

Some Aspects of Fluctuation Driven Phenomena

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ABSTRACT

Fluctuation driven phenomena refer to a broad class of physical systems that are shaped and influenced by randomness. These fluctuations can manifest in various forms such as thermal noise, stochasticity, or even quantum fluctuations. The importance of understanding these phenomena lies in their ubiquity in natural systems, from the formation of patterns in biological systems, to the behavior of phase transitions and universality classes, to quantum computers. In this dissertation, we delve into the peculiar phenomena driven by fluctuations in the following scenarios:

- We study the near-equilibrium critical dynamics of the $O(3)$ nonlinear sigma model describing isotropic antiferromagnets with a non-conserved order parameter reversibly coupled to the conserved total magnetization. We find that in equilibrium, the dynamics is well-separated from the statics and the static response functions are recovered in the limit $\omega \rightarrow 0$, at least to one-loop order in a perturbative treatment with respect to the static and dynamical nonlinearities. Since the static nonlinear sigma model must be analyzed in a dimensional $d = 2 + \varepsilon$ expansion about its lower critical dimension $d_{lc} = 2$, whereas the dynamical mode-coupling terms are governed by the upper critical dimension $d_c = 4$, a simultaneous perturbative dimensional expansion is not feasible, and the reversible critical dynamics for this model cannot be accessed at the static critical renormalization group fixed point. However, in the coexistence limit addressing the long-wavelength properties of the low-temperature ordered phase, we can perform an $\epsilon = 4 - d$ expansion near d_c . This yields anomalous scaling features induced by the massless Goldstone modes, namely sub-diffusive relaxation for the conserved magnetization density with asymptotic scaling exponent $z_T = d - 2$ which may be observable in neutron scattering experiments.
- We investigate the influence of spatial disorder on coined quantum walks. Coined quantum walks describe the time evolution of a quantum particle that is controlled by a quantum coin degree of freedom. We consider one-dimensional walks and use a two-level system as quantum coin. Each time step thus consists of the iterative application of a quantum coin toss and a conditional shift operator. Qualitative differences with classical random walks arise due to superpositioned states and entanglement between walker and coin. We consider spatially inhomogeneous coin tosses with every lattice site having a tossing amplitude. These amplitudes are noisy such that the walk is spatially disordered. We find that disorder deteriorates the ballistic transport properties of non-noisy quantum walks. This leads to an extremely slow spreading of the quantum

walker and potentially induces localization behavior. We investigate this slow dynamics and compare the disordered quantum walk with the standard coined Hadamard walk. Special focus is given to the influence of disorder on entanglement-related properties.

- We apply a perturbative field-theoretical analysis to the symmetric Rock-Paper-Scissors (RPS) model and the symmetric May-Leonard (ML) model, in which three species compete cyclically. We demonstrate that the qualitative features of the ML model are insensitive to intrinsic reaction noise. In contrast, and although not yet observed in numerical simulations, we find that the RPS model acquires significant fluctuation-induced renormalizations in the perturbative regime. We also study the formation of spatio-temporal structures in the framework of stability analysis and provide a clearcut explanation for the absence of spatial patterns in the RPS model, whereas the spontaneous emergence of spatio-temporal structures features prominently in the ML model.
- We delve into the action-to-absorbing phase transition in the Pair Contact Process with Diffusion (PCPD), which naturally generalizes the Directed Percolation (DP) reactions. We revisit the single-species PCPD model in the Doi-Peliti formalism and propose a possible perturbative solution for the model. In addition, we investigate the two-species effective model of PCPD and demonstrate its equivalence to the single-species PCPD at tree-level effective field theory. We also examine the fixed point of the model where all relevant parameters are set to zero. Our analysis reveals that the fixed-point theory is inconsistent with the PCPD critical condition. Thus, combining the effective field theory argument, this inconsistency suggests that the critical theory should already be completely encoded in the single-species model.

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GENERAL AUDIENCE ABSTRACT

Fluctuations are a ubiquitous aspect of the real world. For instance, even though a train schedule may be set, the train may arrive two minutes ahead of schedule or two hours late. Similarly, if you were to flip a coin ten times, you would expect to get five heads and five tails based on simple probability, but in reality, you may not even come close to this result. In classical situations, these fluctuations are a result of our lack of knowledge about the details of the system. However, in quantum mechanics, scientists have demonstrated that fluctuations are inherent to the system, even when every single detail of the system is known. Therefore, understanding fluctuations is crucial to gaining insight into the fundamental laws of the universe.

In most cases, fluctuations are insignificant and the world can be accurately described by a set of deterministic equations. However, there are situations in which fluctuations play a significant role and can greatly deviate the system from the predictions of deterministic equations. In this dissertation, we study the following scenarios where fluctuations dominate and lead to peculiar phenomena:

- Near continuous phase transitions, due to the divergence of the characteristic length, most systems become long-range correlated. This means that the changes at one point can affect another point very far away. We study the critical dynamics of two systems near their phase transitions: antiferromagnetic system in Chapter 2 and a simplified population dynamics model in Chapter 5. Through our analysis, we demonstrate how fluctuations significantly alter the behavior of these systems near their critical points.
- In chapter 3, we examine the impact of spatial disorder on the quantum random walk, a quantum counterpart of the classical random walk or “drunkard’s walk”. Given that the quantum random walk has been shown to have universal quantum computing capabilities, this disorder can be considered as errors in the control of the system. We reveal how disorder effects drastically change the dynamics of the system.
- The formation of patterns is typically studied in deterministic nonlinear systems. In Chapter 4, we analyze pattern formation in stochastic population dynamics models, and demonstrate emergent behavior that goes beyond what is seen in their deterministic counterparts.

Dedicated to human curiosity and the endless exploration of the unknown. This work stands as a testament to the unwavering spirit of those who strive to seek answers and uncover new discoveries, even amidst challenges such as struggles in research and break-up. May it serve as a reminder to keep faith and persevere in the pursuit of knowledge and understanding, no matter the obstacles one may encounter.

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Chapter 1

Background

Albert Einstein once made the famous declaration, “*God doesn’t play dice with the universe.*” However, our understanding of the universe has since evolved, and it is now understood that the world is inherently probabilistic, with fluctuations being an integral part of it. The Copenhagen Interpretation even posits that perhaps the divine entity is a wild gambler after all.

In physics, the study of fluctuation-driven phenomena is a central theme. In this chapter, we will delve into this topic by introducing simple models in which fluctuations play a significant role. We will also explore useful techniques to analyze and address fluctuations in various distinct systems. At the end of this chapter, we describe the structure of this dissertation.

