shed new lights on previous NPRG out of equilibrium results.

5.4. LPA for reaction-diffusion

As a first application of the methods described in the preceding chapter, we briefly study one of the simplest out of equilibrium systems presenting a phase transition, BARW-DP, defined by the reactions $2A \xrightarrow{\lambda} \emptyset$ and $A \xrightarrow{\sigma} 2A$, in the context of one of the simplest approximations within the NPRG, the Local Potential Approximation. More generally, we can write an LPA ansatz for the reaction-diffusion processes considered in this work [45, 50], which reads

$$\Gamma_k^{LPA}[\tilde{\psi},\psi] = \int d^d x\, dt \left\{ \tilde{\psi}\left(\partial_t - D\nabla^2\right)\psi + V_k(\tilde{\psi},\psi) \right\} \tag{5.59}$$

where the running potential $V_k(\tilde{\psi},\psi)$ contains all the physical information of the uniform and stationary modes of the theory (see section 4.2 above), and the dynamical part does not get renormalized at this order of approximation. An equation for the effective potential can be obtained by substituting the ansatz (5.59) into the Wetterich equation, Eq. (5.8), and evaluating in a uniform and static field configuration Ψ, given that

$$V_k(\Psi) = \frac{1}{\Omega}\Gamma_k\Big|_{\Psi(x)=\Psi} \tag{5.60}$$

with Ω the system space-time volume.

The Wetterich equation for the effective average action depends on the second derivative with respect to Ψ of this functional. Therefore we differentiate

Eq. (5.59) twice with respect to the fields $\Psi(q)$, $\Psi(q')$ and evaluate the result in a uniform field configuration to obtain

$$\hat{\Gamma}_k^{(2)}(q,-q) = \begin{pmatrix} V_k^{(2,0)} & -i\omega + D\mathbf{q}^2 + V_k^{(1,1)} \\ i\omega + D\mathbf{q}^2 + V_k^{(1,1)} & V_k^{(0,2)} \end{pmatrix} \tag{5.61}$$

where $V_k^{(n,m)}$ stands for the derivatives of the effective potential with respect to the stationary and uniform fields

$$V_k^{(n,m)}(\tilde{\psi},\psi) = \frac{\partial^{n+m} V_k(\tilde{\psi},\psi)}{\partial\psi^n \partial\tilde{\psi}^m} \tag{5.62}$$

The form of Eq. (5.61) and the general properties sketched above enforce the following form for the cutoff matrix

$$\hat{R}_k(q) = \begin{pmatrix} 0 & R_k(\mathbf{q}^2) \\ R_k(\mathbf{q}^2) & 0 \end{pmatrix} \tag{5.63}$$

so that the inverse propagator matrix $\hat{\Gamma}_k^{(2)} + \hat{R}_k$ is written

$$\hat{\Gamma}_k^{(2)}(q,-q) + \hat{R}_k(q) = \begin{pmatrix} V_k^{(2,0)} & -i\omega + D\mathbf{q}^2 + V_k^{(1,1)} + R_k(\mathbf{q}^2) \\ i\omega + D\mathbf{q}^2 + V_k^{(1,1)} + R_k(\mathbf{q}^2) & V_k^{(0,2)} \end{pmatrix} \tag{5.64}$$

We must now invert this matrix in order to obtain the full propagator $\hat{G}_k[\Psi]$. It is useful to remember that in Fourier space, matrix inversion takes the form

$$\hat{A}_{ij}(p,-p)\hat{B}_{jk}(p,-p) = \delta_{ij} \tag{5.65}$$

and we find

$$\left[\hat{\Gamma}_k^{(2)}(q,-q) + \hat{R}_k(q)\right]^{-1} = \frac{1}{\omega^2 + \left(D\mathbf{q}^2 + R_k(\mathbf{q}^2) + V_k^{(1,1)}\right)^2 - V_k^{(0,2)} V_k^{(2,0)}} \times \begin{pmatrix} -V_k^{(0,2)} & i\omega + D\mathbf{q}^2 + V_k^{(1,1)} + R_k(\mathbf{q}^2) \\ -i\omega + D\mathbf{q}^2 + V_k^{(1,1)} + R_k(\mathbf{q}^2) & -V_k^{(2,0)} \end{pmatrix} \tag{5.66}$$

Taking now into account the Itô prescription procedure explained above, we can write an expression for the propagator matrix $\hat{G}_k[\Psi]$ by modifying the $G_k^{(1,1)}$ components of Eq. (5.66) with suitable ε factors

$$\left[\hat{\Gamma}_k^{(2)}(q,-q) + \hat{R}_k(q)\right]^{-1} = \frac{1}{\omega^2 + \left(D\mathbf{q}^2 + R_k(\mathbf{q}^2) + V_k^{(1,1)}\right)^2 - V_k^{(0,2)} V_k^{(2,0)}} \times \begin{pmatrix} -V_k^{(0,2)} & e^{-i\varepsilon\omega}\left(i\omega + D\mathbf{q}^2 + V_k^{(1,1)} + R_k(\mathbf{q}^2)\right) \\ e^{i\epsilon\omega}\left(-i\omega + D\mathbf{q}^2 + V_k^{(1,1)} + R_k(\mathbf{q}^2)\right) & -V_k^{(2,0)} \end{pmatrix} \tag{5.67}$$

Now we have all the ingredients needed to obtain a NPRG flow equation for the effective potential. For this, we must multiply the matrix (5.67) by the matrix $\partial_k \hat{R}_k(q)$ and take the trace. Taking away an obvious volume factor from the resulting Wetterich equation, we can write an equation for $V_k(\psi,\bar{\psi})$

$$\partial_k V_k(\Psi) = \frac{1}{2}\int_q \partial_k R_k(\mathbf{q}) \times \\ \frac{e^{i\epsilon\omega}\big(-i\omega + D\mathbf{q}^2 + V_k^{(1,1)} + R_k(\mathbf{q})\big) + e^{-i\epsilon\omega}\big(i\omega + D\mathbf{q}^2 + V_k^{(1,1)} + R_k(\mathbf{q})\big)}{\omega^2 + \big(D\mathbf{q}^2 + R_k(\mathbf{q}) + V_k^{(1,1)}\big)^2 - V_k^{(0,2)}V_k^{(2,0)}} \tag{5.68}$$

The integration over ω can be performed by using simple residues techniques, to yield the flow equation

$$\partial_k V_k(\Psi) = \frac{1}{2}\int_{\mathbf{q}} \partial_k R_k(\mathbf{q}) \left(\frac{D\mathbf{q}^2 + V_k^{(1,1)} + R_k(\mathbf{q})}{\sqrt{\big(D\mathbf{q}^2 + R_k(\mathbf{q}) + V_k^{(1,1)}\big)^2 - V_k^{(0,2)}V_k^{(2,0)}}} - 1 \right) \tag{5.69}$$

The -1 term in the r.h.s. stems from the Itô prescription, and would not be there otherwise. Thus, at the LPA order, the Itô prescription contributes with just a constant term and does not change the physical results of the NPRG equations. This would no longer be true at higher orders of the derivative expansion.

Eq. (5.69) must be supplemented by an initial condition $V_\Lambda(\Psi)$ for the potential. Notice that up to now no mention was given to the specific details of the theory under study, other than the form of the non-running kinetic part of the effective action. Thus, Eq. (5.69) describes in fact the LPA flow of any reaction-diffusion system with only one intracting species, such as any BARW system. Also, it has to be minimally modified in order to account for the flow of the KPZ system in the Cole-Hopf representation, this modification stemming from Galilean symmetry, which forbids the use of a frequency-independent regulator of the form (5.63).

For the specific case of BARW-DP, in the shifted case the initial condition reads (after a suitable rescaling of the fields [52, 45, 50])

$$V_\Lambda(\psi,\bar{\psi}) = \bar{\psi}\psi\Big(\sqrt{\frac{\lambda\sigma}{2}}(\psi-\bar{\psi}) + \lambda\bar{\psi}\psi\Big) \tag{5.70}$$

which, together with (5.69), can be used to analyze the behaviour of BARW-DP. In principle, all types of interaction-like terms in the potential are generated by the NPRG flow for lower values of k. Notice though that the initial potential is proportional to $\bar{\psi}\psi$. Following the general arguments given above, this property is preserved along the flow. It is in fact convenient, in order to enforce this in

any numerical implementation, to define

$$V_k(\psi,\bar{\psi}) = \bar{\psi}\psi U_k(\psi,\bar{\psi}) \tag{5.71}$$

A closed flow equation for U_k can be obtained without much effort. It is useful to use the identity

$$\frac{1}{\sqrt{1-xA}} - 1 = \frac{xA}{\sqrt{1-xA}(1+\sqrt{1-xA})} \tag{5.72}$$

The final result reads

$$\begin{aligned}\partial_k U_k(\Psi) = \frac{1}{2}\int_{\mathbf{q}} \partial_k R_k(q) \Bigg\{ & \frac{\left(2U^{(0,1)} + \bar{\psi}U^{(0,2)}\right)\left(2U^{(1,0)} + \psi U^{(2,0)}\right)}{\left(\bar{\psi}U^{(0,1)} + \psi U^{(1,0)} + \psi\bar{\psi}U^{(1,1)} + U + Dq^2 + R_k(q)\right)^2} \\ & \times \frac{1}{\sqrt{1 - \frac{\psi\bar{\psi}\left(2U^{(0,1)}+\bar{\psi}U^{(0,2)}\right)\left(2U^{(1,0)}+\psi U^{(2,0)}\right)}{\left(\bar{\psi}U^{(0,1)}+\psi U^{(1,0)}+\psi\bar{\psi}U^{(1,1)}+U+Dq^2+R_k(q)\right)^2}}} \\ & \times \frac{1}{\left(\sqrt{1 - \frac{\psi\bar{\psi}\left(2U^{(0,1)}+\bar{\psi}U^{(0,2)}\right)\left(2U^{(1,0)}+\psi U^{(2,0)}\right)}{\left(\bar{\psi}U^{(0,1)}+\psi U^{(1,0)}+\psi\bar{\psi}U^{(1,1)}+U+Dq^2+R_k(q)\right)^2}} + 1\right)} \Bigg\}\end{aligned} \tag{5.73}$$

BARW-DP presents an important symmetry, called rapidity symmetry (this name has to do with the equivalent Reggeon field theory). In terms of ϕ and $\bar{\phi}$ fields the BARW-DP action is symmetric under the exchanges

$$\phi(t) \to -\bar{\phi}(-t) \qquad \phi(t) \to -\bar{\phi}(-t) \tag{5.74}$$

This symmetry is preserved by the NPRG flow. It can also be written in terms of the ψ_1 and ψ_2 real fields. In this rapidity symmetry simply reads

$$\psi_1(t) \to -\psi_1(-t) \qquad \psi_2(t) \to \psi_2(-t) \tag{5.75}$$

In order to ensure that the numerical implementation of the LPA flow Eq. (5.73) respects this symmetry of BARW-DP it is useful to re-write the running effective potential V_k in terms of invariants under this symmetry, such as

$$\rho = \psi\bar{\psi} = \frac{\psi_1^2 + \psi_2^2}{2} \qquad \varsigma = \frac{1}{i}(\psi - \tilde{\psi}) = \psi_2 \tag{5.76}$$

We could also use a field expansion to study the system as a set of coupled ordinary differential equations, as explained in section 4.2 before. We can then propose an ansatz for the potential up to a given order in ψ and $\bar{\psi}$.

$$V_k(\psi,\bar{\psi}) = \rho \sum_{n,m} v_{nm}\rho^n \varsigma^m \tag{5.77}$$

The flow equations for the couplings are easily obtained with the help of a symbolic manipulation program such as Mathematica.

Finally, we could also use a mixed strategy, expanding the functional dependency of the effective potential in one of the fields, while leaving the full functional dependence in the other. In this case a natural choice [45, 44, 46, 50] would be to expand in the dependence of the less physical $\tilde{\psi}$ response fields, such as

$$V_k(\psi,\bar{\psi}) = \rho \sum_m b_m(\varsigma)\rho^m \tag{5.78}$$

5.5. Previous NPRG results for out of equilibrium systems

The NPRG formalism in its modern form emerged in the early nineties [201, 71, 147], but it was not before around ten years ago that it began to be applied to out of equilibrium problems. Here we briefly review some important milestones.

In [45], BARW-DP, defined by the reactions $A \to 2A$, $2A \to \emptyset$, was for the first time studied within this formalism, by means of a LPA truncated in the fields. Also a slightly improved version of the LPA, including running field-independent renormalization factors, (which we call LPA', see below) was used in order to have a better determination of critical exponents. The Itô prescription was not correctly implemented, but as we have seen, this bears no consequences at the level of the LPA. Critical exponents and a phase diagram where found for the transition in $d = 2$ and $d = 3$, in particular contradicting previous perturbative RG results which showed no phase transition for $d > 2$. In [44] these results were improved by calculating phase diagrams for higher values of d and comparing with Monte Carlo simulations. A phase transition was found to happen for all studied values of d. All these results were confirmed [50] using higher order truncations in the field, as well as a mixed type of field expansion, with a functional dependency kept in one of the fields while expanding in the second one.

In [46], BARW-PC, defined by $A \to 3A$, $2A \to \emptyset$ was studied, and NPRG was used to sketch the flow diagram around the non-perturbative PC fixed point in $d = 1$ (we will discuss more on this subject below). The study was once again performed within the LPA truncated in the fields. Agreement was found with the predictions of 1-loop perturbative field theory with respect to the upper critical dimension $d_c^{(1)} = 4/3$ for the PC/GV phase transition. Critical exponents were calculated, yielding better results, when compared to Monte Carlo, than previous perturbative calculations [52].

The NPRG has been also used to study critical dynamics close to equilibrium, where detailed balance is satisfied. In particular, in [41], a study at the level of the second order derivative expansion of model A was performed. Model A describes the purely dissipative relaxation of a non-conserved scalar field ϕ, and is described by the Langevin equation

$$\partial_t \phi(x) = -D\frac{\delta H[\phi]}{\delta \phi(x)} + \eta(x) \tag{5.79}$$

where the white noise term η is such that detailed balance is satisfied, and the Hamiltonian H is the Ginzburg-Landau ϕ^4 Hamiltonian, belonging to the Ising universality class. Critical exponents where found in very good agreement with previous results.

The NPRG technique has also been applied, quite successfully, to the study of the KPZ equation presented above. After some failed attempts within the derivative expansion [49], a BMW-inspired type of approximation was introduced [42], and later improved [43, 127], describing the whole momentum and frequency dependency, while truncating the field dependency. In particular, in [43], scaling functions stemming from the NPRG results where found to be in excellent agreement with the exact solution of the KPZ equation in $d = 1$ [180, 175]. Qualitative results for critical exponents and flow diagrams show great promise for this method in dimensions $d > 1$, where much less is known in an analytical way.

Recently, a review article has appeared which discusses the whole out of equilibrium NPRG formalism for stationary states [41]. There is the first place where the subtleties concerning the implementation of Itô's prescription within the NPRG were discussed. An application of the NPRG in the supersymmetric formalism, useful when detailed balance is present, was also presented, as well as a particular study in the case of model A dynamics.

Also, some recent progress has been made in the application of the NPRG techniques to the PCPD universality class [97], showing the existence of the build-up of a cusp instability during the RG flow. This is completely out of reach of a perturbative calculation, and probably signals the formation of bound states, where the dynamics is no longer well described in terms of the density field ϕ, at least perturbatively.

NPRG techniques were also used to study quantum boson systems out of equilibrium [126, 106]. This was performed by extending the Keldysh formalism to the NPRG context. The Keldysh formalism is mainly used when dealing with quantum systems, and also involves the introduction of a second field degree of freedom, analogous to the response field $\tilde{\phi}$ within the formalisms exploited here. However, in the case of [126], NPRG methods has been used to find full

time-dependent quantities, and not only stationary properties, for boson systems relaxing to thermal equilibrium. The results obtained with this method show a very good agreement with experiments [182].

The real time (or real frequency) Keldysh NPRG can also be used for studying correlated Fermi systems in non-equilibrium [89, 110, 122]. First applications, partly reviewed in [141] indicate that also for these type of problems the NPRG constitutes a useful tool. So far only steady state regimes were studied.

It should also be mentioned that much progress has been made recently on the study of out of equilibrium systems (including its full time dependence) within a formalism related to the NPRG, that of the 2PI vertex functionals [20].

We see, thus, that this work sits in the context of a (still) incipient but very promising field. The methods presented up to now have a very broad range of applicability, so that many different problems can eventually be tackled, while the results obtained up to now can also be improved in various ways, by going further in the order of the approximations, or by using new types of approximations of the NPRG equations altogether. We are sure to see many developments regarding the applications of NPRG techniques to out of equilibrium problems in the next few years.