1.1 Random Walks on a Line

One of the simplest models with stochasticity is the random walk. It describes a particle hopping from one site to another with specific probabilities. Despite its simplicity, the random walk model has been found to effectively capture a wide range of phenomena, such as diffusion in liquids (see, for example [1]) or polymer statistics (see, for example, [2, 3, 4]). The variants of random walk are also used to design algorithms in computer sciences (see, for example, [5, 6]).

Assuming the walker is on a line with equal probabilities of jumping to the left and right at each unit time, the system can be described by the probability of the walker $P(n, t)$ at site n and at time t . The dynamics is thus determined by the following recurrence relation

$$P(n, t) = \frac{1}{2} [P(n - 1, t - 1) + P(n + 1, t - 1)]. \quad (1.1)$$

While taking the continuous time limit, this recurrence relation becomes what is known as the master equation, which reads

$$\partial_t P(n, t) = \frac{1}{2} [P(n - 1, t) + P(n + 1, t)]. \quad (1.2)$$

Although the master equation is very useful in analyzing the systems with fluctuations, it is far too intimidating to use a master equation to deal with this simple model. The distribution

$P(n, t)$ can be exactly calculated by simply counting. Assume we start from site 0, sitting at site n at time t simply means the walker has jumped to the right $(t + n)/2$ times and to the left $(t - n)/2$ times. Thus, the probability of staying at site n at time t is given by

$$P(n, t) = \frac{t!}{\left(\frac{t-n}{2}\right)!\left(\frac{t+n}{2}\right)!} 2^{-t}. \quad (1.3)$$

Interestingly, while $t \gg n$, the central limit theorem tells us that the probability distribution can be approximated by a Gaussian distribution:

$$P(n, t) = \frac{1}{\sqrt{2\pi(\Delta n)^2}} \exp\left(-\frac{(n - \bar{n})^2}{2(\Delta n)^2}\right) \quad (1.4)$$

where $\bar{n} = 0$ is the average value of n and Δn is the standard deviation. As $\Delta n \propto \sqrt{t}$, the system behaves diffusively.

This simple random walk model can be expanded by incorporating multiple particles and interactions among them, such as the branching and annihilation random walk, as discussed in [7, 8]. In Chapters 4 and 5, we will examine phase transitions and pattern formation in these generalized random walk systems, also known as reaction-diffusion systems.

1.2 Langevin Equation and Janssen-De Dominicis Functional

A straightforward generalization of the random walk discussed in the previous section is having a particle moving in a certain potential $V(x)$ with random dragging forces, which was first studied by Paul Langevin [9]. The motion of the particle is described by the Langevin equation:

$$m\partial_t^2 x(t) = -m\zeta\partial_t x(t) - \frac{\delta V}{\delta x} + f(t) \quad (1.5)$$

where m is the mass of the particle, $-m\zeta\partial_t x(t)$ is a friction force which is proportional to the velocity of the particle and $f(t)$ is a random force. In the case of strong damping, i.e. $\zeta\dot{x} \gg \ddot{x}$, the inertial term $m\partial_t^2 x(t)$ can be ignored and the above Langevin equation is re-written as

$$\partial_t x(t) = -\Gamma \frac{\delta V}{\delta x} + r(t) \quad (1.6)$$

with $\Gamma = 1/m\zeta$ and $r(t) = f(t)/m\zeta$. The expectation of the random force can always be set to zero by incorporating its non-zero component into the potential V . In the long-time limit, it is assumed that the random force is Markovian, i.e. temporally local. As a result, we have

$$\langle r(t) \rangle = 0, \quad \langle r(t)r(t') \rangle = \lambda\delta(t - t') \quad (1.7)$$

for some noise correlation coefficient λ . If we further assume the medium is at thermal equilibrium, the fluctuation-dissipation theorem uniquely determines the coefficient $\lambda = 2\Gamma k_B T$, where k_B is the Boltzmann constant and T is the temperature.

In 1948, the renowned physicist Richard Feynman introduced a path integral formalism for quantum mechanics [10]. Decades later, in 1976, Janssen [11] and De Dominicis [12] independently presented a way to represent the Langevin dynamics through a path integral. To write the Langevin equation as a path integral, an additional response variable $\tilde{x}$ is introduced, representing the random force $r(t)$. The probability distribution of $x(t)$ is then given by:

$$P[x(t)] = \int \mathcal{D}[i\tilde{x}(t)] \exp(-\mathcal{A}), \quad (1.8)$$

where $\mathcal{A}$ is the Janssen-De Dominicis functional

$$\mathcal{A} = \int_t \left[\tilde{x} \partial_t x + \Gamma \tilde{x} \frac{\delta V}{\delta x} - \lambda \tilde{x}^2 \right]. \quad (1.9)$$

Finally, the expectation value of an arbitrary observable $O[x(t)]$ can be calculated as

$$\langle O[x(t)] \rangle = \int \mathcal{D}[x(t)] O[x(t)] \int \mathcal{D}[i\tilde{x}(t)] \exp(-\mathcal{A}). \quad (1.10)$$

Surprisingly, this formalism derived purely from classical Langevin dynamics can be connected to the Schwinger-Keldysh (SK) formalism [13] for non-equilibrium quantum dynamics by disregarding higher order terms of the so-called quantum fields in the SK formalism. This connection opens up the possibility of better understanding the relationship between classical and quantum fluctuations.

The Janssen-De Dominicis formalism has proven to be highly successful in studying critical dynamics in the renormalization group framework, as demonstrated in numerous works (for an overview, see [14]). In Chapter 2, this formalism will be applied to study the critical dynamics of antiferromagnets.

1.3 Anderson Localization

Another intriguing phenomenon induced by fluctuations is Anderson localization, which was first predicted by Philip Anderson in 1958 [15]. Anderson showed that as the level of disorder increases, some electron systems can undergo a phase transition from being conductors to insulators, due to the interference of scattered waves causing localization.

This phenomena can be studied through a simple one-dimensional model described by the following Hamiltonian:

$$H = W \sum_i \epsilon_i c_i^\dagger c_i + \sum_{\langle i,j \rangle} \left(c_i^\dagger c_j + c_j^\dagger c_i \right), \quad (1.11)$$

where c and $c^\dagger$ are fermionic ladder operators and $\langle i, j \rangle$ denotes nearest neighbors i and j . The first term represents an onsite random potential, with ϵ_i randomly drawn from the range $[-1, 1]$ and W indicating the disorder strength. The second term describes nearest-neighbor hopping. For convenience, we consider the case when $W = 1$ here. Since there are no electron-electron interactions in the Hamiltonian, we can consider a single-electron system described by the ansatz state $|\Psi\rangle = \sum_i \phi(i) c_i^\dagger |0\rangle$. By inserting this ansatz state into the stationary Schrödinger equation, we obtain the following recurrence relation given by the transfer matrices $\hat{T}_i$:

$$\begin{bmatrix} \phi(n) \\ \phi(n-1) \end{bmatrix} = \prod_{i=1}^{n-1} \hat{T}_i \begin{bmatrix} \phi(1) \\ \phi(0) \end{bmatrix}, \quad \hat{T}_i = \begin{bmatrix} E - \epsilon_i & -1 \\ 1 & 0 \end{bmatrix} \quad (1.12)$$

where E is the eigenenergy. It has been shown that as n approaches infinity, $|\phi(n)|^2$ decays exponentially, with $|\phi|^2 \sim \exp(-n/\xi)$, where ξ is the localization length [16, 17]. This indicates that the electron wavefunctions in a disordered lattice can become localized, meaning they are confined to a small region in space and do not extend throughout the entire lattice. The presence of random potentials in the system scatters the wavefunctions and causes them to interfere destructively, leading to localization.

Similar localization phenomena have been observed in a variety of physical systems, including electrons in disordered solids, light in disordered optical media, and acoustic waves in disordered materials [18, 19, 20, 21]. In Chapter 3, we will study the localization behavior of quantum random walks with spatial disorders.

1.4 Continuous Phase Transitions and Landau's Paradigm

The scaling behavior near continuous phase transitions is strongly impacted by fluctuations. To understand these critical phenomena, Lev Landau proposed a symmetry-breaking paradigm [22], which has proven to be successful in describing most phase transitions encountered.¹ The paradigm suggests that phase transitions can be identified by a local order parameter that represents a particular symmetry group G . Two phases are separated by a critical point, where the symmetry is spontaneously broken at the “ground state” level.²

This paradigm can be understood through a zero-dimensional toy model that possesses $\mathbb{Z}_2$ symmetry. The free energy of the model reads

$$F = \alpha m^2 + \beta m^4. \quad (1.13)$$

It is clear from the above expression that the free energy is invariant under the transformation $m \rightarrow -m$, making it $\mathbb{Z}_2$ symmetric. A schematic graph of the free energy F as a function

¹Recently, phase transitions beyond Landau's Paradigm are found in highly entangled systems, see, for example [23, 24].

²In thermal phase transitions, the ground state refers to the state with lowest free energy.

of m is shown in Fig. 1.1. When β is positive and α is also positive, the only ground state is located at $m = 0$, preserving the $\mathbb{Z}_2$ symmetry of the system. However, if α becomes negative, two degenerate ground states appear, which are symmetric over $m = 0$. Despite this, the system will settle into only one of the two ground states, breaking the symmetry. A continuous phase transition happens at $\alpha = 0$ between the symmetric and the symmetry-breaking phases.

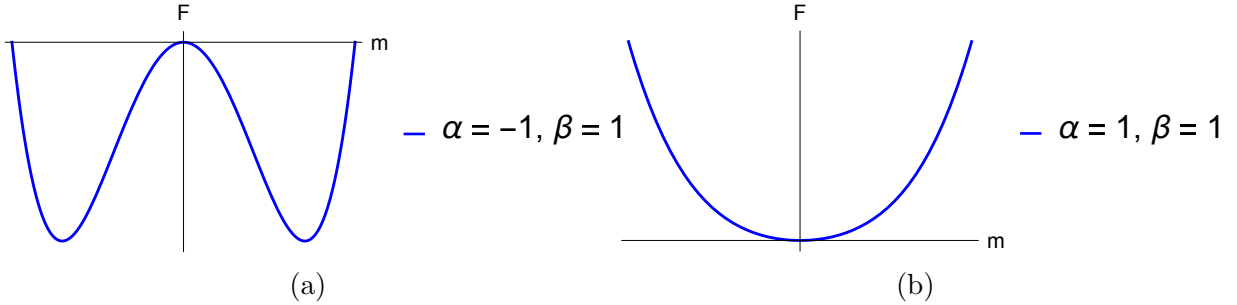


Figure 1.1: A schematic graph of the free energy F as a function of m is shown for (a) $\alpha = -1$ and $\beta = 1$, and (b) $\alpha = 1$ and $\beta = 1$.

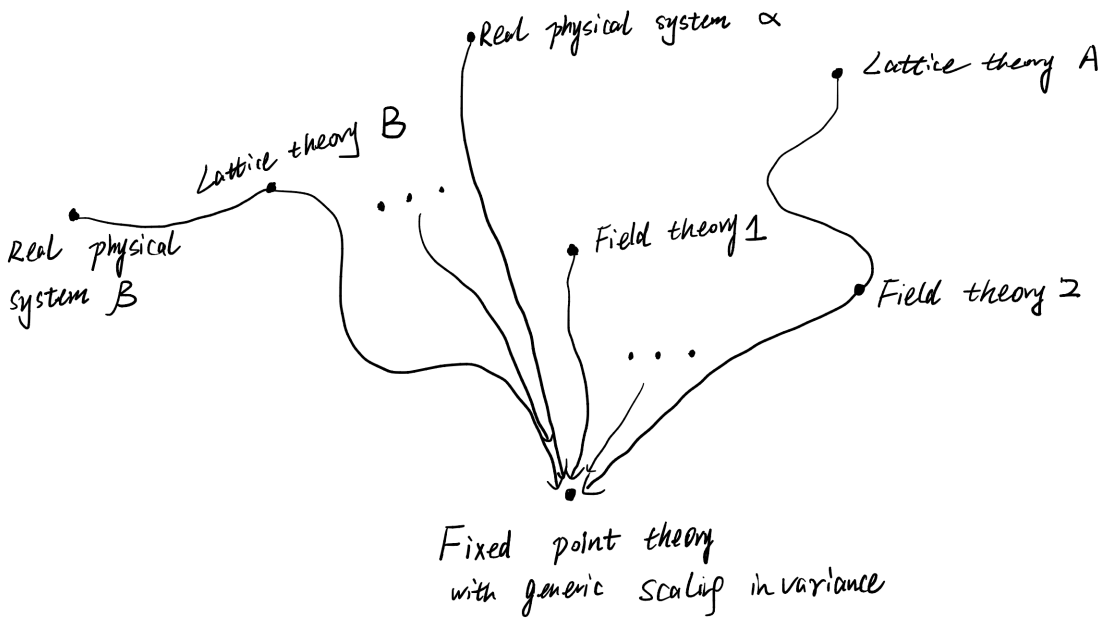
In Landau's original theory of symmetry breaking for continuous phase transitions [22], the mean-field approach was employed, neglecting the effects of fluctuations. To rectify this, the renormalization group method can be applied, as will be discussed in the following section. This paradigm, despite its limitation, has been successful in qualitatively explaining the vast majority of continuous phase transitions.