5.6. Full functional dependence on the fields

As mentioned before, all previous NPRG results for out of equilibrium systems were obtained by performing some sort of field expansion. This is a natural first step, given that the formalism is written in terms of two fields, or, when available, in terms of at least two symmetry invariants of the theory. This poses a much harder problem than the single invariant field dependency in the case of Ising or $O(N)$ scalar field models.

In the case of reaction-diffusion systems NPRG studies have been performed at the level of the LPA (as well as the slightly improved LPA' described above). The use of more refined approximations was made difficult by a lack of a clear understanding of the subtleties related with the use of the Itô prescription, discussed in section 5.2.

There are then two clear pathways for improving our knowledge of BARW systems. On one hand, we can, still using a field truncation, improve the level of the approximation, by going for example to the $\mathscr{O}(\partial^2)$ DE. This would be a rather straightforward generalization of known results. On the other hand, it would be very satisfying from the methodological point of view to be able to study the full functional dependency in the fields for these theories. It is widely known [63, 98] that field truncations can often be misleading, presenting for example spurious fixed points, and in general lose one of the main advantages

of functional NPRG methods over other approaches.

On top of that, a full field description should be used if we want to obtain the probability distribution of the order parameter for reaction-diffusion systems, which would be a natural and very interesting generalization of the study made in the Ising case.

When performing such a full field LPA study of BARW systems we were confronted with unexpected difficulties, which in retrospect seem to be related to the construction of a suitable well-defined Γ_k effective action. In particular, its definition in terms of the usual Legendre transform Γ_k^L, Eq. (5.56) above.

Indeed, when numerically integrating Eq. (5.73) for BARW-DP and BARW-PC we found hard numerical problems, most notably the presence of poles which entered the field region under consideration. Numerical integration of the flow equation was only possible in a limited field region, and for fine tuned numerical discretization parameters. When such a solution was numerically feasible, it yielded the same values for the critical exponents as previous truncated approximations [45, 50].

These problems did not appear in previous NPRG studies. Now we understand why a field expansion can yield the correct values for the critical exponents, and why the expansion in one invariant was numerically not very stable. Indeed, when performing a field expansion in terms of the fields ψ_1 and ψ_2 for example, a natural separation arises between contributions to the effective potential which are even and odd in ψ_2. That is

$$V_k^L(\psi_1,\psi_2) = \sum_{n,m} a_{mn}\psi_1^n\psi_2^m \tag{5.80}$$

implies

$$V_k(\psi_1,\psi_2) = \sum_{n,m} (i)^m a_{mn}\psi_1^n\psi_2^m \tag{5.81}$$

and one obtains the same description at any order of the expansion in ψ_2, because the factors of i simplify between left and right sides of NPRG flow equations. Problems arise only when a full field description is sought for. The understanding of these subtleties can be seen as one of the main contributions of this work.

Once we implement the reality prescription described above, the corrected flow equation reads, in terms of the fields ψ_1 and ψ_2

$$\partial_k V_k(\psi_1,\psi_2) = \frac{1}{4}\int \frac{d^dq}{(2\pi)^d} \frac{\partial_k R_k(q)}{\sqrt{1-\frac{\left(\frac{V^{(2,0)}-V^{(0,2)}}{2}\right)^2+\left(V^{(1,1)}\right)^2}{\left(R_k(q)+\frac{V^{(2,0)}+V^{(0,2)}}{2}\right)^2}}} \tag{5.82}$$

with initial condition, for BARW-DP

$$\partial_k V_\Lambda(\psi_1,\psi_2) = \left(\frac{\psi_1^2+\psi_2^2}{2}\right)\left(\sqrt{2\lambda\sigma}\, i\psi_2 + \lambda\left(\frac{\psi_1^2+\psi_2^2}{2}\right)\right) \tag{5.83}$$

The definition (5.56) allows us then to integrate the LPA equations in terms of a complex potential $V_k(\psi_1,\psi_2) \in \mathbb{C}$ depending on the pair of real fields, ψ_1 and ψ_2. In the case of BARW-DP, the LPA flow equation (5.82) can be rewritten in terms of the rapidity invariants (5.76), and it can be checked that no poles appear at the level of the initial condition for arbitrary values of the invariant fields. This solves the difficulties pointed out before. However, the use of an explicit time-stepping algorithm leads to instabilities when solving this flow equation, which we think have a purely numerical origin. The implementation of more refined numerical methods to solve the BARW-DP LPA equation is currently underway.

5.7. Comments

In this chapter we presented some aspects and particularities of the NPRG method when applied to out of equilibrium, and in particular reaction-diffusion, systems. Apart from the doubling of the degrees of freedom stemming from the construction of a field theory, further complications arise due to causal properties, the Itô prescription, and reality conditions for the fields. Some of these properties have not been fully discussed before in the literature, and work is underway to fully exploit them while performing a DE type of approximation for these systems.

The NPRG appears to be much less forgivable with respect with these fundamental properties, if we make a comparison with e.g. the usual perturbative expansion. On the one hand this implies that much work must be devoted to fully integrate these and other subtleties into the formalism. On the other hand, in our opinion the NPRG procedure ends up yielding a much better understanding of the physics of these systems.

Next, we are going to use a different approach to study some of these BARW systems. Instead of augmenting the order in the DE, we have chosen to perform a new type of expansion around pure annihilation.

Chapitre 6

Some exact results in BARW

Exact solutions for simple systems are very important in physics. They serve as exemplars but also as a basis to obtain a better understanding of a subject, and as a possible starting point for perturbative approaches. There is a good number of such solutions for strongly correlated systems at thermal equilibrium, obtained by powerful methods like Conformal Field Theory, Bethe ansatz or large N methods.

Much less is known in an exact way in the case of out of equilibrium systems, where such methods cannot be generalized to these less-structured systems. Of course there are some exceptions to this general rule, and some exact solutions have indeed been found for some specific systems [8], and in particular for reaction-diffusion systems in $d = 1$ [186]. Recently, an exact solution has been found for KPZ in $d = 1$ [56, 180, 32, 2, 175], by using the Cole-Hopf version of the theory, and thanks to a series of mappings into theories in which random matrix methods could be used. This solution has a great deal of interest, and it serves as an excellent testing ground for approximation methods to be used in similar system. For example, this has been recently done for the NPRG formalism as applied to KPZ in [43, 127].

In fact, RG techniques are seldom used to arrive to an exact result. When such an exact solution is possible, it is generally found by using less convoluted methods. Sometimes it is possible to recover an exact solution by means of a RG procedure, but, as we have discussed before, the main reason to use the RG (and the NPRG in particular) is to apply powerful approximation schemes, such as the loop expansion, the DE, or the BMW method.

In this chapter we use the NPRG to prove an exact relation that allows us to obtain closed equations for any vertex in PA, which in principle yields a full and exact description of the system in any dimension. This relation, which is easy to see at the perturbative level (and we show it non-perturbatively), was not previously noticed in the literature, apart from some particular cases, as

far as we know. Even though PA is a relatively simple system where no phase transition is found, its response functions are non-trivial, and in particular non-Gaussian.

With this exact characterization of PA at hand, we then introduce what we call the σ-expansion, an expansion in the branching rate around the solution of PA. With the σ-expansion we can rewrite low branching rate quantities in BARW in terms of PA vertices, which allows us to obtain exact answers for some questions in these systems. It is important to begin by stressing that this expansion is qualitatively distinct to the usual perturbative expansion, in that it is a perturbation around a non-trivial, non Gaussian theory. This type of expansion, analogous to what is usually performed in equilibrium around Conformal Field Theories, is also a first in the out of equilibrium literature, as far as we know.

We begin this chapter by studying in detail pure annihilation. The closed equations for any vertex in PA to which we arrive could be further exploited, but we restrain here to those which are going to be useful later on, when treating BARW at low branching rates.

In section 6.2 we introduce the σ-expansion in the context of BARW-DP. This expansion allows us, in particular, to obtain the minimum threshold value λ_{th} for the annihilation rate in order to have an inactive phase. This threshold value is non-universal, and, being a low branching quantity, the first order of the σ-expansion allows us to obtain it in an exact way. Later on, in section 6.3 we apply our method to BARW-PC, showing the existence of an unexpected RG fixed point structure.

This chapter is based on publications [14] and [15].

6.1. Pure Annihilation

In this section we study the simplest case of a reaction-diffusion system, that is, PA, in which the only reaction in the system is annihilation by pairs of diffusing particles $2A \to \emptyset$, with a probability rate λ. Later we use the exact solution for this particular system as the starting point of a perturbative expansion, in order to study more general BARW at small branching rates. It is easy to prove [189, 172] that this system belongs to the same universality class as pure coagulation, in which the only reaction is $A + A \to A$. In the following we consider mainly the PA model but the pure coagulation case can be analyzed in a similar way, as discussed in section 6.2.2 below.

After implementing the Doi-Peliti procedure and performing a shift in the response fields, Eq. (3.70), the bare action S^{PA} can be written [52, 189]

$$S^{PA}[\bar{\phi},\phi] = \int_x \left(\bar{\phi}(\partial_t - D\nabla^2)\phi + \lambda\bar{\phi}(\bar{\phi}+2)\phi^2 \right). \tag{6.1}$$

As said before, we only analyze the steady state of the system, where all correlation functions are zero, since the system always reaches the empty state in the long time limit. However, even in this state, the response functions are non trivial and are governed in the IR (that is, for momenta and frequencies smaller than the scale set by λ) by a non-trivial fixed point of the RG equations, for $d < 2$. Therefore we speak of 'correlation functions' in a generalized sense, including response functions.

As it stands, this theory shows a certain similarity with the standard ϕ^4 scalar field theory studied before. However, symmetry and causality properties allow for a greatly simplified analysis, which goes beyond what can be done in standard equilibrium theories. The complexities of out of equilibrium physics are here working in our favor. We first show that for the PA model all $\Gamma^{(n,m)}$ functions can be obtained from the $\Gamma^{(n,n)}$, vertices with the same number of incoming and outgoing legs. This is quite clear perturbatively, but we give in the following a non-perturbative proof based on a Ward identity for a $U(1)$ transformation. Secondly, we deduce a general identity yielding a closed equation for any $\Gamma^{(n,m)}$. It is easy to verify that the $\Gamma^{(1,1)}$, $\Gamma^{(2,1)}$ and $\Gamma^{(2,2)}$ vertices thus obtained coincide with the results of [52, 172, 202, 206]. We show later how we can compute $\Gamma^{(3,3)}$ from our method.

6.1.1. $U(1)$ Ward identity

Let us start by studying a generalization of PA with a modified action $\tilde{S}^{PA}$, where couplings for the cubic and quartic terms are independent.

$$\tilde{S}^{PA}[\bar{\phi},\phi] = \int_x \left(\bar{\phi}(\partial_t - D\nabla^2)\phi + \lambda_3\bar{\phi}\phi^2 + \lambda_4\left(\bar{\phi}\phi\right)^2\right). \tag{6.2}$$

Consider now the infinitesimal field transformation

$$\begin{aligned}\phi(x) &\to (1+\epsilon)\phi(x)\\ \bar{\phi}(x) &\to (1-\epsilon)\bar{\phi}(x)\end{aligned} \tag{6.3}$$

When $\lambda_3 = 0$ this is a symmetry of the action, but the cubic term breaks it explicitly. We can nevertheless obtain a Ward identity [208] associated with this transformation by performing (6.3) as a change of variables in the partition function $\mathcal{Z}[J,\bar{J}]$

$$0 = \epsilon\int_x \langle J\phi - \bar{J}\bar{\phi} + \lambda_3\phi^2\bar{\phi}\rangle_{J,\bar{J}} \tag{6.4}$$

Here the mean value $\langle\ldots\rangle_{J,\bar{J}}$ is computed in the presence of the sources J and $\bar{J}$. The term proportional to λ_3 can be written as a derivative w.r.t. λ_3 of the generating functional of connected correlation functions. By Legendre transforming

Eq. (6.4), one deduces the Ward identity

$$-\lambda_3 \frac{\partial \Gamma}{\partial \lambda_3} + \int_x \left(\psi \frac{\delta \Gamma}{\delta \psi} - \bar{\psi} \frac{\delta \Gamma}{\delta \bar{\psi}} \right) = 0 \tag{6.5}$$

This equation can be derived w.r.t. ψ and $\bar{\psi}$ fields and evaluated at zero field, yielding

$$(n-m)\Gamma^{(n,m)} = \lambda_3 \frac{\partial \Gamma^{(n,m)}}{\partial \lambda_3} \tag{6.6}$$

where $\Gamma^{(n,m)} = \Gamma^{(n,m)}(x_1, \ldots, x_n, \bar{x}_1, \ldots, \bar{x}_m; \psi = 0, \bar{\psi} = 0)$.

Since, perturbatively, $\Gamma^{(n,m)}$ can only involve positive powers of λ_3, this equation shows that $\Gamma^{(n,m)} \sim \mathcal{O}(\lambda_3^{n-m})$ when $n \geq m$, and that for PA, $\Gamma^{(n,m)}$ contains exactly $(n-m)$ third-order bare vertices. We conclude that all $\Gamma^{(n,n)}$ vertices can be computed directly from the action with $\lambda_3 = 0$ and that

$$\Gamma^{(n,m)} = 0 \qquad \text{if } n < m \tag{6.7}$$

which simplifies the study of this system.

Moreover, given this result, one can conclude that for any correlation function, the perturbative expansion in λ_3 is, being in fact a polynomial, exact at a *finite* order. In order to calculate the connected correlation function $G^{(n,m)}$ with $n > m$, one can expand the functional integral at order λ_3^{n-m} :

$$G^{(n,m)}(x_1, \ldots, x_n, \bar{x}_1, \ldots, \bar{x}_m) = \lambda_3^{n-m} \langle \phi(x_1) \ldots \phi(x_n) \bar{\phi}(\bar{x}_1) \ldots \bar{\phi}(\bar{x}_m) \Big(\int_x \bar{\phi} \phi^2 \Big)^{n-m} \rangle_c \Big|_{J=\bar{J}=0, \lambda_3=0} \tag{6.8}$$

(using the unique decomposition of $G^{(n,m)}$ in terms of 1PI vertices [208]) reducing its calculation to the knowledge of correlation functions of the $\lambda_3 = 0$ model (which only contains $\Gamma^{(n,n)}$ vertices). This shows that the building blocks of the PA model are the vertex functions with an equal number of incoming and outgoing legs, that can be directly calculated from the modified theory with $\lambda_3 = 0$.

6.1.2. An identity for the $\Gamma^{(n,m)}$ vertices

We now present an identity that allows us to obtain a closed equation for any $\Gamma^{(n,m)}$. It can be most conveniently written at the diagrammatic level : any diagram contributing to $\Gamma^{(n,m)}$ which includes at least one loop has the structure shown in Fig. 6.1 (that is to say : any 1PI perturbative diagram begins with a 4-legs bare vertex, at all orders in a perturbative expansion, and even beyond a perturbative expansion, as will be explained below).

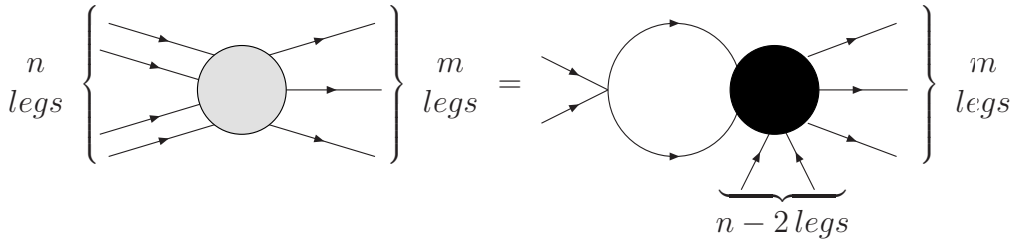

FIGURE 6.1 – Generic form of a diagram contributing to $\Gamma^{(n,m)}$ and that involves at least one loop in PA. Left hand side : diagrammatic representation of a generic $\Gamma^{(n,m)}$ vertex. Right hand side : general structure for such vertices in PA, the black blob is a connected and amputated Green function that has to comply with some requisites, see text.

The black blob denotes a sub-diagram that is constrained by the condition that the full diagram must be 1PI. In particular, it means that this sub-diagram must be connected (and with amputated external legs). Now, any connected diagram with n incoming and m outgoing legs has a unique tree decomposition in terms of 1PI sub-diagrams having at most these numbers of legs. By summing all possible diagrams and permutations compatible with the 1PI structure of the full diagram, we obtain a closed equation that relates any $\Gamma^{(n,m)}$ with vertices $\Gamma^{(s,l)}$ with a lower number of legs. A non-perturbative proof (not based on an all-order analysis) of this general property can be given by using NPRG techniques. We detail it in section 6.1.3.