1.5 Coarse-Graining and Renormalization Group

The concept of effective theories in physics, developed due to scale separation in physical phenomena, has proven to be a valuable tool in the absence of a comprehensive theory of microscopic physics. By integrating out known microscopic details, the coarse-graining process allows for the development of theories that describe phenomena at specific scales. While the idea of coarse-graining may seem simple, its systematic mathematical formulation is challenging. The concept of the renormalization group, which provides a systematic method for coarse-graining, was first introduced in the field of relativistic quantum electrodynamics by Gell-Mann and Low [25]. Later in 1966, Kadanoff also developed a block-transformation renormalization procedure and applied it to critical phenomena [26]. Kenneth Wilson realized the equivalence between the renormalization in quantum electrodynamics and the block-transformation proposed by Kadanoff and proposed a systematic renormalization group method for the first time [27, 28]. In 1972, Wilson and Fisher published a seminal paper [29] examining the critical scaling of the Ising model using dimensionally regularized renormalization group techniques. This method was further explored in a sequence

of papers by Kenneth Wilson and collaborators (see, for example, [30, 31, 32]). Since then, the Renormalization Group (RG) method has been one of the most important tools to study critical phenomena.

The RG concept is straightforward. Physical theories are defined on a specific length or energy scale, and the parameters in the models are dependent on the scale parameter l . By starting from a microscopic theory and gradually coarsening it, the effective theory changes as the scale parameter changes, governed by the RG flow equations. In a continuous phase transition near the critical point, the correlation length becomes divergent, leading to scale invariance in the system. This corresponds to a fixed point of the RG flows. As the RG process loses information, different microscopic theories can lead to the same fixed point, resulting in universal behavior in systems with diverse microscopic details. This concept is schematically illustrated in Fig. 1.2, where different microscopic systems converge to a common fixed point with scale invariance.



RG flow & Universality

Figure 1.2: The Renormalization Group (RG) flow and universality class concept is illustrated schematically. Through the RG flow, various microscopic theories converge to a common fixed point theory exhibiting generic scale invariance and therefore exhibit universal behavior in their scaling characteristics.

In Chapters 2 and 5, we will utilize the dimensionally regularized renormalization group method to explore the dynamic critical phenomena of antiferromagnetic systems during relaxation and the active-to-absorbing phase transitions in the reaction-diffusion system

known as the Pair Contact Process with Diffusion.

1.6 Structure of this Dissertation

The chapters of this dissertation are structured as follows: In chapter 2, we apply the renormalization group method to investigate the critical dynamics of the antiferromagnetic $O(3)$ nonlinear σ model with conserved magnetization. In chapter 3, the localization phenomenon in the disordered quantum random walk is studied via numerical simulations. We explore pattern formation and the active-to-absorbing phase transition in certain reaction-diffusion systems in chapter 4 and 5, respectively. A comprehensive conclusion to the dissertation is provided in chapter 6, which includes a summary of the above chapters.

Chapter 2

Critical Dynamics of the Antiferromagnetic $O(3)$ Nonlinear Sigma Model with Conserved Magnetization

This chapter is adapted from our publication [33],

*Louie Hong Yao and Uwe C. Täuber, “Critical dynamics of the antiferromagnetic $O(3)$ nonlinear sigma model with conserved magnetization”, *Phys. Rev. E* (2022) 105, 064128, Copyright (2022) by the American Physical Society.*

2.1 Introduction

The universal scaling behavior near critical points and in low-temperature ordered phases with spontaneously broken continuous symmetries has been studied extensively in both equilibrium thermal as well as quantum systems since the 1960s. Many different powerful methods have been developed, most prominently Monte Carlo computer simulations and renormalization group (RG) analysis, carried out either perturbatively analytically (see, for example, Refs. [29, 30, 34]) or non-perturbatively numerically (e.g., Refs. [35, 36, 37]); we also note the recently developed “conformal bootstrap” approach [38, 39, 40].

Yet for systems driven away from thermal equilibrium, more complicated and intriguing issues arise. It is well-known that systems in the same static equilibrium universality class may in fact display distinct universal dynamic scaling features. $O(n)$ -symmetric magnetic systems constitute a paradigmatic example: The associated order parameter may either freely relax to equilibrium or be constrained by a strict conservation law for the total magnetization, whence the magnetization density relaxes diffusively. These two different variants are described by the relaxational models A and B in Hohenberg and Halperin’s classification [14]. In addition to purely relaxational kinetics, the order parameter may be reversibly dynamically coupled to other conserved modes (c.f., models E, G, and J).

To distinguish different dynamic universality classes near equilibrium, a distinct critical

exponent, the dynamic scaling exponent $z \geq 1$, was introduced to capture the phenomenon of critical slowing down of a critical system's kinetics [41, 42]. As this term implies, near a critical point the order parameter is governed by slow algebraic relaxation rather than the standard exponential decay with finite characteristic relaxation time t_r . This power law behavior can be described by a scaling law for the relaxation time $t_r \sim \xi^z$, where $\xi \sim |T - T_c|^{-\nu}$ ($\nu > 0$) denotes the diverging correlation length of the system; or equivalently by the leading wavevector dependence of the order parameter damping coefficient $D(q) \sim |q|^z$ that determines the peak linewidth in the associated scattering cross section.

One important historical approach to theoretically classify dynamic universal behavior was mode-coupling theory, wherein reversible dynamical coupling terms were added to the relaxation dynamics, and the resulting stochastic equations of motion subsequently solved by means of a Hartree-Fock like self-consistent factorization approximation. This methodology was originally proposed by Fixman for binary fluids [43], later reformulated by Kadanoff and Swift [44] and Kawasaki, who also extended this treatment to magnetic systems [45, 46, 47]. In a theory incorporating dynamical mode-coupling terms, the order parameter is coupled to other slow hydrodynamic modes, which originate from conservation laws, during the system's relaxation. For example, in the still purely relaxational models C / D, a static coupling term between a real scalar field and the order parameter is introduced into the Hamiltonian to keep the total energy conserved [14, 48, 49, 50]. Furthermore, when the conserved modes correspond to specific order parameter symmetries, additional reversible dynamical terms can be introduced via the Lie algebra Poisson brackets between the order parameter and the conserved modes [49, 50, 51, 52, 53, 54, 55, 56].

In this work, we utilize the field-theoretic perturbative dynamical renormalization group approach to study the near-equilibrium relaxation dynamics of the antiferromagnetic $O(3)$ nonlinear sigma model with conserved total magnetization. We specifically account for the reversible hydrodynamic mode couplings between the conserved magnetization density fields and the non-conserved staggered magnetization serving as the order parameter for the continuous para- to antiferromagnetic phase transition. For magnetic systems, these purely dynamical contributions originate from the microscopic spin precession in the local effective field. In an antiferromagnetically ordered phase, in contrast with purely relaxational kinetics, the mode coupling of the staggered magnetization to the conserved standard magnetization density causes the emergence of propagating spin wave modes (magnons) with linear dispersion $\omega(q) = c|q|$ and quadratic wave vector dependence of the damping $D(q) \sim q^2$ [see Eq. (2.20) below]. At $T = T_c$, strong order parameter fluctuations induce the critical damping $D(q) \sim \lambda(q) \sim |q|^{z_c}$ for both the order parameter and the magnetization densities, with the well-established dynamic critical exponent $z_c = d/2$ in dimensions $2 < d < d_c = 4$, which represents the upper critical dimension for this model G dynamical universality class [14, 49, 50]. This exponent value differs markedly from the corresponding mean-field values $z_0 = 2$ and the purely relaxational model A result $z_c = 2 + c' \eta$, where η denotes the static Fisher critical exponent η and c' is a universal constant. These classical results have been amply confirmed experimentally, e.g., perhaps most convincingly in neutron scattering ex-

periments for the isotropic antiferromagnet RbMnF_3 [57] as well as in detailed numerical simulations, for example in Refs. [58, 59, 60].

In thermal equilibrium, the $O(n)$ nonlinear sigma model represents a paradigmatic field theory to describe ferromagnetic or antiferromagnetic systems exhibiting rotational symmetry in order parameter space [61, 62]. It exhibits spontaneous symmetry breaking and a continuous phase transition at a critical temperature T_c , and its static thermodynamic critical properties are well-established to be in the same universality class as the $O(n)$ -symmetric Landau–Ginzburg–Wilson ϕ^4 theory in equilibrium. Out of equilibrium, the $O(n)$ nonlinear sigma model has to our knowledge only been studied under the restrictive assumption of purely relaxational (model A) dynamics. In 1980, Bausch, Janssen, and Yamazaki calculated the associated dynamical critical exponent z and compared it with the corresponding scaling exponent of the relaxational $O(n)$ -symmetric Landau–Ginzburg–Wilson theory [63]. Only comparatively recently in 2006, Fedorenko and Trimper evaluated the critical aging scaling behavior for the purely relaxational $O(n)$ nonlinear sigma model with non-conserved order parameter [64]; not surprisingly, it belongs to the model A universality class. Although the $O(n)$ -symmetric Landau–Ginzburg–Wilson model with mode-coupling terms have been widely studied in the literature (for overviews, see Refs. [49, 50]), the $O(n)$ nonlinear sigma model with non-dissipative reversible mode-mode couplings appears to have not drawn similar attention.

We couple the three-component non-conserved staggered magnetization order parameter of the nonlinear sigma model to the conserved magnetization density vector field. We employ coupled Langevin-type stochastic partial differential equations to describe the dynamics of this system and construct the associated Janssen–De Dominicis functional [11, 65, 66]. In the resulting field theory framework, we apply the standard transverse fluctuation loop expansion to perturbatively compute the model’s dynamical response functions to the first nontrivial order in the nonlinear couplings. Indeed, to one-loop order, the dynamics cleanly separates from the statics, and in the low-frequency limit $\omega \rightarrow 0$, we properly recover the static susceptibilities. However, it turns out that the ordinary dimensional $d = 2 + \varepsilon$ expansion about the lower critical dimension $d_c = 2$ that captures the nonlinear sigma model’s universal static critical properties is not capable to access the critical dynamics in the presence of reversible mode couplings.

Hence we turn our attention to the ordered-phase or coexistence fixed point; to this end, we tune the effective temperature to zero and employ an $\epsilon = 4 - d$ expansion scheme near the dynamical upper critical dimension $d_c = 4$ to retrieve the universal dynamical scaling behavior in the coexistence regime. Solving the one-loop RG flow equations, we find that the dynamic scaling exponents for both the order parameter and for the magnetization density flow to the same fixed point values as in the Sasvári–Schwabl–Szépfalusy (SSS) model [67]. Hence we obtain Gaussian dynamical scaling exponents $z_D = 2$ and $z_\lambda = 2$ for the order parameter and transverse magnetization components, implying a mean-field form for the ensuing spin wave dispersion, but our results remarkably yield anomalous sub-diffusive relaxation for the longitudinal magnetization density, described by $z_\Gamma = d - 2$. This

result indicates that the $O(n)$ nonlinear sigma model with conserved total magnetization belongs to the same dynamical universality class as the SSS model. Intriguingly, although the critical regime is conceptionally not approachable with an ϵ expansion near the upper critical dimension $d_c = 4$, the numerical solutions of the near-critical RG flow equations initially approach the known critical values, recovering the dynamic critical exponent $z_c = d/2$, before they ultimately cross over to their asymptotic scaling behavior at the ordered-phase coexistence fixed point.

This chapter is organized as follows: In the following section, we introduce the near-equilibrium dynamics of the antiferromagnetic nonlinear sigma model with conserved total magnetization, properly incorporating the crucial non-dissipative mode coupling terms. We formulate the coupled Langevin stochastic equations for the order parameter and the magnetization density, construct the corresponding Janssen–De Dominicis functional, and utilize this formalism to derive the explicit one-loop expressions for the dynamic response functions. In Section 2.3, we discuss the ensuing scaling behavior of the model near its RG fixed points. We argue that the critical fixed point is not reachable in this perturbative approach. Subsequently we present a thorough scaling analysis via the dimensionally regularized perturbative RG method near the ordered phase or coexistence fixed point. We numerically solve the resulting RG flow equations and compare our findings with the SSS model, and discuss relevant experimental consequences. We conclude with a brief summary and outlook. The Appendix contains additional pertinent technical details for the one-loop perturbative analysis. It also addresses the feasibility of the critical dynamics of the nonlinear sigma model with conserved total energy as well as a conserved order parameter field.

2.2 Nonlinear Sigma Model with Conserved Total Magnetization

In this section, we introduce the near-equilibrium dynamics of the $O(3)$ -symmetric antiferromagnetic nonlinear sigma model with conserved total magnetization. Its time evolution subject to random thermal fluctuations is described by appropriate coupled generalized Langevin equations, and the corresponding Janssen–De Dominicis response field theory functional that encodes this stochastic nonlinear dynamics. We employ dynamic perturbation theory to derive explicit results for the dynamic response functions to one-loop order in the fluctuation expansion with respect to the transverse modes. The ensuing dynamic scaling behavior will be discussed in the next section.