Notice that, as explained in the previous section, $\Gamma^{(n,n)}$ vertices can be calculated at $\lambda_3 = 0$. Now, for $\lambda_3 = 0$ the $U(1)$ transformation (6.3) is a symmetry of the action, and the fields ψ and $\bar{\psi}$ play symmetric roles. Accordingly, a construction analogous to Fig. 6.1 can be performed singularizing two outgoing legs in the case of $\Gamma^{(n,n)}$ vertices.

In order to be concrete, let us analyze the identity given in Fig. 6.1 for the simplest vertices. For $\Gamma^{(1,1)}$ this gives a well-known non-renormalization property : there is no correction to $\Gamma^{(1,1)}$ in PA. This is due to the fact that no diagram such as the one presented in Fig. 6.1 can be drawn with a single incoming leg. This no-field-renormalization condition implies that the critical exponents η and z have their mean field values, $\eta = 0$ and $z = 2$. Concerning $\Gamma^{(2,2)}$, the result is less trivial. As said before, this vertex can be calculated in the $\lambda_3 = 0$ theory. Given that there are only two incoming legs and that in a theory with Z_2 symmetry all connected diagrams with four external legs are 1PI, one arrives at the closed equation (see Fig. 6.2) which reads :

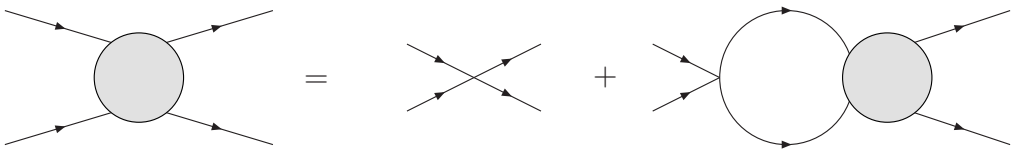

FIGURE 6.2 – Closed equation for $\Gamma^{(2,2)}$ in PA.

$$\Gamma^{(2,2)}(p_1,p_2,\bar{p}_1,\bar{p}_2) = 4\lambda_4 - 2\lambda_4 \int_q G(q) \times G(p_1+p_2-q)\Gamma^{(2,2)}(q,p_1+p_2-q,\bar{p}_1,\bar{p}_2) \quad (6.9)$$

whose solution is of the form

$$\Gamma^{(2,2)}(p_1,p_2,\bar{p}_1,\bar{p}_2) = 4l_4(p_1+p_2) \quad (6.10)$$

that is, $\Gamma^{(2,2)}(p_1,p_2,\bar{p}_1,\bar{p}_2)$ depends only on p_1+p_2. By substituting (6.9) in (6.10) we find

$$l_4(p) = \frac{\lambda_4}{1+2\lambda_4 \int_q G(q)G(p-q)} \quad (6.11)$$

For $\Gamma^{(2,1)}$ the identity in Fig. 6.1 becomes that of Fig. 6.3, which can be written as

$$\Gamma^{(2,1)}(p_1,p_2,\bar{p}) = 2\lambda_3 - 2\lambda_4 \int_q G(q) \times G(p_1+p_2-q)\Gamma^{(2,1)}(p_1+p_2-q,q,\bar{p}) \quad (6.12)$$

We can show (see below) that this implies that $\Gamma^{(2,1)}(p_1,p_2,\bar{p})$ depends only on $\bar{p}$. We thus define

$$\Gamma^{(2,1)}(p_1,p_2,\bar{p}) = 2l_3(\bar{p}) \quad (6.13)$$

By substituting Eq. (6.13) into Eq. (6.12) we find

$$l_3(\bar{p}) = \frac{\lambda_3}{1+2\lambda_4 \int_q G(q)G(\bar{p}-q)} \quad (6.14)$$

Dividing $\Gamma^{(2,1)}$ by $\Gamma^{(2,2)}$ one observes that their ratio is equal to $\lambda_3/(2\lambda_4)$, so that the relation between three and four point vertices is not renormalized. Of course, for the actual PA model one must take $\lambda_3 = 2\lambda_4 = 2\lambda$, and $l(p) = l_4(p) =$

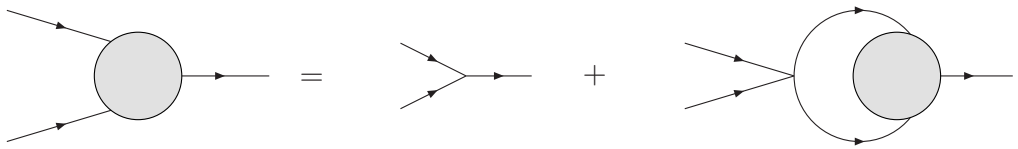

FIGURE 6.3 – Diagrammatic identity for $\Gamma^{(2,1)}$ in PA.

$l_3(p)/2$. In the rest of this chapter, we only consider this case unless otherwise stated.

Let us now show, by using NPRG equations, that these expressions are in fact non-perturbative (they are valid beyond an all-order perturbative analysis). These expressions have already been obtained before for the vertices with two incoming legs [52, 172, 202], as a sum over bubbles. The interesting point is that the present analysis applies to any $\Gamma^{(n,m)}$ vertex in PA. As an example, the equation for $\Gamma^{(3,3)}$ is obtained below. Unfortunately, for $n > 2$ the corresponding equations must be solved numerically.

6.1.3. Non-perturbative proof of the closed equation for $\Gamma^{(n,m)}$

Here we use the NPRG in order to show the general diagrammatic property seen in Fig. 6.1, which relates $\Gamma^{(n,m)}$ with λ and vertices of at most (n,m) legs. First, observe that we can write the property we want to show in terms of a specific form for Γ_k, the average effective action for the theory at any scale k

$$\Gamma_k = S^{PA} + \int_x \psi^2(x) \int_{x',x''} G_k(x'-x) G_k(x''-x) \tilde{\Gamma}_k[x',x'',\psi,\bar{\psi}] \tag{6.15}$$

with

$$\begin{aligned} \frac{\delta \tilde{\Gamma}_k[x',x'',\psi,\bar{\psi}]}{\delta \psi(\mathbf{x},t)} &= 0 \qquad \text{if } t < \max(t',t'') \\ \frac{\delta \tilde{\Gamma}_k[x',x'',\psi,\bar{\psi}]}{\delta \bar{\psi}(\mathbf{x},t)} &= 0 \qquad \text{if } t < \max(t',t'') \end{aligned} \tag{6.16}$$

Indeed, this form ensures that any $\Gamma_k^{(n,m)}$ vertex will consist in a series of bare terms given by the action S^{PA}, together with renormalized terms which always begin (temporally speaking) by a bare $(2,2)$ vertex.

The property we want to show is obviously true at the bare level, with $\tilde{\Gamma}_\Lambda = 0$. Now we proceed in an iterative way, assuming that the property we want to prove is true at a RG scale k_0, and checking that it continues to be valid for a scale $k_0 - \delta k$.

By hypothesis then, we take that at $k = k_0$ all vertices $\Gamma_{k_0}^{(n,m)}$ can be decomposed as a diagram containing a λ_4 bare vertex (with two simultaneous incoming ψ legs) and a $\tilde{\Gamma}_{k_0}^{(n,m)}$, this last function being constrained by the condition that the full diagram must be 1PI. As explained before, the NPRG equations for any vertex $\Gamma_k^{(n,m)}$ can be represented diagrammatically by 1-loop diagrams, where vertices and propagators are read from $\Gamma_k + \Delta S_k$. To those diagrams one must apply the operator $\tilde{\partial}_k$ introduced before, in order to obtain $\partial_k \Gamma_k^{(n,m)}$. Each one of these terms consists in a number of $\Gamma_k^{(l,s)}$ vertices joined together by an internal loop of propagators. We can distinguish between internal lines, pertaining to the internal loop, and external lines.

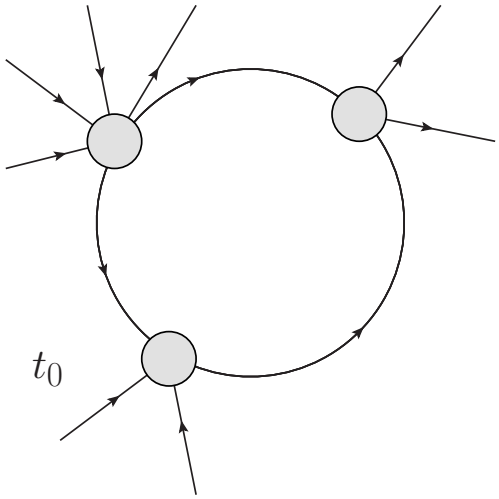

FIGURE 6.4 – A diagram contributing to $\partial_k \Gamma_k^{(n,m)}(t_1, \ldots, t_n, \tilde{t}_1, \ldots, \tilde{t}_m)$.

Consider then a typical diagram contributing to $\partial_k \Gamma_k^{(n,m)}(t_1, \ldots, t_n, \tilde{t}_1, \ldots, \tilde{t}_m)$, where we emphasize the time dependence of the vertices. See Fig. 6.4. We now define as t_0 the smallest time for any incoming external leg, $t_0 = \min(t_1, \ldots, t_k)$. Its corresponding leg is attached to one of the vertices in the loop, and by hypothesis at $k = k_0$, the two smallest times in this vertex must correspond to an incoming bare λ_4 vertex. We have then two possibilities to consider :

1) Both t_0 legs are external legs. This means that $\partial_k \Gamma_k^{(n,m)}$ can also be decomposed in the form (6.16). Which implies the desired property for $k = k_0 - \delta k$

2) Only one t_0 leg is an external leg, and the other one is an internal incoming leg. Thus, given the non-renormalization of the causal propagators, there must be another vertex with an outgoing leg at a time smaller than t_0. But at

$k = k_0$ this vertex should have at least two incoming legs with a corresponding time previous to t_0. At least one of these incoming legs must be external, contradicting our assumption.

The desired property is then preserved all along the NPRG flow, up to and including the physically most relevant case $k = 0$, showing that it is a fully non-perturbative relation, as announced before.

6.1.4. Comparison with non-relativistic many-body theory

The NPRG formalism for reaction-diffusion systems as presented up to now can be related very directly to the NPRG formalism in the case of non-relativistic many body theory [79, 80, 82]. Indeed, there have been some recent studies of few-body physics of identical non-relativistic bosons, related for example to the Efimov effect [146, 81]. The field theory action for these systems reads

$$S[\phi] = \int d\tau \int d^d x \left\{ \phi^* \left(\partial_\tau - \frac{\nabla^2}{2M_\phi} - \mu \right) \phi + \lambda_\phi \left(\phi^* \phi \right)^2 \right\} \tag{6.17}$$

in terms of a bosonic field ϕ (which is appropriate to describe identical bosons). The microscopic interaction strength λ_ϕ is seen to be related to the s-wave scattering length. An imaginary time formulation is used, with τ being integrated from 0 to $1/T$ in the Matsubara formalism. μ stands for the chemical potential in this context. We are only interested here in few-body properties in the vacuum, i.e. for vanishing temperature $T = 0$ and particle density $n = 0$, energies can be measured in units of momentum squared which leads to $2M_\phi = 1$. In the case we are interested thus, we end up with the action

$$S[\phi] = \int d\tau \int d^d x \left\{ \phi^* \left(\partial_\tau - \nabla^2 \right) \phi + \lambda_\phi \left(\phi^* \phi \right)^2 \right\} \tag{6.18}$$

which is basically the same as our action for the modified PA theory, with only λ_4 vertices.

Given property (6.6) above, it is immediate to see that only vertices of the form $\Gamma^{(n,n)}$ are non-zero, which coincides with the expected conservation of the number of particles in the system. Also, by the same reasoning as above, it is easy to see that the propagator is not renormalized. These results were already known in the literature.

However, in [82, 146, 81, 80], a property is invoked which states that the NPRG equations for the $\Gamma_k^{(n,n)}$ must decouple from the flow of all the $\Gamma_k^{(m,m)}$ with $m > n$. This coincides with the intuitive expectation that, as no particles are created, the $n-$body properties should not depend of higher order correlations. We have seen that this is indeed the case for the $\Gamma^{(2,2)}$ vertex, but in [82, 146, 81] this property is also used for the case of the $\Gamma^{(3,3)}$ vertex.

Unfortunately, as we have mentioned, the causality properties which ultimately lead to the closure of the flow equation for the $\Gamma^{(2,2)}$ vertex are not enough to justify this decoupling in the case of higher order vertices. We think there is a mistake in the proposed proof of this decoupling property for general n in [80], of which we give a counter-example for the $\Gamma^{(3,3)}$ vertex.

Indeed, consider Fig. 6.5. This diagram represents a non-vanishing contribution to the flow of the $\Gamma_k^{(4,4)}$ vertex. Notice that its form allows for the development, along the flow, of a time ordering of the external legs of $\Gamma_k^{(4,4)}$, in which an outgoing $\bar{\psi}$ leg is evaluated at a time earlier than that of one of the incoming ψ legs (as legs p_4 and $\bar{p}_1$ in the figure). This happens even though both the propagator and the $\Gamma^{(2,2)}$ vertex are strictly causal, in the sense that all incoming ψ legs must have corresponding times smaller than those of all outgoing $\bar{\psi}$ legs.

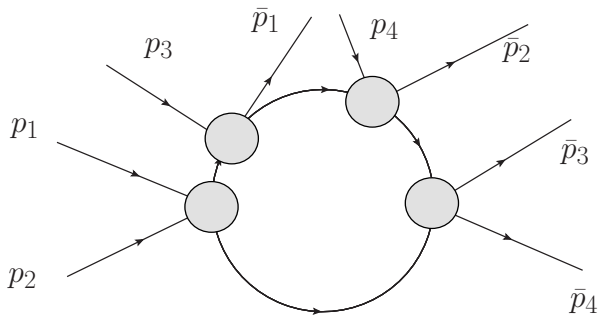

FIGURE 6.5 – A non-zero contribution to the NPRG flow of $\Gamma^{(4,4)}$ in nonrelativistic many-body theories.

Now, the $\Gamma^{(4,4)}$ vertex enters into the flow of $\Gamma_k^{(3,3)}$ in the tadpole diagram shown in Fig. 6.6. If $\Gamma_k^{(4,4)}$ were strictly causal in the sense defined above, then this diagram would not contribute to the flow, given that the closed propagator loop of the tadpole requires $\Gamma_k^{(4,4)}$ to have one incoming leg with a corresponding time larger than that of one of its outgoing leg. But this is precisely the kind of term which can be constructed with diagram 6.5. This shows that the flow of $\Gamma_k^{(4,4)}$ does indeed enter into the calculation of $\Gamma_k^{(3,3)}$, and therefore this last vertex is not decoupled. More precisely, the decoupling probably takes place, but not in such a naive way. This same argument can be generalized to higher order vertices.

Notice that this non-decoupling of higher order vertices can be also seen at the perturbative level. Figure Fig. 6.7 shows a contribution of the $\Gamma^{(4,4)}$ 1PI vertex to one possible $\Gamma^{(3,3)}$ perturbative diagram.

PA, and therefore non-relativistic many-body theory, has in conclusion a causal structure which is a little more complex than the one which was pro-

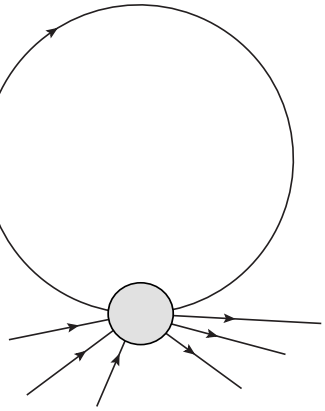

FIGURE 6.6 – A non-zero contribution to the NPRG flow of $\Gamma^{(3,3)}$ in nonrelativistic many-body theories.

posed in [80]. We circumvented this difficulty by proving property (6.15), which allows us to find closed equations for any vertex. Thus, we see that there is indeed a decoupling, but it is not seen at the level of the NPRG equations, or at least not without some further information.

6.1.5. Study of the $\Gamma^{(3,3)}$ vertex in PA

As a first nontrivial example of the use of the closed equation for $\Gamma^{(n,n)}$ in PA, here we study the $\Gamma^{(3,3)}$ vertex. Unfortunately, as we will see, this procedure is not enough to find a complete analytical solution for the vertex. To find a solution we would need a numerical analysis of the resulting equation, beyond the scope of the present work.