2.2.1 Dynamics with Conserved Total Magnetization

We consider a rotationally symmetric three-component antiferromagnet described by the $O(3)$ nonlinear sigma model with the coarse-grained mesoscopic Hamiltonian [61]

$$\mathcal{H}[\vec{n}] = \int d^d x \left[\frac{\rho}{2} \left(\nabla \vec{n}(x) \right)^2 - h \sigma \right], \quad (2.1)$$

where $\vec{n}(x) = (\vec{\pi}(x), \sigma(x))$ denotes the staggered magnetization vector that serves as order parameter for an antiferromagnet, and the constraint $\vec{n}^2 = 1$ is imposed at all locations x . ρ represents the order parameter stiffness and h is a (fictitious) external conjugate thermodynamic field pointed along the direction of σ . (Note that positions x and later, the corresponding wavevectors and momenta p , are d -dimensional spatial vectors. We drop their vector labels in order to not confuse them with the three-component vector fields in order parameter space.)

To describe the interaction of the antiferromagnet with the conserved total magnetization, we introduce the magnetization density $\vec{M}(x, t)$ in the Hamiltonian (2.1),

$$\mathcal{H}[\vec{M}, \vec{n}] = \int d^d x \left[\frac{1}{2\chi} \vec{M}(x)^2 + \frac{\rho}{2} \left(\nabla \vec{n}(x) \right)^2 - h \sigma \right], \quad (2.2)$$

where χ denotes the static magnetic susceptibility. The conservation of the total magnetization is intimately related to the underlying $O(3)$ invariance for the order parameter. Indeed, $\vec{M}$ is the generator of the rotational symmetry, and hence satisfies the standard angular momentum Lie algebra Poisson brackets

$$\begin{aligned} \{M_\alpha(x), M_\beta(y)\} &= -\epsilon_{\alpha\beta\gamma} M_\gamma(x) \delta^{(d)}(x - y), \\ \{M_\alpha(x), n_\beta(y)\} &= -\epsilon_{\alpha\beta\gamma} n_\gamma(x) \delta^{(d)}(x - y), \end{aligned} \quad (2.3)$$

where $\alpha, \beta, \gamma = 1, 2, 3$, and Einstein's summation rule over repeated indices is implemented (unless otherwise specified).

Generalized Langevin equations for “slow” modes ϕ with respect to an effective Hamiltonian $\mathcal{H}[\phi]$ take the form

$$\dot{\phi} = \{\phi, \mathcal{H}\} - D(i\nabla)^a \frac{\delta \mathcal{H}}{\delta \phi} + \eta, \quad (2.4)$$

where $a = 0, 2$ corresponds to nonconserved and conserved relaxation dynamics, respectively, D denotes the relaxation rate or diffusion constant, and η represents Gaussian stochastic noise. With the Hamiltonian (2.2) and Poisson brackets (2.3), the following coupled Langevin dynamics of the antiferromagnetic order parameter $\vec{n}$ and the rescaled conserved magnetization density $\vec{m} = \vec{M}/\sqrt{\rho\chi}$ ensue [14, 50],

$$\begin{aligned} \dot{\vec{m}} &= c \vec{n} \times \nabla^2 \vec{n} + \lambda \nabla^2 \vec{m} + \vec{\eta}, \\ \dot{\vec{n}} &= -c \vec{n} \times \vec{m} + D \left(\nabla^2 \vec{n} + \tilde{h} \right) + \vec{\zeta}. \end{aligned} \quad (2.5)$$

Here

$$c = \sqrt{\rho/\chi} , \quad u = k_B T / \rho \quad (2.6)$$

are the spin wave velocity and scaled effective temperature, and $\tilde{h} = \rho h$. $\vec{\eta}(x, t)$ and $\vec{\zeta}(x, t)$ represent independent additive Gaussian white noise terms with vanishing means $\langle \vec{\eta} \rangle = 0 = \langle \vec{\zeta} \rangle$ and the second moments

$$\begin{aligned} \langle \eta_\alpha(x_1, t_1) \eta_\beta(x_2, t_2) \rangle &= -2\lambda u \delta_{\alpha\beta} \delta(t_1 - t_2) \nabla^2 \delta^{(d)}(x_1 - x_2) , \\ \langle \zeta_\alpha(x_1, t_1) \zeta_\beta(x_2, t_2) \rangle &= 2Du \delta_{\alpha\beta} \delta(t_1 - t_2) \delta^{(d)}(x_1 - x_2) . \end{aligned} \quad (2.7)$$

The corresponding Janssen–De Dominicis response functional becomes [11, 12]

$$\begin{aligned} \mathcal{A}[\tilde{m}_\alpha, \tilde{n}_\alpha, m_\alpha, n_\alpha] &= \int dt d^d x \left[\tilde{m}_\alpha (\partial_t - \lambda \nabla^2) m_\alpha + \tilde{n}_\alpha (\partial_t - D \nabla^2) n_\alpha - Du \tilde{n}_\alpha \tilde{n}_\alpha \right. \\ &\quad \left. + \lambda u \tilde{m}_\alpha \nabla^2 \tilde{m}_\alpha + c \epsilon_{\alpha\beta\gamma} (\tilde{n}_\alpha n_\beta m_\gamma - \tilde{m}_\alpha n_\beta \nabla^2 n_\gamma) \right] , \end{aligned} \quad (2.8)$$

and the probability distribution $P[\vec{m}, \vec{n}]$ for any specific configuration $m_\alpha(x, t)$, $n_\alpha(x, t)$ is

$$P[\vec{m}, \vec{n}] \propto \delta(\vec{n}^2 - 1) \int \mathcal{D}[i\tilde{m}_\alpha, i\tilde{n}_\alpha] e^{-\mathcal{A}[\tilde{m}_\alpha, \tilde{n}_\alpha, m_\alpha, n_\alpha]} . \quad (2.9)$$

As a consequence of the stringent local constraint $\vec{n}(x, t)^2 = 1$, only two components of the three-dimensional order parameter field $\vec{n} = (\vec{\pi}, \sigma)$ are independent, while the third one is completely determined, $\sigma^2 = 1 - \vec{\pi}^2$. One may thus integrate out the “longitudinal” σ mode and only consider the “transverse” $\vec{\pi}$ fluctuations. In order to properly implement the constraint in the ensuing stochastic dynamics, one also needs to impose the noise field for the order parameter $\vec{\zeta}$ to be perpendicular to the instantaneous order parameter itself. In the framework of the associated Janssen–De Dominicis functional this implies $\tilde{n}_\alpha n_\alpha = 0$ [63, 64].

Deep in the ordered phase, the transverse Goldstone mode fluctuations $\vec{\pi}^2$ should be small and one may expand

$$\begin{aligned} \sigma &= \sqrt{1 - \vec{\pi}^2} = 1 - \frac{\vec{\pi}^2}{2} + \mathcal{O}(\pi^4) , \\ \tilde{\sigma} &= -\tilde{\pi}_i \pi_i / \sqrt{1 - \vec{\pi}^2} = -\tilde{\pi}_i \pi_i - \frac{1}{2} \tilde{\pi}_i \pi_i \vec{\pi}^2 + \mathcal{O}(\pi^4) \end{aligned} \quad (2.10)$$

(where $i = 1, 2$), which allows the elimination of the σ component and the associated $\tilde{\sigma}$ field. The resulting Janssen–De Dominicis functional becomes $\mathcal{A} = \mathcal{A}_h + \mathcal{A}_{\text{int}}$ with

$$\begin{aligned} \mathcal{A}_h &= \int_{t,x} \left[\tilde{m}_i (\partial_t - \lambda \nabla^2) m_i + \tilde{m}_3 (\partial_t - \Gamma \nabla^2) m_3 - c \epsilon_{ij} \tilde{\pi}_i m_j + c \epsilon_{ij} \tilde{m}_i \nabla^2 \pi_j - c \tilde{h} \epsilon_{ij} \tilde{m}_i \pi_j \right. \\ &\quad \left. + \tilde{\pi}_i (\partial_t - D \nabla^2 + D \tilde{h}) \pi_i - Du \tilde{\pi}_i \tilde{\pi}_i + \lambda u \tilde{m}_i \nabla^2 \tilde{m}_i + \Gamma u \tilde{m}_3 \nabla^2 \tilde{m}_3 + \mathcal{O}(\pi^4) \right] \end{aligned} \quad (2.11)$$

and

$$\begin{aligned} \mathcal{A}_{\text{int}} = \int_{t,x} & \left[\frac{\tilde{\pi}_i \pi_i}{2} \left(\partial_t - D \nabla^2 + D \tilde{h} \right) \vec{\pi}^2 - Du(\tilde{\pi}_i \pi_i)^2 + c \epsilon_{ij} \tilde{\pi}_i \pi_j m_3 - c \epsilon_{ij} \tilde{m}_3 \pi_i \nabla^2 \pi_j \right. \\ & \left. - c \epsilon_{ij} (\tilde{\pi}_k \pi_k) \pi_i m_j + \frac{c \epsilon_{ij}}{2} \tilde{\pi}_i m_j \vec{\pi}^2 - \frac{c \epsilon_{ij}}{2} (\tilde{m}_i \nabla^2 \pi_j) \vec{\pi}^2 + \frac{c \epsilon_{ij}}{2} \tilde{m}_i \pi_j \nabla^2 \vec{\pi}^2 + \mathcal{O}(\pi^4) \right], \end{aligned} \quad (2.12)$$

where $\int_{t,x} \dots = \int dt d^d x \dots$ and $i, j, k = 1, 2$.

A cutoff in the $\vec{\pi}^2$ expansion naturally introduces explicit symmetry breaking and manifestly leaves us in the ordered phase region, which is governed by a so-called coexistence RG fixed point [68]. The explicit symmetry breaking induces anisotropy for the different order parameter components. In anticipation of different renormalizations for the transverse and longitudinal components of the conserved magnetization, we thus introduce a distinct diffusivity Γ for the m_3 component of the magnetization density. Yet this explicit symmetry breaking is expected to be resolved by the RG flow upon approaching the critical point, where one should recover $\Gamma = \lambda$.

2.2.2 Dynamic Response Functions

To retrieve the dynamical response functions for our model, we introduce source terms to $\vec{\pi}$ and $\vec{M}$ in the Hamiltonian (2.2)

$$\mathcal{H}_s[\vec{M}, \vec{\pi}] = - \int d^d x \left(\rho J_i \pi_i + c M_\alpha H_\alpha \right), \quad (2.13)$$

where $i = 1, 2$ and $\alpha = 1, 2, 3$. The thus induced source terms in the Janssen–De Dominicis functional are

$$\begin{aligned} \mathcal{A}_s = \int_{t,x} & \left[\lambda \tilde{m}_i \nabla^2 H_i + \Gamma \tilde{m}_3 \nabla^2 H_3 - D \tilde{\pi}_i J_i - c \tilde{m}_3 \epsilon_{ij} \pi_i J_j + c \epsilon_{ij} \tilde{m}_i J_j - \frac{c \epsilon_{ij}}{2} \tilde{m}_i J_j \vec{\pi}^2 \right. \\ & \left. - c \epsilon_{ij} \tilde{\pi}_i \pi_j H_3 + c (\tilde{\pi}_k \pi_k) \epsilon_{ij} \pi_i H_j + c \epsilon_{ij} \tilde{\pi}_i H_j - \frac{c \epsilon_{ij}}{2} \tilde{\pi}_i H_j \vec{\pi}^2 - c \epsilon_{ij} \tilde{m}_i m_j H_3 \right. \\ & \left. + c \epsilon_{ij} \tilde{m}_i H_j m_3 - c \tilde{m}_3 \epsilon_{ij} m_i H_j + \mathcal{O}(\pi^4) \right]. \end{aligned} \quad (2.14)$$

With the usual definition of the dynamical response functions

$$\begin{aligned} \chi_{ij}(x, t; x', t') &= \left. \frac{\delta \langle \pi_i(x, t) \rangle_s}{\delta J_j(x', t')} \right|_{H=0, J=0}, \\ R_{ij}(x, t; x', t') &= \left. \frac{\delta \langle m_i(x, t) \rangle_s}{\delta H_j(x', t')} \right|_{H=0, J=0}, \quad R_{\parallel}(x, t; x', t') = \left. \frac{\delta \langle m_3(x, t) \rangle_s}{\delta H_3(x', t')} \right|_{H=0, J=0}, \end{aligned} \quad (2.15)$$

and the probability distribution given by the Janssen–De Dominicis functional, one may express the response functions in terms of the correlation functions in the field theory,