As explained before, every diagram for $\Gamma^{(3,3)}$ is of the form shown in Fig. 6.1. The black blob that appears in the figure can be decomposed in a sum of 1PI diagrams, as shown in Fig 6.8. If we analyze the possible 1PI contributions we end up with the two diagrams shown in Fig. 6.9. Using the known form for $l(p)$, Eq. (6.11) and the corresponding symmetry factors, the equation corresponding to

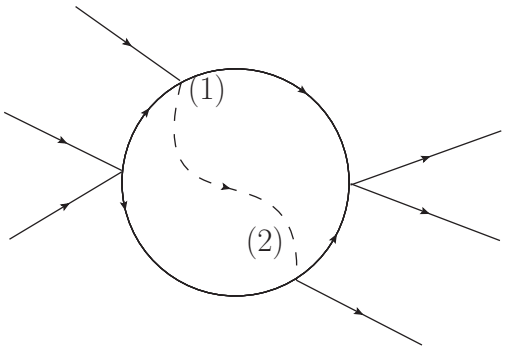

FIGURE 6.7 – A diagram contributing to $\Gamma^{(3,3)}$ in perturbation theory. It is obtained from $\Gamma^{(4,4)}$ by joining an outgoing with an incoming leg. This contribution is non-zero, and in particular notice that particle number conservation is never violated, but that the outgoing leg (1) of $\Gamma^{(4,4)}$ must occur at a smaller time than that of the incoming (2) leg.

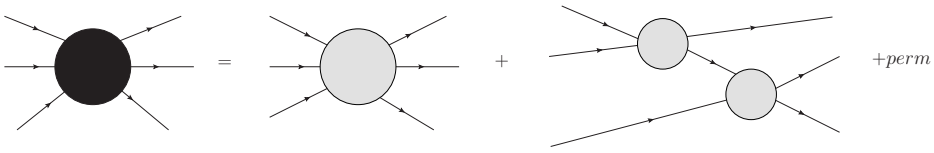

FIGURE 6.8 – 1PI contributions to the connected (3,3) correlation function in PA.

this diagram reads

$$
\begin{aligned}
&\Gamma^{(3,3)}(p_1,p_2,p_3,\tilde{p}_1,\tilde{p}_2,\tilde{p}_3) = \\
&\quad 64\lambda\Big(\int_q G(q)G(p_1+p_2-q)\Big[l(\tilde{p}_2+\tilde{p}_3)G(p_3+q-\tilde{p}_1)l(q+p_3) \\
&\quad + l(\tilde{p}_1+\tilde{p}_3)G(p_3+q-\tilde{p}_2)l(q+p_3) + l(\tilde{p}_1+\tilde{p}_2)G(p_3+q-\tilde{p}_3)l(q+p_3) \\
&\quad + \int_q G(q)G(p_1+p_3-q)l(p_2+q)\Big[G(p_2+q-\tilde{p}_1)l(\tilde{p}_2+\tilde{p}_3) \\
&\quad + G(p_2+q-\tilde{p}_2)l(\tilde{p}_1+\tilde{p}_3) + G(p_2+q-\tilde{p}_3)l(\tilde{p}_1+\tilde{p}_2)\Big] \\
&\quad + \int_q G(q)G(p_2+p_3-q)l(p_1+q)\Big[G(p_1+q-\tilde{p}_1)l(\tilde{p}_2+\tilde{p}_3) \\
&\quad + G(p_1+q-\tilde{p}_2)l(\tilde{p}_1+\tilde{p}_3) + G(p_1+q-\tilde{p}_3)l(\tilde{p}_1+\tilde{p}_2)\Big]\Big) \\
&\quad - 2\lambda\int_q G(q)\Big(G(p_1+p_2-q)\Gamma^{(3,3)}(q,p_1+p_2-q,p_3,\tilde{p}_1,\tilde{p}_2,\tilde{p}_3) \\
&\quad + G(p_1+p_3-q)\Gamma^{(3,3)}(q,p_1+p_3-q,p_2,\tilde{p}_1,\tilde{p}_2,\tilde{p}_3) \\
&\quad + G(p_2+p_3-q)\Gamma^{(3,3)}(q,p_2+p_3-q,p_1,\tilde{p}_1,\tilde{p}_2,\tilde{p}_3)\Big) \qquad (6.19)
\end{aligned}
$$

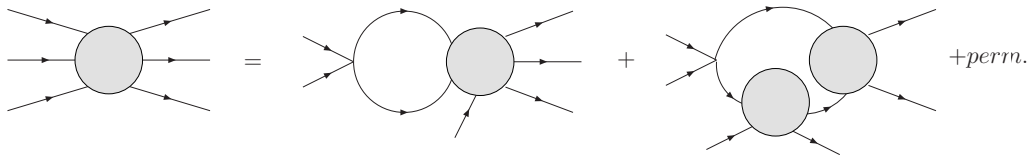

FIGURE 6.9 – Closed equation for $\Gamma^{(3,3)}$ in PA.

This equation shows a very symmetric structure, which suggests the ansatz (stable by iterations)

$$\Gamma^{(3,3)}(p_1,p_2,p_3,\tilde{p}_1,\tilde{p}_2,\tilde{p}_3) = f(p_1+p_2,p_3,\tilde{p}_1+\tilde{p}_2,\tilde{p}_3) + \text{permutations} \quad (6.20)$$

where in fact the last dependence (in $\tilde{p}_3$ in the equation) is redundant due to momentum conservation. The corresponding equation for f is

$$\begin{aligned} f(p_a,p_b,\tilde{p}_a,\tilde{p}_b) = 64\lambda\, l(\tilde{p}_a)\int_q G(q)G(p_a-q)G(p_b+q-\tilde{p}_b)l(p_b+q) \\ -2\lambda\int_q G(q)G(p_a-q)\Big[f(p_a,p_b,\tilde{p}_a,\tilde{p}_b)+f(q+p_b,p_a-q,\tilde{p}_a,\tilde{p}_b) \\ +f(p_a+p_b-q,q,\tilde{p}_a,\tilde{p}_b))\Big] \end{aligned} \quad (6.21)$$

and, using the explicit form for $l(p)$ this can be rewritten as

$$\begin{aligned} f(p_a,p_b,\tilde{p}_a,\tilde{p}_b) = 64 l(p_a)l(\tilde{p}_a)\int_q G(q-p_b)G(q-\tilde{p}_b)G(p_a+p_b+q)l(q) \\ -4l(p_a)\int_q G(q)G(p_a-q)f(p_a+p_b-q,q,\tilde{p}_a,\tilde{p}_b) \end{aligned} \quad (6.22)$$

where a change of variables has also been performed inside the integrals. Eq. (6.22) is specially interesting given that it is only written in terms of dressed propagators an vertices (there is no longer an explicit dependence in λ).

In order to get rid of the incoming and outgoing dressed $l(p)$ vertices we can define

$$\chi(p_a,p_b,\tilde{p}_a,\tilde{p}_b) = \frac{f(p_a,p_b,\tilde{p}_a,\tilde{p}_b)}{l(p_a)\tilde{l}(p_a)} \quad (6.23)$$

whose equation reads

$$\begin{aligned} \chi(p_a,p_b,\tilde{p}_a,\tilde{p}_b) = 64\int_q G(q-p_b)G(q-\tilde{p}_b)G(p_a+p_b+q)l(q) \\ -4\int_q G(q)G(p_a-q)l(p_a+p_b-q)\chi(p_a+p_b-q,q,\tilde{p}_a,\tilde{p}_b) \end{aligned} \quad (6.24)$$

This expression can be further simplified, but in the long run a numerical study is unavoidable to solve it. Notice also that this expression is not explicitly symmetric with respect to the change $p \to \tilde{p}$. It is easy though to find such a symmetric expression, by combining this expression with the one obtained by using the equation stemming from the diagrammatic ansatz with the λ bare vertex in the outgoing legs of the diagram. This symmetric equation does not turn out to be simpler to solve than (6.24).

6.1.6. Galilean Symmetry

There is a less evident symmetry in PA, which we call Galilean symmetry. It manifests itself in terms of an action with only kinetic and quartic terms, but as we have seen this is enough for the study of the $\Gamma^{(n,n)}$ vertex functions in PA. This would also be useful for the study of the Cole-Hopf version of KPZ [202].

The action

$$S = \int_{x,t} \{\bar{\phi}(\partial_t - \Delta)\phi + \lambda(\bar{\phi}\phi)^2\} \tag{6.25}$$

is invariant under the following Galilean transformations, with v an infinitesimal vector

$$\delta\phi = \frac{1}{2}(x\cdot v)\phi + t\, v\cdot\nabla\phi$$
$$\delta\bar{\phi} = -\frac{1}{2}(x\cdot v)\bar{\phi} + t\, v\cdot\nabla\bar{\phi}$$

The Ward identity for this symmetry reads

$$\int_{x,t}\left(\delta\phi\Big|_{\phi\to\psi}\frac{\delta\Gamma}{\delta\psi} - \delta\bar{\phi}\Big|_{\bar{\phi}\to\bar{\psi}}\frac{\delta\Gamma}{\delta\bar{\psi}}\right) = 0 \tag{6.26}$$

which allows us to obtain some identities for the vertex functions. Differentiating w.r.t. ψ and $\bar{\psi}$ we find

$$\left(\frac{1}{2}y\cdot v - t_y v\cdot\nabla_y\right)\frac{\delta^2\Gamma}{\delta\psi(y)\delta\bar{\psi}(z)} + \left(-\frac{1}{2}z\cdot v - t_z v\cdot\nabla_z\right)\frac{\delta^2\Gamma}{\delta\bar{\psi}(z)\delta\psi(y)} +$$
$$\int_{x,t}\left(\delta\psi\frac{\delta^3\Gamma}{\delta\psi(x)\delta\psi(y)\delta\bar{\psi}(z)} - \delta\bar{\psi}\frac{\delta^3\Gamma}{\delta\bar{\psi}(x)\delta\psi(y)\delta\bar{\psi}(z)}\right) = 0$$

evaluating at zero field and using translation invariance yields

$$\left(\frac{1}{2}y\cdot v - t_y v\cdot\nabla_y\right)\frac{\delta^2\Gamma}{\delta\psi(y)\delta\bar{\psi}(0)} = 0 \tag{6.27}$$

where t_y is the time associated with the y coordinate. Performing the Fourier transform

$$\left(\frac{i}{2}\partial_{\mathbf{q}} + \mathbf{q}\partial_{\omega}\right)\Gamma^{(1,1)}(\mathbf{q}^2,\omega) = 0 \tag{6.28}$$

from where one can deduce that

$$\Gamma^{(1,1)}(\mathbf{q}^2,\omega) = f(\mathbf{q}^2 + i\omega) \tag{6.29}$$

a known result.

The $\Gamma^{(1,1)}$ case is relatively easy because it only involves one momentum q. It is more difficult to obtain useful information from Galilean invariance for higher order vertices. In the case of the $(2,2)$ vertex the Ward identity yields, after Fourier transforming

$$\left(\frac{i}{2}\partial_{\mathbf{q}_1} + \mathbf{q}_1\partial_{\omega_1} - \frac{i}{2}\partial_{\mathbf{q}_2} + \mathbf{q}_2\partial_{\omega_2} + \frac{i}{2}\partial_{\mathbf{q}_3} + \mathbf{q}_3\partial_{\omega_3} - \frac{i}{2}\partial_{\mathbf{q}_4} + \mathbf{q}_4\partial_{\omega_4}\right) \times \delta^{(d+1)}(\sum_i q_i)\Gamma^{(2,2)}(q_1,q_3,q_2,q_4) = 0 \tag{6.30}$$

where the delta function appears due to translation invariance. We then must use

$$\sum_i q_i\partial_{\omega_i}\delta(\sum_i \omega_i)\delta^{(d)}(\sum_i \mathbf{q}_i) = \sum_i \mathbf{q}_i\delta^{(d)}(\sum_i \mathbf{q}_i)\delta'(\sum_i \omega_i) = 0 \tag{6.31}$$

and, for the derivatives w.r.t. $\mathbf{q}$ (x represent any component for the momenta)

$$\left(\partial_{\mathbf{q}_1} - \partial_{\mathbf{q}_2} + \partial_{\mathbf{q}_3} - \partial_{\mathbf{q}_4}\right)\left[\delta(\sum_i \omega_i)\delta^{(d)}(\sum_i \mathbf{q}_i)\right]\Big|_x = \delta(\sum_i \omega_i)\delta^{(d-1)}(\sum_i \mathbf{q}_i)(1-1+1-1)\delta'(\sum_i \mathbf{q}_i^{(x)}) = 0$$

so that we can choose not take into account derivatives of the delta function. We rewrite equation (6.30) in terms of more useful variables

$$\Gamma^{(2,2)} = \Gamma^{(2,2)}\left(\omega_1,\omega_2,\omega_3,\mathbf{q}_1^2,\mathbf{q}_2^2,\mathbf{q}_3^2,\alpha = 2\mathbf{q}_1\cdot\mathbf{q}_2,\beta = 2\mathbf{q}_1\cdot\mathbf{q}_2,\gamma = 2\mathbf{q}_2\cdot\mathbf{q}_3\right) \tag{6.32}$$

This turns out not to be enough to fully characterize the $(2,2)$ vertex. This kind of problem is also present when studying higher order vertices, as in the case of the $\Gamma^{(3,3)}$ vertex, which can be used for the study of d_c in BARW-even.

For the case of the $(2,2)$ vertex, we can use additional information available from our independent study of it. We know that in fact

$$\Gamma^{(2,2)} = \Gamma^{(2,2)}\left(\omega = \omega_1 + \omega_3, q = (\mathbf{q}_1 + \mathbf{q}_3)^2\right) \tag{6.33}$$

allowing us to write

$$\Big(2(\mathbf{q}_1+\mathbf{q}_3)\partial_{\mathbf{q}^2}-i(\mathbf{q}_1+\mathbf{q}_3)\partial_\omega\Big)\Gamma^{(2,2)}(\omega,\mathbf{q}^2)=0 \tag{6.34}$$

which leads to

$$\Gamma^{(2,2)}(\omega,\mathbf{q}^2)=f\left(\frac{\mathbf{q}^2}{2}+i\omega\right) \tag{6.35}$$

Which is again a known result.

We tried to use these relations to help us with the case of the $\Gamma^{(3,3)}$ vertex, where we can write the Ward identity (using our standard notations for momenta)

$$\begin{aligned}\Big(\frac{i}{2}\partial_{\mathbf{p}_1}+\mathbf{p}_1\partial_{\nu_1}+\frac{i}{2}\partial_{\mathbf{p}_2}+\mathbf{p}_2\partial_{\nu_2}+\frac{i}{2}\partial_{\mathbf{p}_3}+\mathbf{p}_3\partial_{\omega_3}-\frac{i}{2}\partial_{\tilde{\mathbf{p}}_1}+\tilde{\mathbf{p}}_1\partial_{\tilde{\omega}_1}\\ -\frac{i}{2}\partial_{\tilde{\mathbf{p}}_2}+\tilde{\mathbf{p}}_2\partial_{\tilde{\omega}_2}-\frac{i}{2}\partial_{\tilde{\mathbf{p}}_3}+\tilde{\mathbf{p}}_3\partial_{\tilde{\omega}_3}\Big)\Gamma^{(3,3)}(p_1,p_3,p_2,p_4)=0\end{aligned} \tag{6.36}$$

which is too generic to obtain any useful information. We tried to see if the $d\to\infty$ limit allowed to obtain some ansatz for a general solution, but this turned up to be a dead end for the study of the $\Gamma^{(3,3)}$ vertex.

Even though the closed equations for the $\Gamma^{(n,n)}$ PA vertices must be solved numerically if $n>2$, the existence of this type of closed equations is important as it highlights the decoupling of $\Gamma^{(n,n)}$ vertices (n-body interaction in the language of non-relativistic many-body theory) from higher order vertices. This, together with the perturbative expansion in λ_3 described before, is enough to yield a satisfying decoupling property for all PA vertices.

Now that we have a method to calculate all correlation functions in PA, we can study BARW by means of a perturbative expansion in the branching rate σ. We stress that a perturbative expansion on a coupling constant around a non-Gaussian model, such as PA, is a priori difficult to perform.

To end this section, notice that all the results above are independent of the space dimension d. This allows us to make predictions independently of the upper critical dimension d_c of the BARW systems studied below.

6.2. BARW - DP

In this Section we consider the simplest BARW-DP model, where the only reactions are $A\xrightarrow{\sigma}2A$ and $2A\xrightarrow{\lambda}\emptyset$. The microscopic action for this model reads, after the shift in the response fields

$$S^{DP}=\int_x\Big(\bar\phi(\partial_t-D\nabla^2)\phi+\lambda\bar\phi(\bar\phi+2)\phi^2-\sigma\bar\phi(\bar\phi+1)\phi\Big) \tag{6.37}$$

We now show how to perform a systematic expansion in σ while keeping a finite λ. This expansion is particularly well suited for properties of the model that take place at small σ, but at values of λ that can be out of reach of a perturbative expansion around the Gaussian theory. It is important to notice that, in order to perform the σ-expansion at arbitrarily high orders, it is necessary to calculate all PA vertices $\Gamma^{(n,m)}$ exactly.

As mentioned before, the transition between the active and the absorbing phases in BARW-DP takes place, for $d > 2$, at values of λ larger than a threshold λ_{th}, se Fig. 2.4 above, which makes the calculation of the phase diagram impossible within the usual perturbative analysis in these dimensions. The LPA phase diagram for the theory has been shown in Fig. 2.4 above. As this threshold corresponds to σ arbitrarily small, the value of λ_{th} is computable in an exact way at the leading order of the expansion in σ that we detail in the following. We stress, however, that the calculation of this quantity is just a specific example of an application of the expansion in σ, which may be used for more general purposes.

In order to analyze BARW-DP it is useful to consider, as in PA, a generalization of S^{DP} with independent couplings. We then consider the action

$$\tilde{S}^{DP} = \int_x \left(\bar{\phi}(\partial_t - D\nabla^2)\phi + \lambda_3 \bar{\phi}\phi^2 + \lambda_4 (\bar{\phi}\phi)^2 - \sigma_2 \bar{\phi}\phi - \sigma_3 \bar{\phi}^2 \phi \right) \tag{6.38}$$

As in the case of PA, one can deduce a Ward identity for the $U(1)$ transformations (6.3), which in this case reads

$$-\lambda_3 \frac{\partial \Gamma}{\partial \lambda_3} + \sigma_3 \frac{\partial \Gamma}{\partial \sigma_3} + \int_x \left(\psi \frac{\delta \Gamma}{\delta \psi} - \bar{\psi} \frac{\delta \Gamma}{\delta \bar{\psi}} \right) = 0 \tag{6.39}$$

that leads us to

$$(n-m)\Gamma^{(n,m)} = \lambda_3 \frac{\partial \Gamma^{(n,m)}}{\partial \lambda_3} - \sigma_3 \frac{\partial \Gamma^{(n,m)}}{\partial \sigma_3} \tag{6.40}$$

where $\Gamma^{(n,m)}$ is a function of $(x_1, \ldots, x_n, \bar{x}_1, \ldots, \bar{x}_m)$. The solution of (6.40) implies the following relation for $\Gamma^{(n,m)}$

$$\Gamma^{(n,m)}(\sigma_2, \sigma_3, \lambda_3, \lambda_4) = \sigma_3^{m-n} \gamma^{(n,m)}(\sigma_2, \sigma_3 \lambda_3, \lambda_4) \tag{6.41}$$

for $m > n$, with $\gamma^{(n,m)}$ a regular function of its arguments (in particular for $\sigma_3 = 0$). This is nothing but the well known result of perturbation theory, which states, putting aside a re-scaling of vertices, that cubic couplings appear only via their product. At leading order in σ_3, Eq. (6.41) shows that

$$\Gamma^{(n,m)} \sim \mathcal{O}(\sigma_3^{m-n}) \qquad \text{for } n < m \tag{6.42}$$

and that the calculation at leading order can be done at $\lambda_3 = 0$.

In order to perform the σ_3-expansion one can consider the generating functional $\mathcal{Z}[J,\bar{J}]$ and expand the exponential term

$$\mathcal{Z} = \int \mathcal{D}\phi\mathcal{D}\bar{\phi}\exp\Big(-\tilde{S}^{DP}\big|_{\sigma_3=0} + \int_x J\phi + \bar{J}\bar{\phi}\Big)\sum_{k=0}^{\infty}\frac{1}{k!}\Big(\sigma_3\int_x \bar{\phi}^2\phi\Big)^k \tag{6.43}$$

In this way, the calculation to any order in σ_3 of any correlation function is reduced to the calculation of higher order correlation functions in a modified PA that includes a mass-like σ_2 term. It is worth mentioning that the methods presented in the previous Section work as well in the model including a σ_2 term. When and if this σ_2 term is not necessary to make the theory IR safe it is possible to expand in σ_2 as well as σ_3 and this is what we are going to do in practice.

As a final comment with respect to the σ-expansion, it is important to notice that it generates a *convergent* series, something not very common when dealing with perturbative expansions in field theories. Indeed, in usual perturbative approaches one expands in the coupling constant corresponding to the term of highest order in powers of the fields in the action, which is the one that ensures the stability of the functional integral. Here we do otherwise : we expand in σ_3 which is not the coupling that rules the stability of the model at large fields. This convergence property can be most easily seen by working with a zero dimensional toy model

$$Z = \int dx\, e^{-\lambda x^4+\sigma x^3} \tag{6.44}$$

Defining

$$f_n(x) = \sum_i^n e^{-\lambda x^4}\frac{1}{n!}\sigma^n x^{3n} \tag{6.45}$$

we see that the integrands

$$0 \le f_n(x) \le Ae^{-\frac{\lambda}{2}x^4} \tag{6.46}$$

for some large enough constant A. From the dominated convergence theorem [83] we know that the sequence of integrals of functions $f_n(x)$ converge to the integral of the function $f(x) = \lim_{n\to\infty} f_n(x)$. A similar reasoning applies in the case of the $(d+1)$-dimensional model, at least for the model defined on a lattice and in a finite volume.

6.2.1. Threshold of the active-to-absorbing transition

Let us consider as a specific example the calculation of the threshold λ_{th} for the existence of an active-to-absorbing phase transition in BARW-DP. No-

tice that this threshold value is non-universal, as would be a critical temperature in an equilibrium model. Intuitively, even though at mean field the branching reaction should win over the annihilation reaction in this system, a coarse-graining argument shows than an effective spontaneous decay reaction is generated in the system. Indeed, the reaction $A \xrightarrow{\mu_R} \emptyset$ is generated by the chain of reactions

$$A \to 2A \to \emptyset$$

which takes place at a coarse-grained level. This effective spontaneous decay is relevant in the RG sense, and, given the right values of the microscopic λ and σ rates, can end up dominating the large scale physics, and in particular allowing for the existence of an absorbing phase.

In order to check for the presence of a phase transition in our formalism, it is enough to study the behavior of $\Delta = \Gamma^{(1,1)}(p=0)$ as a function of the annihilation rate λ. In fact, we can detect this phase transition by looking for the zeroes of Δ, the effective mass, which correspond to a divergence in the correlation length [63]. Given that λ_{th} corresponds to the transition value of λ when $\sigma \to 0^+$, an analysis at leading order in σ allows for an exact calculation of λ_{th}. Following the lines of the previous discussion, an equation for $\Gamma^{(1,1)}(p)$ at order $\mathcal{O}(\sigma)$ can be represented in the diagrammatic form of Fig. 6.10, that can be written

$$\begin{aligned}\Gamma^{(1,1)}(p) &= -\sigma + \sigma \int_q G(q)G(p-q)\Gamma^{(2,1)}(q, p-q, -p) + \mathcal{O}(\sigma^2) \\ &= -\sigma + 4\sigma l(p) \int_q G(q)G(p-q) + \mathcal{O}(\sigma^2) \end{aligned} \tag{6.47}$$

In the second line of (6.47) we have evaluated the propagator $G(p)$ and the vertex $\Gamma^{(2,1)}(q, p-q, -p)$ at order zero in σ, and consequently replaced this last function by $4l(p)$ (see Eq. (6.11), remember that we consider $l(p) = l_4(p)$).

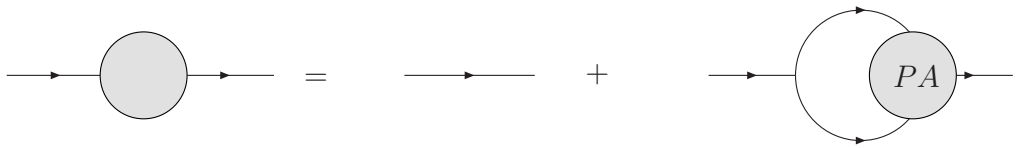

FIGURE 6.10 – Equation for $\Gamma^{(1,1)}$ at first order in σ in BARW-DP.

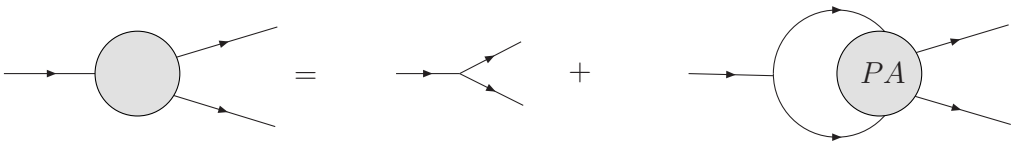

FIGURE 6.11 – Closed equation for $\Gamma^{(1,2)}$ at first order in σ in BARW-DP.

As a side note, observe that we could have just as well written an equivalent equation for $\Gamma^{(1,2)}$ (see Fig. 6.11), which reads at order σ

$$\begin{aligned}\Gamma^{(1,2)}(p_1,\bar{p}_1,\bar{p}_2) &= -2\sigma + 2\sigma\int_q G(q)G(p_1-q)\Gamma^{(2,2)}(p_1-q,q,\bar{p}_1,\bar{p}_2) + \mathcal{O}(\sigma^2)\\ &= -2\sigma + 8\sigma l(p_1)\int_q G(q)G(p_1-q) + \mathcal{O}(\sigma^2)\end{aligned} \tag{6.48}$$

were in the second equality, as before, the $\Gamma^{(2,2)}(q,p_1-q,\bar{p}_1,\bar{p}_2)$ vertex is taken at order σ^0, that is, taken to be equal to $4l(p_1)$. Expressions (6.47) and (6.48) imply that

$$\Gamma^{(1,2)}(p_1,\bar{p}_2,\bar{p}_3) = 2\Gamma^{(1,1)}(p_1) + \mathcal{O}(\sigma^2) \tag{6.49}$$

Which states that at first order in σ, the bare relation between the $(1,1)$ and $(1,2)$ vertices is maintained.

Returning to our problem, we can look for a second order phase transition by studying the behavior of Δ. One needs the non-universal value $l(p=0)$ that can be obtained by evaluating Eq. (6.11) at $p=0$:

$$l(p=0) = \frac{\lambda}{1+2\lambda I(d)} \tag{6.50}$$

where

$$I(d) = \int_q G(q)G(-q) \tag{6.51}$$

By substituting the expression for $l(p=0)$, and evaluating (6.47) at $p=0$ one arrives at

$$\Delta = -\sigma + 4\sigma\frac{\lambda I(d)}{1+2\lambda I(d)} + \mathcal{O}(\sigma^2) \tag{6.52}$$

which for $\Delta = 0$ implies a threshold value

$$\lambda_{th} = \frac{1}{2I(d)} \tag{6.53}$$

To evaluate λ_{th}, we need to take into account that the properties of a phase diagram are not universal and depend on the specific form of the theory at small

distances. This is as in equilibrium statistical mechanics, where critical temperatures depend on the specific form of the lattice. We consider two particular microscopic forms for the model. The first one corresponds to the model defined on a hyper-cubic lattice with lattice spacing a. The second corresponds to a 'continuum' version where a UV cut-off is imposed at a finite (but large) scale Λ.

For the hyper-cubic lattice, the propagator reads

$$G(q) = \frac{1}{i\omega + \frac{2D}{a^2}\sum_{i=1}^{d}(1-\cos(aq_i))}, \tag{6.54}$$

and the integral in (6.53) becomes

$$\begin{aligned} I(d) &= \int \frac{d\omega}{2\pi} \int_{-\pi/a<q_i\leq\pi/a} \frac{d^d q}{(2\pi)^d} G(q)G(-q) \\ &= \frac{1}{2}\int_{-\pi/a<q_i\leq\pi/a} \frac{d^d q}{(2\pi)^d} \frac{1}{\frac{2D}{a^2}\sum_{i=1}^{d}(1-\cos(aq_i))} \\ &= \frac{a^{2-d}}{4D}\int_{-\pi<q_i\leq\pi} \frac{d^d q}{(2\pi)^d} \frac{1}{\sum_{i=1}^{d}(1-\cos(q_i))} \end{aligned} \tag{6.55}$$

where the integral over ω has been performed by using the residues' theorem and a rescaling of q has been performed. The remaining integral must be calculated numerically. In Table 6.1, the value of the resulting threshold coupling is given. Previous results from Monte-Carlo simulations and approximated NPRG equations [44, 155] are in good agreement with these exact ones. The same general structure of the phase diagram, with threshold values for annihilation rates, has also been shown to exist in other models in the DP universality class [156].

An interesting property observed in [44] is that λ_{th} seems to grow linearly with d. In [47], a single-site approximation scheme that is argued to become exact in the large d limit on a hyper-cubic lattice was analyzed, and this linear behavior was obtained. In order to analyze such a behavior here, it is necessary to find the large-d limit for the integral $I(d)$. For this purpose it is useful to rewrite it in the following form :

$$I(d)Da^{d-2} = \frac{1}{4d}\int_{-\pi<q_i\leq\pi} \frac{d^d q}{(2\pi)^d} \frac{1}{1-\left(\sum_{i=1}^{d}\cos(q_i)\right)/d} \tag{6.56}$$

To solve it, one can imagine the various $\cos(q_i)$ as random variables with zero mean. By the strong law of large numbers, their mean $\left(\sum_{i=1}^{d}\cos(q_i)\right)/d$ tends to zero, except in a zero measure set. We are then tempted to substitute the limit inside the integrand and obtain

$$I(d)Da^{d-2} \overset{d\to\infty}{\sim} \frac{1}{4d}. \tag{6.57}$$

d	3	4	5	6
λ_{th}/Da^{d-2} (this work)	3.96	6.45	8.65	10.7
λ_{th}/Da^{d-2} (Monte-Carlo) [44]	3.99	6.48	8.6	10.8

TABLE 6.1 – Values of the threshold coupling λ_{th} for various dimensions d. Comparison of present exact results with Monte-Carlo [44].

This step is non trivial from a rigorous mathematical point of view, but turns out to be correct by using elaborate methods of real analysis [15]. As a consequence,

$$\lambda_{th}/Da^{2-d} \overset{d\to\infty}{\sim} 2d \tag{6.58}$$

in agreement with previous results [47].

It is interesting to observe that expression (6.53) only depends on quantities that are calculated exactly in the Local Potential Approximation (LPA) of the NPRG, the lowest order of the Derivative Expansion. Only vertices at zero momenta are used and their exact equation turns out to be the same as the one that comes from the LPA. This a posteriori explains the success of the LPA in reconstructing the phase diagram of this model with such a good precision [44].

However, as mentioned before, the phase diagram is a non-universal property that depends on the precise definition of the model in the ultraviolet. In particular, the value of the integral $I(d)$ is different if calculated on a discrete lattice or in the continuum with a given ultraviolet regularization. In the previous study done within the NPRG [44], a continuum version of the model was implemented, but the initial bare condition was imposed at a finite (but large) value of the microscopic scale Λ, which serves as a UV cut-off. In order to be able to compare our continuum non-universal results with those obtained in [44] we choose an UV regularization compatible with the NPRG procedure.

In the continuum regularized case, the integral to be calculated in order to make a direct comparison with previous LPA results is (with the tilde indicating this second regularization)

$$\begin{aligned}\tilde{I}(d) &= \frac{1}{(4\pi)^{d/2}\Gamma(d/2)\,D}\int_0^\Lambda dq\, q^{d-1}\Big(\frac{1}{q^2}-\frac{1}{\Lambda^2}\Big)\\ &= \frac{\Lambda^{d-2}}{(4\pi)^{d/2}\Gamma(d/2)\,D}\,\frac{2}{d(d-2)}.\end{aligned} \tag{6.59}$$

This yields for this particular regularization

$$\tilde{\lambda}_{th} = \frac{\Lambda^{2-d}(4\pi)^{d/2}\Gamma(d/2)\,Dd(d-2)}{4} \tag{6.60}$$

Given that this integral is calculated in a closed form by using exclusively quantities evaluated at momentum $p = 0$, we can check that it coincides exactly with the LPA equation for this same quantity. Indeed, our result recovers the numerical LPA solution of the NPRG of [44] within a nine digit accuracy.

We can also compare the results coming from both lattice and continuum regularizations, as has been done in [44, 48]. As is explained there, one cannot do such comparison without fixing the relation between Λ and the lattice spacing a. In [44], this relation was fixed by multiplying the continuum results by $\exp(c(2-d))$ and fitting the constant number c, finding a very reasonable agreement up to $d = 7$. However, we observe in the present results that the agreement is lost in higher dimensions where the continuum version leads to

$$\tilde{\lambda}_{th}\Lambda^{d-2}/D \overset{d\to\infty}{\sim} \frac{(2\pi\, d/e)^{d/2}\sqrt{\pi}\, d^{5/2}}{4}. \tag{6.61}$$

This indicates that the agreement between both results is only valid for a limited range of dimensions. In order to relate the results in a larger range of dimensions, one must consider a d-dependent relation between Λ and a or, as done here, take into account the precise ultraviolet regularization considered.

Finally, it is convenient to point out that for $d \leq 2$ an IR divergence of the integral in (6.53) takes place. This makes $\lambda_{th} = 0$ in those dimensions, in agreement with the results of [52]. For this reason, for $d \leq 2$ it is not useful to expand the model at small σ for a finite λ in order to study the phase transition. Moreover, this also shows that in these dimensions the transition is dominated by IR effects, and correspondingly most of the dependence on the microscopic behaviour of the model is absent. On the contrary, for $d > 2$, the determination of λ_{th} is dominated by the UV behaviour of the model, and neglecting the quartic term $\lambda\phi^2\bar{\phi}^2$ term, as is done in the usual perturbation theory on power counting arguments, prevents us from determining λ_{th}. Our calculation shows how to take into account this term, which on one hand is IR irrelevant, and on the other hand is crucial for determining in high d the correct phase diagram.

6.2.2. The system $A \to 2A$, $2A \to A$

As an important side note, we can also take a look at the BARW system defined by equations

$$A \xrightarrow{\sigma} 2A \qquad 2A \xrightarrow{\lambda'} A \tag{6.62}$$

together with diffusion. This systems is indistinguishable from BARW-DP from a mean field or perturbative theory viewpoint [173], amounting to a redefinition of what we call the three point vertex λ_3.

As mentioned before when introducing PA, we can consider the pure coagulation system $2A \xrightarrow{\lambda'} A$ by following the same route as with PA, finding essentially the same results, aside from the aforementioned redefinition of λ_3. This redefinition, though, turns out to have important consequences in our formalism

We can perform a σ-expansion in this system, which would allow us to determine the value λ'_{th} of the annihilation rate to have a phase transition in $d > 2$. By doing the same calculations at order σ as in the previous section (see Fig. 6.10 and Eq. (6.52) above) we arrive at

$$\Delta = -\sigma + 2\sigma \frac{\lambda' I(d)}{1 + 2\lambda' I(d)} \tag{6.63}$$

$$= \frac{-\sigma}{1 + 2\lambda' I(d)} \tag{6.64}$$

which remains negative for any λ'. This means that there is no λ'_{th} above dimension 2 (or, at least, that the transition line does nos cross the $\sigma = 0$ axis), and that therefore the system always ends up in the active phase : there is no phase transition.

We emphasize that here, as opposed to perturbation theory, the predictions for the two systems, BARW-DP and the system defined by Eq. (6.62) differ completely. We end up with a completely different phase diagram for these two systems, which was expected from Monte Carlo simulations. Moreover, this can be understood by the fact that the effective coupling $A \to \emptyset$ can not be generated by coarse-graining in this system.

With this comment we finish our presentation of the σ-expansion as applied to BARW-DP. Much more could be done by going to higher orders in the expansion. For example, we can easily extract from the order σ^2 the linear behaviour of the phase transition line in the $\lambda - \sigma$ plane (cf. Fig. 2.4 above). We could also look at universal exponents, but in that case the results would be approximate, given that the fixed point value for σ in this transition is not particularly small. Instead of doing that, let us now move forward to the study of BARW-PC.

6.3. BARW - PC

Let us now consider BARW-PC, corresponding to the Parity Conserving / Generalized Voter universality class, with reactions $A \xrightarrow{\sigma} 3A$ and $2A \xrightarrow{\lambda} \emptyset$. In this case, it is convenient not to shift the response field in order to make explicit the $\phi \to -\phi$, $\hat{\phi} \to -\hat{\phi}$ symmetry associated with conservation of the parity of the

number of particles. The microscopic action for the BARW-PC model reads

$$S^{PC}[\phi,\hat{\phi}] = \int_x \left(\hat{\phi}(\partial_t - D\nabla^2)\phi + \lambda(\hat{\phi}^2 - 1)\phi^2 + \sigma(1-\hat{\phi}^2)\phi\hat{\phi}\right) \tag{6.65}$$

where the last term corresponds to the branching reaction $A \to 3A$ with rate σ.

The case $\sigma = 0$ corresponds to Pure Annihilation, now written in terms of the non-shifted $\hat{\phi}$ field. This version of Pure Annihilation can again be solved following the same ideas as previously. Here, as opposed to the shifted case, we have the additional constraint that $\Gamma^{(n,m)} = 0$ if $(n+m)$ is odd.

Let us now show that in this version of PA

$$\Gamma^{(n,m)} \sim \mathcal{O}(\lambda^{(n-m)/2}) \quad \text{for } n \geq m \tag{6.66}$$

and zero otherwise. We again define a generalized action $\tilde{S}^{PC}$ with independent λ_2 and λ_4 couplings as in Eq. (6.2)

$$\tilde{S}^{PC}[\phi,\hat{\phi}] = \int_x \left(\hat{\phi}(\partial_t - D\nabla^2)\phi - \lambda_2\phi^2 + \lambda_4\hat{\phi}^2\phi^2 + \sigma_2\hat{\phi}\phi - \sigma_4\hat{\phi}^3\phi\right) \tag{6.67}$$

First we set σ_2 and σ_4 equal to zero, in order to be in PA, and exploit the $U(1)$ Ward identity for the infinitesimal transformation

$$\begin{aligned} \phi(x) &\to (1+\epsilon)\phi(x) \\ \hat{\phi}(x) &\to (1-\epsilon)\hat{\phi}(x) \end{aligned} \tag{6.68}$$

The argument is completely analogous to the one shown in Section 6.1, yielding (for $\sigma_2 = \sigma_4 = 0$)

$$(n-m)\Gamma^{(n,m)} = 2\lambda_2 \frac{\partial \Gamma^{(n,m)}}{\partial \lambda_2} \tag{6.69}$$

(with, as before, $\Gamma^{(n,m)}$ a function of $(x_1,\ldots,x_n,\bar{x}_1,\ldots,\bar{x}_m)$) from which Eq. (6.66) follows.

It is easy to check that the equation for $\Gamma^{(2,2)}$ remains the same as in the shifted case, Eq. (6.9), and we thus define the function $l(p)$ again by means of Eq. (6.11). The vertex $\Gamma^{(2,0)}$ can be studied by following similar lines, and is found to be related to $l(p)$, by $\Gamma^{(2,0)}(p) = -2l(p)$. Also as before, $\Gamma^{(1,1)}$ is easily proven not to be renormalized in this version of PA.

Since we are interested in studying the σ-expansion around PA, it is useful to establish the equivalent of Eq. (6.42) regarding the order in σ of the $\Gamma^{(n,m)}$. We again work with generalized couplings σ_2 and σ_4, using the modified action (6.67) and we arrive, by using the $U(1)$ Ward identity deduced from (6.68) (an identity similar to Eq. (6.39)) at the relationship

$$\Gamma^{(n,m)}(\sigma_2,\sigma_4,\lambda_2,\lambda_4) = \sigma_4^{(m-n)/2}\gamma^{(n,m)}(\sigma_2,\sigma_4\lambda_2,\lambda_4) \tag{6.70}$$

for $m > n$, with $\gamma^{(n,m)}$ a regular function of its arguments (in particular for $\sigma_4 = 0$). This implies that $\Gamma^{(n,m)} \sim \mathcal{O}(\sigma^{(m-n)/2})$ if $m > n$. The details of the calculations leading to this property are completely analogous to those shown before in the case of BARW-DP.

6.3.1. The stability of the PA fixed point

One striking feature of the PC model is the existence of an active-to-absorbing phase transition in $d = 1$, whereas mean field predicts that the system always reaches the active phase at large times. This phase transition is believed to be related to a change of stability of the PA fixed point in a dimension d_c between one and two. Perturbatively, and also within the LPA, this change of stability occurs in the following way (see a schematic representation of this scenario in Fig. 6.12 [52, 46]). On one hand, in $d = 2$, the Gaussian and PA fixed points merge so that, for dimensions close to two, the relevance of the branching reaction $A \xrightarrow{\sigma} 3A$ can be proven by canonical power counting arguments (which shows that the system is in the active phase for any $\sigma > 0$). On the other hand, at 1- and 2-loop orders an (upper) critical dimension $d_c > 1$ is found such that for $d < d_c$ the coupling σ becomes irrelevant around the PA fixed point which therefore becomes fully attractive (proving that for $d < d_c$ the system is in the absorbing phase at small σ). This change of stability occurs because a new fixed point, F^{PC}, crosses the PA fixed point at d_c and in this dimension they exchange their stability. Below d_c, this new fixed point is in the physically relevant quadrant $\lambda \geq 0$, $\sigma \geq 0$, has one unstable direction, and is thus associated with the phase transition. The PA fixed point is then fully attractive for $d < d_c$ and describes the absorbing phase. Notice that the value of d_c changes significantly between one-loop – where $d_c = 4/3$ – and two-loops where $d_c \simeq 1.1$ (within the LPA $d_c \sim 4/3$ was also found [46]).

Some of these facts seem to be confirmed by other methods. In $d = 1$, an active to absorbing phase transition is found in Monte-Carlo simulations of this model which indeed belongs to a new universality class [157, 118], and an exactly soluble model expected to be in the same universality class as BARW-PC shows a negative scaling dimension for σ : $d_\sigma = -1$ at that dimension [186]. This result ($d_\sigma = -1$) is identical to the prediction at order ϵ [52]. At two loop order, though, this value for d_σ changes and gets smaller in magnitude, $d_\sigma \simeq -0.137$ at $d = 1$ [52]. As will be argued in the following, this significative difference between MC and 2-loop results can be seen as a first indication that the results of [186] are not entirely valid for this system.

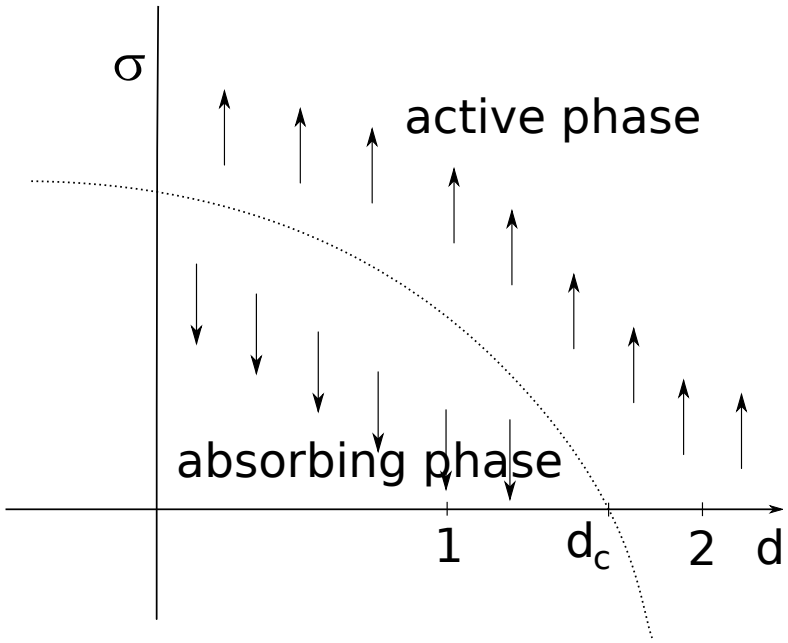

FIGURE 6.12 – Sketch of the relevance of the σ perturbation in BARW-PC around the PA fixed point as a function of the dimension, as expected from [52, 46]. The arrows show the direction of the RG flow for the coupling σ towards the IR. Above d_c, σ is relevant, whereas it is irrelevant below d_c. The dashed line represents the location of the fixed point F^{PC} that crosses the PA fixed point at d_c and that is associated with a phase transition below d_c.

We now reanalyze the stability of the PA fixed point in the presence of the PC creation reaction, $A \xrightarrow{\sigma} 3A$, that we can determine exactly since our analysis is exact at small σ. The relevance of this coupling can be obtained from the flow of either $\Gamma^{(1,1)}$ or $\Gamma^{(1,3)}$, since both these functions are of order σ. However, the RG flow of $\Gamma^{(1,1)}$ depends on the somewhat difficult to study $\Gamma^{(3,1)}$ vertex of PA (see Fig. 6.13), and we prefer to study $\Gamma^{(1,3)}$.

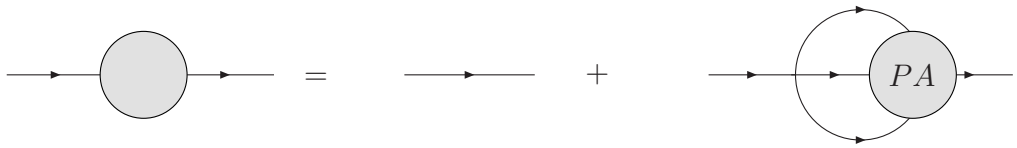

FIGURE 6.13 – Closed equation for $\Gamma^{(1,1)}$ in BARW-PC, at first order in σ.

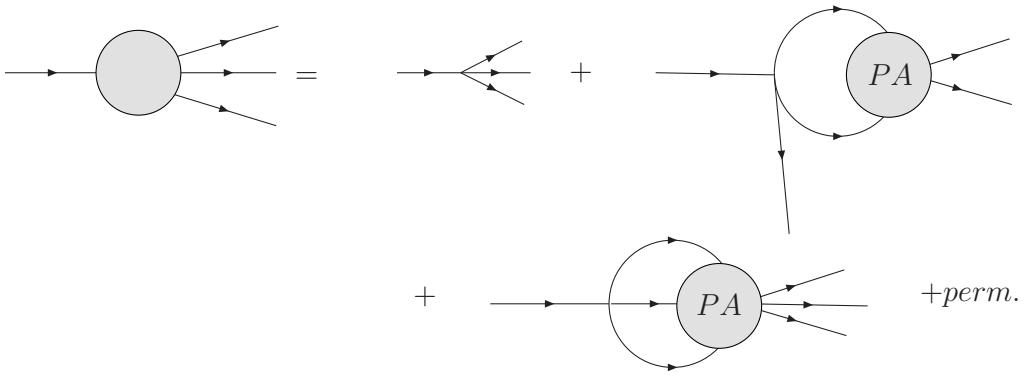

FIGURE 6.14 – Closed equation for $\Gamma^{(1,3)}$ in BARW-PC at first order in σ.

At first order in σ, any diagram for $\Gamma^{(1,3)}$ is of the form shown in Fig. 6.14. As can be seen on this figure, it involves the bare σ vertex as well as the PA $\Gamma^{(2,2)}$ and $\Gamma^{(3,3)}$ 1PI vertices. As it stands, though, we would have to solve the independent equation for $\Gamma^{(3,3)}$ in order to make progress (an analysis of which can be found in Section 6.1.5, where it is shown that its equation requires numerical methods to be solved). Moreover, this expression is not well suited for the analysis of universal properties, because it is expressed in terms of the bare vertex and not in terms of the full $\Gamma^{(1,3)}$ vertex. Fortunately, the fact that we only deal with PA vertices allows us to find an easier relationship for $\Gamma^{(1,3)}$, using the already known property which allows us to find closed forms for PA vertices. Notice that $\Gamma^{(2,2)}$ and $\Gamma^{(3,3)}$ have always two possible closed decompositions, being vertex of the form $\Gamma^{(n,n)}$ (as discussed before). Specifically, we can rewrite the equation for $\Gamma^{(1,3)}$ in the form shown diagrammatically in Fig. 6.15, which can be written

$$\begin{aligned}\Gamma^{(1,3)}(p,\tilde{p}_1,\tilde{p}_2,\tilde{p}_3) = -6\sigma \\ -2\lambda\int_q G(q)G(\tilde{p}_1+\tilde{p}_2-q)\Gamma^{(1,3)}(p,q,\tilde{p}_1+\tilde{p}_2-q,\tilde{p}_3) \\ -2\lambda\int_q G(q)G(\tilde{p}_1+\tilde{p}_3-q)\Gamma^{(1,3)}(p,q,\tilde{p}_1+\tilde{p}_3-q,\tilde{p}_2) \\ -2\lambda\int_q G(q)G(\tilde{p}_2+\tilde{p}_3-q)\Gamma^{(1,3)}(p,q,\tilde{p}_2+\tilde{p}_3-q,\tilde{p}_1) \quad (6.71)\end{aligned}$$

The highly symmetric form of this equation suggests the following ansatz for the functional form of $\Gamma^{(1,3)}$ (which can be easily checked by iteration)

$$\Gamma^{(1,3)}(p,\tilde{p}_1,\tilde{p}_2,\tilde{p}_3) = -2\sigma(p,\tilde{p}_1) - 2\sigma(p,\tilde{p}_2) - 2\sigma(p,\tilde{p}_3) \quad (6.72)$$

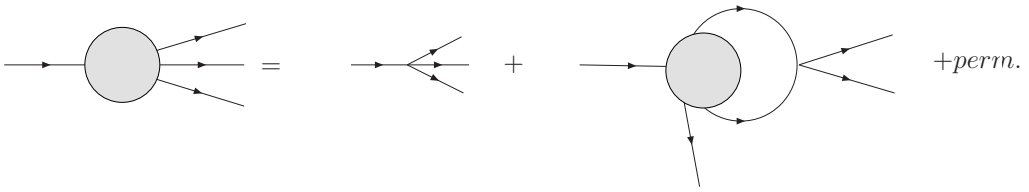

FIGURE 6.15 – Another possible closed equation for $\Gamma^{(1,3)}$ in BARW-PC, at first order in σ.

In terms of $\sigma(p,\tilde{p})$ the equation becomes

$$\sigma(p,\tilde{p}) = \sigma - 2\lambda \int_q G(q)G(p-\tilde{p}-q) \times \Big(\sigma(p,q) + \sigma(p,p-\tilde{p}-q) + \sigma(p,\tilde{p})\Big) \quad (6.73)$$

Using the known expression for $l(p)$, Eq. (6.11), we obtain

$$\sigma(p,\tilde{p}) = \frac{\sigma}{\lambda} l(p-\tilde{p}) - 2l(p-\tilde{p}) \int_q G(q)G(p-\tilde{p}-q) \times \Big(\sigma(p,q) + \sigma(p,p-\tilde{p}-q)\Big) \quad (6.74)$$

For the calculation of d_c, it is enough to analyze the $p = 0$ behavior (we are interested in the IR fixed point structure of the theory). Defining

$$\sigma(\tilde{p}) = \sigma(p=0,-\tilde{p}) \quad (6.75)$$

(notice that we have chosen a minus sign in the definition), and after a change of variables inside the integral, we get

$$\sigma(\tilde{p}) = \frac{\sigma}{\lambda} l(\tilde{p}) - 4l(\tilde{p}) \int_q G(q)G(\tilde{p}-q)\sigma(q) \quad (6.76)$$

From now on we omit the tilde in $\tilde{p}$ for notational simplicity. The quantity we are mostly interested in is d_σ, the scaling dimension of σ in the IR limit

$$\sigma(p) \sim |\mathbf{p}|^{d_\sigma} \qquad \text{for} \quad \nu, |\mathbf{p}|^2 \ll \lambda^{\frac{2}{2-d}} \quad (6.77)$$

The IR behaviour of this function gives information about the stability of the PA fixed point. Indeed, if $d_\sigma > 0$ the branching perturbation becomes irrelevant at long distances, which implies that the PA fixed point is stable under the perturbation. Naive power counting yields $d_\sigma = 2$, which would imply that the branching perturbation σ is relevant for all d, but fluctuations of course change

this value of d_σ, and could even make it negative, which would imply the irrelevance of the σ perturbation.

In order to solve Eq. (6.76) it is useful to define the quantity

$$\hat{\sigma}(p) = \frac{\sigma(p)}{l(p)} \tag{6.78}$$

whose behavior in the IR is expected to be of the form $\hat{\sigma}(p) \sim |\mathbf{p}|^{d-d_\sigma}$ (recall that $l(p) \sim |\mathbf{p}|^{2-d}$ in that regime). The equation for $\hat{\sigma}$ reads

$$\hat{\sigma}(p) = \frac{\sigma}{\lambda} - 4\int_q G(q)G(p-q)\hat{\sigma}(q)l(q) \tag{6.79}$$

Using this exact expression and expanding in $\epsilon = 2-d$ we recover the 1-loop result $d_c = 4/3$, as well as the 2-loop result $d_c \simeq 1.1$ [52]. These results follow from a perturbative series in σ and λ, and from a simultaneous expansion in $\epsilon = 2-d$.

In order to get an exact result for d_σ it is convenient to get rid of the bare reaction rates, as we are interested in the universal IR scaling behavior. Let us start by doing so in the case of $l(p)$, which will be useful in what follows. The IR limit is taken by making $\lambda \to \infty$ (more precisely, by considering $\nu, |\mathbf{p}|^2 \ll \lambda^{2/(2-d)}$, the typical momentum scale set by the bare annihilation rate). This can be done safely for $d < 2$, and is a subtle limit when one studies directly $d = 2$ in order to perform the ϵ-expansion. By exploiting expression (6.11) we obtain the IR behavior

$$\begin{aligned}\left(l^{IR}(p)\right)^{-1} &= 2\int_q G(q)G(p-q) \\ &= 2\int \frac{d^d q}{(2\pi)^d}\int \frac{d\omega}{2\pi}\frac{1}{q^2+i\omega}\frac{1}{(p-q)^2+i(\nu-\omega)}\end{aligned} \tag{6.80}$$

and thus

$$l^{IR}(p) = \frac{(4\pi)^{d/2}}{2^{1-d/2}\Gamma(1-d/2)}\left(\frac{p^2}{2}+i\nu\right)^{1-d/2} \tag{6.81}$$

Now we can return to $\hat{\sigma}$. As we are only interested in its scaling behavior, it proves convenient to subtract to (6.79) its value at zero $\hat{\sigma}(p=0)$, which is zero in the IR for $d < 2$, given that we expect $d_\sigma < d$. This is seen to be true in the ϵ expansion around $d = 2$, and must be true near the sought-for d_c, where d_σ should be zero. Our results will later confirm $d_\sigma < d$. We thus have

$$\hat{\sigma}(p) = -4\int_q \hat{\sigma}(q)l(q)G(q)\Big(G(p-q) - G(-q)\Big) \tag{6.82}$$

This is a complicated equation, and to be able to solve it, we must take into account the scaling invariance we expect from its solution. We exploit scale invariance in order to define the scaling function $\tilde{\sigma}(\tilde{\nu})$

$$\hat{\sigma}(\mathbf{p},\nu) = |\mathbf{p}|^{d-d_\sigma}\tilde{\sigma}(\tilde{\nu}), \qquad \tilde{\nu} = \frac{\nu}{|\mathbf{p}|^2} \tag{6.83}$$

Observe that we are performing a perturbation around the PA fixed point, whose anomalous dimensions are zero (that is, $\eta = 0$, $z = 2$, as already mentioned). Accordingly, the natural scaling variable is $\tilde{\nu} = \nu/|\mathbf{p}|^2$.

We can now write an equation for $\tilde{\sigma}(\tilde{\nu})$, using the form (6.81) for $l(p)$ and choosing as variables $\tilde{\omega} = \omega/q^2$, $\tilde{q} = |q|/|p|$ and $u = \cos\widehat{(\mathbf{p},\mathbf{q})}$

$$\begin{aligned}\tilde{\sigma}(\tilde{\nu}) = -4&\left(\frac{(4\pi)^{d/2}}{2^{1-d/2}\Gamma(1-d/2)}\right)\left(\frac{2\pi^{\frac{d-1}{2}}}{(2\pi)^{d+1}\Gamma\left(\frac{d-1}{2}\right)}\right)\\ &\times\int_0^\infty d\tilde{q}\,\tilde{q}^{d-d_\sigma+1}\int_{-1}^1 du\,(1-u^2)^{\frac{d-3}{2}}\int_{-\infty}^\infty d\tilde{\omega}\,\tilde{\sigma}(\tilde{\omega})\left(\frac{1}{2}+i\tilde{\omega}\right)^{1-d/2}\\ &\times\frac{1}{1-i\tilde{\omega}}\left(\frac{1}{1+i\tilde{\nu}+\tilde{q}^2(1-i\tilde{\omega})-2\tilde{q}u}-\frac{1}{\tilde{q}^2(1+i\tilde{\omega})}\right)\end{aligned} \tag{6.84}$$

This equation is still too complicated to be solved analytically, and requires a numerical solution. But before that, we can show how it can be used to recover the perturbative results of [52] for d_σ. Let us begin by recalling the equation for $\hat{\sigma}$, which reads

$$\hat{\sigma}(p) = \frac{\sigma}{\lambda} - 4\int_q G(q)G(p-q)\hat{\sigma}(q)l(q) \tag{6.85}$$

Using this expression we can recover the 1-loop and 2-loop results for d_σ (and hence d_c). In order to do so it is convenient to get rid of the bare level dependence on λ and σ by writing some sort of RG flow equation. The easiest way to do this is by performing a logarithmic derivative w.r.t. ν, which yields

$$\begin{aligned}\nu\partial_\nu\hat{\sigma}(p) =& -4\nu\partial_\nu\int_q \hat{\sigma}(q)l(q)G(p-q)G(q)\\ =&4i\nu\int_q\hat{\sigma}(q)l(q)G^2(p-q)G(q)\end{aligned} \tag{6.86}$$

This equation can be compared with the corresponding RG equation for $l(p)$, obtained by differentiating Eq. (6.11)

$$\nu\partial_\nu l(p) = -2l^2(p)\nu\partial_\nu\int_q G(p-q)G(q) \tag{6.87}$$

At 1-loop order the q-dependence in $\hat{\sigma}$ should be weak. In the IR one expects this dependence to be dominated by the external momentum p, given that the momentum integral is regular for the values of d we are interested in

$$\nu\partial_\nu\hat{\sigma}(p) \simeq -4\hat{\sigma}(p)l(p)\nu\partial_\nu\int_q G(p-q)G(q) \tag{6.88}$$

which, together with (6.87) yields

$$\nu\partial_\nu\left(\frac{\hat{\sigma}(p)}{l^2(p)}\right) = 0 \tag{6.89}$$

Accordingly, and given that

$$\frac{\hat{\sigma}(p)}{l^2(p)} \xrightarrow{\nu\to\infty} \frac{\sigma}{\lambda^3} \tag{6.90}$$

we have the result

$$\hat{\sigma}(p) \sim \frac{\sigma}{\lambda^3}l^2(p) \tag{6.91}$$

This behaves, when $\nu, |\mathbf{p}|^2 \ll \lambda^{2/(2-d)}$, as

$$\hat{\sigma}(p) \sim |\mathbf{p}|^{2(2-d)} \tag{6.92}$$

Given the definition of d_σ we find

$$d_\sigma = 3d - 4 = 2 - 3\epsilon \tag{6.93}$$

With this expression we find that d_σ changes sign at $d_c = 4/3$ just as expected.

Going now to 2-loop order it is convenient to use the logarithmic derivative of $\hat{\sigma}$

$$\nu\partial_\nu\log\hat{\sigma}(p) = -4i\int_q \frac{l(q)\hat{\sigma}(q)}{\hat{\sigma}(p)}G^2(p-q)G(q) \tag{6.94}$$

We now introduce in the r.h.s. of this equation the 1-loop result $\hat{\sigma}(p) \sim l^2(p)$, to obtain

$$\nu\partial_\nu\log\hat{\sigma}(p) = -4i\int_q \frac{l^3(q)}{l^2(p)}G^2(p-q)G(q) \tag{6.95}$$

We also need the scaling form for $l(p)$, as given by (6.81) before. At this point it is enough in order to obtain d_σ to restrict to $\mathbf{p} = 0$ (given that $\hat{\sigma}(\mathbf{p},\nu) \sim \nu^{\frac{d-d_\sigma}{2}}$)

$$d - d_\sigma = -8i\nu\frac{(4\pi)^{d/2}2^{-\epsilon/2}}{\Gamma\left(\frac{\epsilon}{2}\right)}\int_q \frac{\left(\frac{\mathbf{q}^2}{2}+i\omega\right)^{3\epsilon/2}}{(i\nu)^\epsilon}G(\mathbf{q},\omega)G^2(-\mathbf{q},\nu-\omega) \tag{6.96}$$

which can be evaluated to yield

$$d_\sigma = 2 - 3\epsilon + 3\log\left(\frac{4}{3}\right)\epsilon^2 \tag{6.97}$$

the known 2-loops result [52], which corresponds to $d_c \simeq 1.1$.

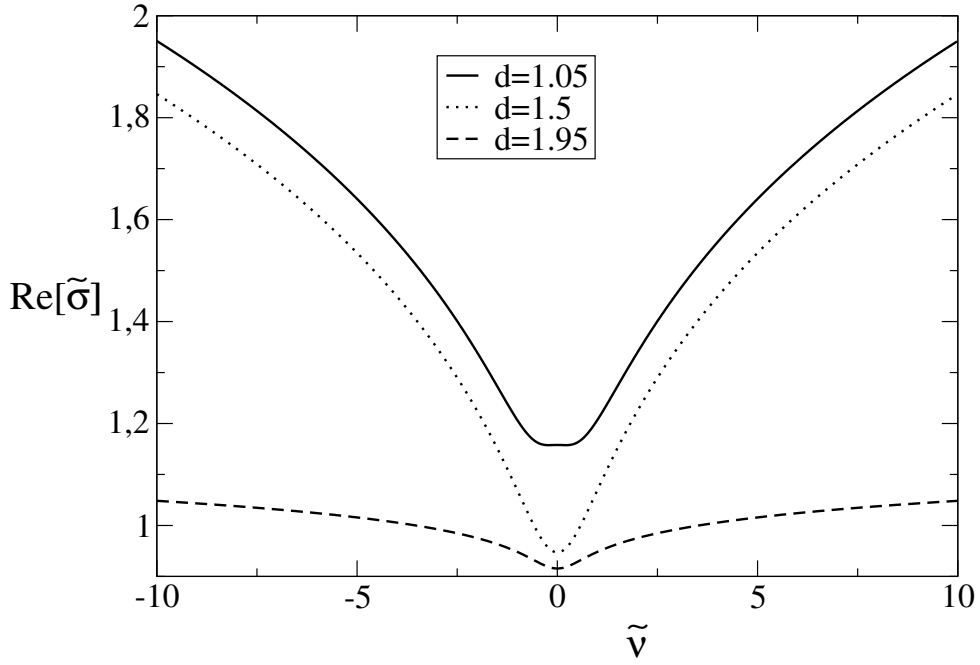

FIGURE 6.16 – $\tilde{\nu}$-dependence of the real part of the scaling function $\tilde{\sigma}(\tilde{\nu})$ for several values of d.

Now, going back to the full numerical solution of equation (6.84), it turns out to be convenient to make an expansion in u, which we observe is rapidly convergent. We then proceed as follows : at each order in the expansion in u we adjust d_σ at a given value of d, by numerically iterating this equation in order to reach a fixed functional form for $\tilde{\sigma}(\tilde{\nu})$ in a lattice of N_ν points with a resolution $\delta\nu$. We have checked the convergence in u and in the numerical parameters $\delta\nu$ and N_ν, used for the computation of integrals. This procedure gives always a converged scaling function $\tilde{\sigma}(\tilde{\nu})$, which confirms a posteriori the scaling form ansatz (6.83). In Fig. 6.16, we show the explicit $\tilde{\nu}$ dependence of the function $\tilde{\sigma}(\tilde{\nu})$ for some values of d. As can be seen, it is a non-trivial function of its argument, which may explain the qualitative difference between our results and previous approximate results. Indeed, notice that LPA and 1-loop analysis are based on a constant coupling σ (without dependence on frequency and momentum). As expected given the perturbative results, this dependence becomes weaker as d approaches 2.

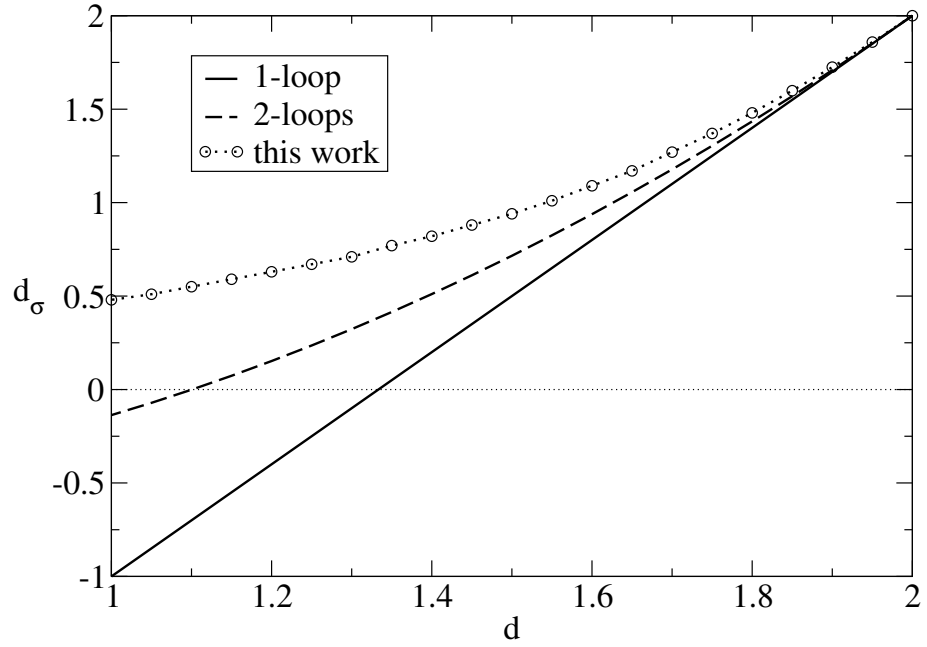

FIGURE 6.17 – Results for d_σ, showing there is no change in the RG relevance for the branching rate σ for $d \in [1,2]$.

This procedure allows us to find the value of d_σ as a function of d, the results of which are plotted, together with previous perturbative results, in Fig. 6.17. There one can see that even if d_σ gets smaller when d decreases, it remains always positive. This is an unexpected result, which deserves a careful discussion. At first sight, the positivity of d_σ implies that the PA fixed point is stable for all $d \in [1,2]$, which would naively imply that no fixed point exists to govern the PC transition (that is known to exist from other methods).

First of all, it is important to observe that this result does not rule out the existence of a new fixed point F^{PC} for small d, corresponding to the PC universality class. A new fixed point can indeed appear but for a nonzero value of the branching rate σ^*, as seen for example in the sketched flow shown in Fig. 6.18. This conjectured scenario would mean in particular that the low branching phase of the model has a behavior different from PA. This behaviour can

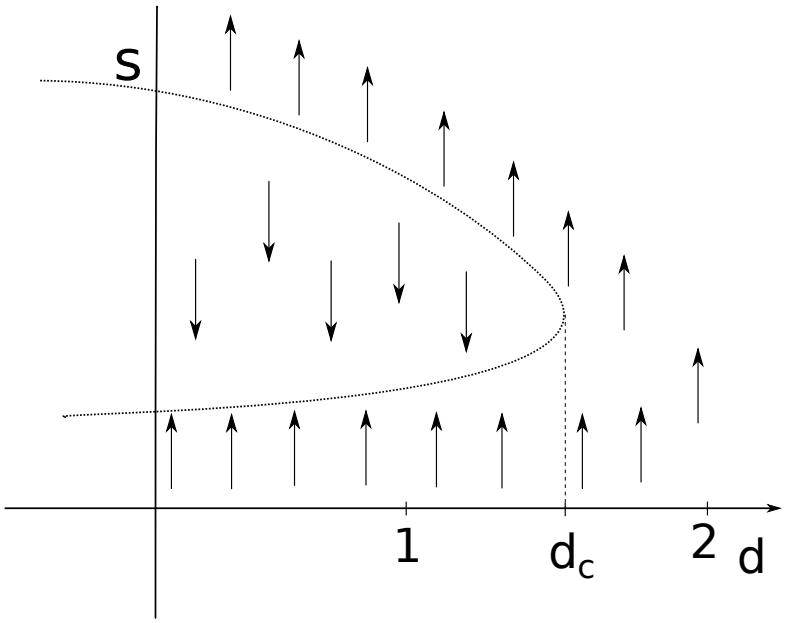

FIGURE 6.18 – Sketch of the relevance of the σ perturbation in BARW-PC, compatible with the results in this work and with simulations.

be studied either by using Monte-Carlo methods or perhaps by means of the NPRG at orders higher than the LPA.

As said before, there exists an exact result in $d = 1$ [186] which seems to indicate that in the PC/GV universality class σ is in fact irrelevant with respect to the PA fixed point. We can explain the difference, by observing that the model used in [186] is defined with $\lambda = \infty$, and indeed presents no phase transition at all for whatever value of σ. Now, the IR limit corresponds to $\nu, |\mathbf{p}|^2 \ll \lambda^{2/(2-d)}$, but this does not allow us to take $\sigma = 0$ when compared to λ. Looking at Eq. (6.79), $\lambda = \infty$ implies $\hat{\sigma} \equiv 0$, so that the relevant direction corresponding to σ is no longer accessible by studying σ as a perturbation. This is true for all d. Indeed, the results of [189] are also compatible with this scenario : in fact they show an irrelevant σ for all d when $\lambda = \infty$. For example, at 1-loop level (approximation valid close to $d = 2$) we have

$$\hat{\sigma}(p) \sim \frac{\sigma}{\lambda^3} l^2(p) \tag{6.98}$$

so that we see explicitly that $\lambda \to \infty$ yields $\hat{\sigma} \equiv 0$, and $\hat{\sigma}$ is no longer associated with the relevant branching direction. The fact is that there is an unstable direction in that dimension, but cannot be identified with the $\hat{\sigma}$ perturbation. Thus, we think that the exact calculation in [186] does not apply to BARW-PC, the system in which we are interested.

Also, there exist a result in [196] in which branching and annihilating systems of particles performing Lévy flight dynamics are studied. In it, the authors show that a change in the value of the Lévy flight exponent can be made to correspond to a change in the dimension d of the corresponding standard BARW system. This is used to recover $d_c = 4/3$ for BARW-PC. The analysis, however, is made by means of a 1-loop perturbative expansion in λ and σ, which explains the coincidence with the results of [52]. A re-analysis of Lévy flight dynamics can be conceived within the approach proposed in this work.

In what respects Monte Carlo studies of the low branching regime of this system, they have until now, as far as we know, also been mostly made in the limit $\lambda \to \infty$ [118, 157] mentioned before. They are compatible with the low branching rate being governed by the PA fixed point, but within the criticisms previously pointed out with respect to this particular $\lambda \to \infty$ limit. We have recently performed a preliminary Monte Carlo study of BARW-PC with a finite annihilation rate λ. The results for the density decay shown in Fig. 6.19, are compatible with the older results with $\lambda \to \infty$, not showing strong deviations from PA behaviour. However, the form of the decay does nos suffice to characterize the universality class. Of course, this matter deserves further study.

Let us emphasize that Fig. 6.18 only shows one of the possible scenarios allowing for the compatibility of all what is known about the PC transition. This scenario is not a result of this work, but only what we consider the simplest possibility. There may well indeed exist other explanations, and we do not pretend that Fig. 6.18 is the final word about this issue.

6.4. Comments

In this chapter we have applied field theoretical methods to answer some non-trivial questions about a class of reaction-diffusion systems. We have proceeded by exploiting the special case of Pure Annihilation, a system which does not present a phase transition but which nonetheless possesses a non-trivial fixed point in the RG sense. In order to do so, we took advantage of its simple structure, as well as the symmetries and causal properties of the system (which in fact allowed us to go beyond perturbation theory). We have then applied an expansion in the branching rate σ around Pure Annihilation, giving us access to the small branching regime of BARW, both with and without an additional parity conserving symmetry.

We have chosen to focus, as a first order example, on some important properties of these systems, usually very difficult to control but that become possi-

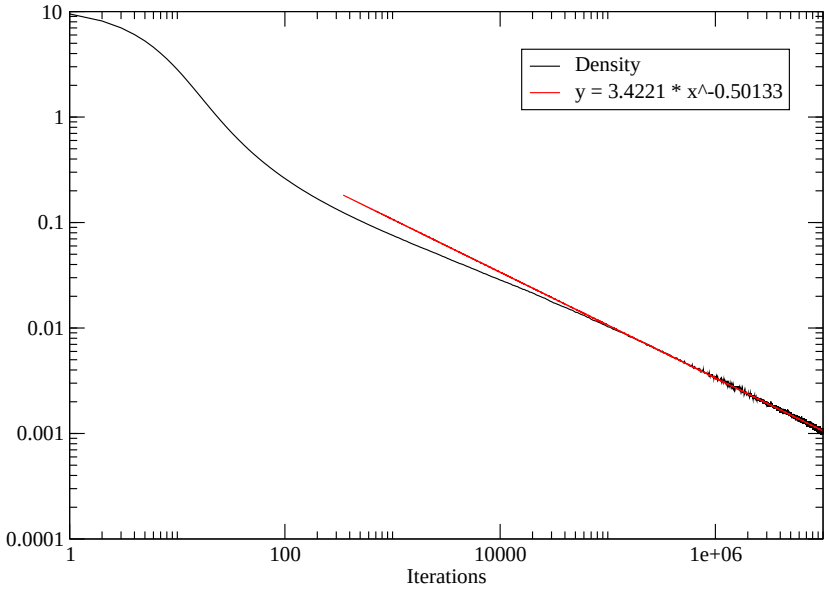

FIGURE 6.19 – (Preliminary) Monte Carlo results for the time dependency of the density in the low branching phase of BARW-PC in $d = 1$. PA-like behavior in $t^{-\frac{1}{2}}$ is observed. System size : 10^6, periodic boundary conditions.

ble to solve within the present method. In the case of the system of reactions $2A \to \emptyset$, $A \to 2A$, which belongs to the DP universality class, we have given an explicit proof of the existence of a phase transition in all space dimensions, already seen in previous numerical solutions of approximated versions of the NPRG flow equations, and in Monte-Carlo simulations. We have moreover calculated exactly the non-universal threshold value for the annihilation rate in order to find this phase transition in two sample systems. This result is beyond the possibilities of usual perturbation theory.

In BARW-PC, where the parity of the number of particles is conserved, we have concentrated on the value d_c of the upper critical dimension, that was previously believed to be between $d = 1$ and $d = 2$. Previous 1-loop and LPA results indicated $d_c \simeq 4/3$. By truncating our equations at one-loop order we were able to recover this approximate result, as well as the two-loop result of [189]. Surprisingly, we have found that the appearance of the PC fixed point associated with d_c must occur at a nonzero value of the branching rate, which would be compatible with a scenario where there exists not one but two new fixed points

for $d < d_c$. Further investigation of this issue should be performed, either by a higher order expansion in σ or by lattice simulations, or by the use of the NPRG method at orders higher than the LPA. Work in some of these directions is already underway.

Let us emphasize that the σ-expansion introduced here represents an expansion around a non-trivial (non-Gaussian) model, which in particular implies, as explained in the text for BARW-DP, that the first order results obtained in this work represent the first term in a convergent series.

The σ-expansion has allowed us to obtain results not accessible with the usual perturbative expansion, while still being (for the most part) analytical. This kind of ideas could in principle be generalized to other field theoretical systems, and future applications can be thought within the study of out of equilibrium systems. In what concerns BARW, a second order expansion in σ would in principle allow for the approximate calculation of critical exponents. Extensions to other out of equilibrium systems can also be conceived, for example in the study of PCPD, or of the Cole-Hopf version of the KPZ equation [202], which has a structure very reminiscent of Pure Annihilation.

Chapitre 7

Concluding remarks

Please understand, I never had a secret chart
to get me to the heart of this
or any other matter
Leonard Cohen

In this work we have applied powerful RG machinery to the study of various strongly correlated systems. While we were mostly interested in out of equilibrium systems, some of the tools we used are best introduced, and should be tested, in the far simpler context of equilibrium statistical mechanics. What we have done here can be seen then as a twofold contribution : we have applied methods and schemes already proven in the equilibrium context, such as the LPA, to out of equilibrium problems, and, in parallel, we have developed new methods within the NPRG for equilibrium systems, which we hope will be useful for the study of more complex systems in the future.

In what regards equilibrium systems, then, we have developed recently proposed schemes in order to obtain universal functions, an exploit mostly without reach for most previous NPRG studies. In particular, we have used the relatively new BMW approximation, in order to extract the momentum dependent universal scaling function of the Ising model, showing a remarkable agreement with theory and experiments, and without the need to adjust any free parameter. This function is really difficult to obtain by other means, so much so that even Monte Carlo techniques usually struggle with it, and there is also evidence that available experimental results are not sufficiently accurate. In fact, as we have seen, the most reliable source of comparison for this universal function is the analytical ansatz due to Bray, which is a well educated guess of the behaviour of this function, given its known regimes and its expected analytical properties. The BMW approximation, then, can be seen as a first justification of Bray's ansatz from first principles.

In parallel, we have used the lattice version of the NPRG formalism in order to obtain, again without any fitting parameter, the probability distribution function of the order parameter of the Ising model in $d = 3$. This family of universal functions can usually only be studied by means of Monte Carlo simulations. By doing so, we also give a physical meaning to the fixed point dimensionless potential v^*.

As stated many times before, our main motivation here was the study of out of equilibrium problems, where much less is known in the first place. As a first prerequisite in order to go deeper than the usual perturbative calculations, we were lead to some formal relations and interesting properties when defining out of equilibrium problems, within both the Doi-Peliti formalism and the Langevin equation approach. Specifically, we have studied the equivalences between these two formalisms when they can both be used to describe a given system, as is the case in reaction-diffusion processes. We think these developments, while in themselves not in any way revolutionary, shed light in some subtleties and common pitfalls on the field of stochastic dynamics.

Also, in this work we have for the first time provided a well-behaved definition of the Legendre transform for out of equilibrium field theories, which plays a fundamental role in the NPRG formalism, even if analysis of the theory in field expansions around $\tilde{\phi} = 0$ (as usually done in perturbation theory) are independent of this definition.

Having then cleared the terrain for a successful application of full functional NPRG techniques to these systems, we concentrated in the application of the LPA to one of the simplest and most important out of equilibrium universality classes, directed percolation. This showed to be a hard task, given the many conceptual and numerical difficulties involved.

In a purely analytical front, we have used the NPRG formalism, as well as other standard field theory techniques, to prove many exact properties in the case of pure annihilation, which in its turn allowed us to study the low branching properties of BARW. This lead to a series of exact results, derived for the first time using these methods. In particular, we calculated the exact non-universal value of the threshold annihilation rate λ_{th} for finding a phase transition in BARW-DP in any dimension. Moreover, we showed the existence of a surprising RG fixed point structure in the case of BARW-PC near $d = 1$, which we have shown to be compatible with all previous known information about the PC/GV transition.

The NPRG formalism has seldom been used to obtain exact results, and we think this work represents is particularly interesting in that sense. We think the same kind of ideas could be useful in many related systems, such as in the Cole-Hopf version of the KPZ equation. Indeed, we think that the results of this work represent a nice introduction to the potentialities of the NPRG methods, and

can very well be used as a possible introduction to them.

Many further applications are left for future work. In the equilibrium context, the BMW approximation deserves to be further exploited, as the first results shown here clearly indicate. Extensions to other scalar field theories, or to different spatial dimensions, are easily conceived, and for example it would be very illuminating to see the BMW approximation applied to the Kosterlitz-Thouless transition. Also, a deeper study should be performed of the broken symmetry phase, following the recent ideas presented in [171]. The possibilities are manifold, and the only bottleneck seems for the moment to be the difficulties of numerical implementation (and the disponibility of man-hours).

Secondly, the work presented here in the probability distribution of the Ising model can be readily improved, by using higher levels of the derivative expansion, or possibly even BMW. The extension to $O(N)$ should also be rather straightforward. Of course, a more ambitious objective would be to generalize this study to the case of reaction-diffusion out of equilibrium systems, such as BARW or PCPD, where there would be much to be learned from these distribution functions.

As for out of equilibrium systems *per se*, a lot is still to be done. At the formal level, it is really prioritary to devise a way to also regularize the frequency dependency of the vertex functions, which would increase the accuracy of our calculations, as well as allow the implementation of more sophisticated approximation schemes, such as BMW or high order derivative expansion. Also, frequency regularization would constitute a first step toward the study of time dependent problems, such as ageing or coarsening dynamics. Last, but not least, we believe that not regularizing the frequencies may be the cause of some of the numerical instabilities that we observe. The difficulty with this modification, as already stated, resides in finding an effective regulator term which would not break the causality properties of the theory.

In other fronts, it would be interesting to apply even low level approximations for the case of many species reaction-diffusion systems, such as DEP or Lotka-Volterra. We are sure the NPRG would provide useful contributions to the understanding of these systems. Also, the pursuit of orders higher than the LPA in the derivative expansion for BARW systems are within easy reach using the methods of this work. Simultaneously, the σ-expansion presented here can be taken to higher orders, with the hope to find more concluding evidence for our BARW-PC scenario, as well as to be able to obtain approximate values for critical exponents and related quantities.

On top of that, some non reaction-diffusion out of equilibrium systems share many of the properties of the systems studied here, with the already mentioned Cole-Hopf version of the KPZ equation being perhaps the easiest example. Work is already underway in some of these areas.

We also hope this work has helped the reader to see the (still) promising capabilities of the NPRG approach, when considering complex systems in and out of thermal equilibrium. The results presented in this work are just a small part of an increasing set of non-perturbative studies, starting to yield results not reachable by usual, more established, methods. We are now pushing the ideas of Wilson to its logical continuation, with often spectacular results. These methods, of course, have a much larger range of applicability, and we are sure to see lots of new developments within them in the following years.

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