$$\begin{aligned}
\chi_{ij}(x, t; x', t') &= D \langle \pi_i(x, t) \tilde{\pi}_j(x', t') \rangle + c \epsilon_{kj} \langle \pi_i(x, t) [\tilde{m}_3 \pi_k](x', t') \rangle - c \epsilon_{kj} \langle \pi_i(x, t) \tilde{m}_k(x', t') \rangle \\
&\quad + \frac{c}{2} \epsilon_{kj} \langle \pi_i(x, t) [\tilde{m}_k \vec{\pi}^2](x', t') \rangle + \mathcal{O}(\pi^4) , \\
R_{ij}(x, t; x', t') &= -\lambda \langle m_i(x, t) \nabla^2 \tilde{m}_j(x', t') \rangle - c \epsilon_{kj} \langle m_i(x, t) [\tilde{\pi}_l \pi_l \pi_k](x', t') \rangle \\
&\quad + \frac{c}{2} \epsilon_{kj} \langle m_i(x, t) [\tilde{\pi}_k \vec{\pi}^2](x', t') \rangle - c \epsilon_{kj} \langle m_i(x, t) [\tilde{m}_k m_3](x', t') \rangle \\
&\quad + c \epsilon_{kj} \langle m_i(x, t) [\tilde{m}_3 m_k](x', t') \rangle - c \epsilon_{kj} \langle m_i(x, t) \tilde{\pi}_k(x', t') \rangle + \mathcal{O}(\pi^4) , \\
R_{\parallel}(x, t; x', t') &= -\Gamma \langle m_3(x, t) \nabla^2 \tilde{m}_3(x', t') \rangle + c \epsilon_{ij} \langle m_3(x, t) [\tilde{m}_i m_j](x', t') \rangle \\
&\quad + c \epsilon_{ij} \langle m_3(x, t) [\tilde{\pi}_i \pi_j](x', t') \rangle + \mathcal{O}(\pi^4) .
\end{aligned} \tag{2.16}$$

We note that the correlation functions with subscript s are calculated in the presence of external source terms, while the correlation functions without subscripts are calculated without external sources.

We have evaluated the dynamical response functions to one-loop order with respect to the transverse fields, which corresponds to a first-order perturbation in the effective temperature u for the statics and the parameter $u c^2$ for dynamical quantities. By means of a Dyson equation resummation of the one-loop order results, the dynamical susceptibilities can be written in the following compact form [67],

$$\begin{aligned}
\chi_{ij}(p, \omega) &= \delta_{ij} \chi(p, 0) \left[1 + \frac{i\omega}{-i\omega + \Delta(p, \omega) + C(p, \omega)^2 / [-i\omega + \Lambda(p, \omega)]} \right] , \\
R_{ij}(p, \omega) &= \delta_{ij} R(p, 0) \left[1 + \frac{i\omega}{-i\omega + \Lambda(p, \omega) + C(p, \omega)^2 / [-i\omega + \Delta(p, \omega)]} \right] , \\
R_{\parallel}(p, \omega) &= \frac{\Lambda_{\parallel}(p, \omega)}{-i\omega + \Lambda_{\parallel}(p, \omega)} ;
\end{aligned} \tag{2.17}$$

some additional computation details can be found in Appendix A. Here we have used the static susceptibilities

$$\chi(p, 0) = \frac{1}{p^2 + \tilde{h}} \left[1 - u \int_k \frac{1}{k^2 + \tilde{h}} \right] , \quad R(p, 0) = 1 , \tag{2.18}$$

with $\int_k \dots = \int \dots d^d k / (2\pi^d)$ and introduced the abbreviations

$$\begin{aligned}
 C(p, \omega) &= c(p^2 + \tilde{h})^{1/2} \left[1 - \frac{u}{2} \int_k \frac{1}{k^2 + \tilde{h}} \right], \quad \Lambda(p, \omega) = \lambda p^2, \\
 \Delta(p, \omega) &= D(p^2 + \tilde{h}) - D(p^2 + \tilde{h}) \frac{c^2 u}{D} \int_k \frac{1}{k^2 + \tilde{h}} \\
 &\quad \times \frac{i\omega - \Gamma(p-k)^2 - \lambda k^2}{[-i\omega + i\omega_+(k) + \Gamma(p-k)^2] [-i\omega + i\omega_-(k) + \Gamma(p-k)^2]}, \\
 \Lambda_{\parallel}(p, \omega) &= \Gamma p^2 - 2c^2 u \int_k \frac{[k^2 - (p-k)^2] [i\omega - \lambda k^2 - D(p-k)^2 - D\tilde{h}]}{(k^2 + \tilde{h}) [(p-k)^2 - \tilde{h}] [\omega - \omega_+(k) - \omega_+(p-k)]} \\
 &\quad \times \frac{[i\omega - \lambda(p-k)^2 - D\tilde{h}] [i\omega - \lambda k^2 - \lambda(p-k)^2] + 2c^2(k^2 + \tilde{h})}{[\omega - \omega_-(k) - \omega_+(p-k)] [\omega - \omega_-(k) - \omega_-(p-k)] [\omega - \omega_+(k) - \omega_-(p-k)]}, \tag{2.19}
 \end{aligned}$$

with the Gaussian (mean-field) spin wave dispersion relation

$$\omega_{\pm}(p) = -\frac{i}{2} \left[(D + \lambda) p^2 + D\tilde{h} \right] \pm \sqrt{c^2(p^2 + \tilde{h}) - \frac{1}{4} \left[(D - \lambda) p^2 + D\tilde{h} \right]^2}. \tag{2.20}$$

In the limit $\omega \rightarrow 0$, the static response functions are recovered. Thus, the dynamics is cleanly separable from the statics. From the results (2.19), we also see that in comparison with the SSS model in the ordered phase [67], all contributions from transverse magnetization fluctuations are absent, as a result of the truncated $\vec{\pi}^2$ expansion.

2.3 Dimensional ϵ Expansion and Scaling Properties

In this section, we will implement the dimensional ϵ expansion to approach the scaling behavior near RG fixed points. We start by explaining why a straightforward $d = 2 + \epsilon$ expansion as appropriate for the static behavior of the nonlinear sigma model fails to capture its dynamics in the vicinity of the critical fixed point. We then explore the dynamical scaling behavior at the ordered “coexistence” phase fixed point with an $\epsilon = 4 - d$ expansion near the model’s dynamical upper critical dimension, and subsequently discuss the intriguing crossover features of the ensuing RG flows.

2.3.1 Failure of the (Static) $2 + \epsilon$ Expansion at the Critical Fixed Point

In the static nonlinear sigma model, it is well-known that perturbatively the transverse fluctuation loops scale according to $\vec{\pi}^2 \propto u \sim T$ and consequently the $\epsilon = d - 2$ expansion

corresponds to a low-temperature expansion about the critical temperature $T_c = 0$ in two dimensions. The effective temperature u has scaling dimension ϵ , which suggests it is marginal near the model's *lower* critical dimension $d_{lc} = 2$. Therefore, the standard procedure to perturbatively access the critical behavior of the nonlinear sigma model relies on an ϵ expansion near $d_{lc} = 2$. However, the effective dynamical coupling for the reversible mode-coupling terms is $c^2 u$, as can be inferred from Eq. (2.19). Its naive scaling dimension is $[c^2 u] = 4 - d$, resulting in a dynamical *upper* critical dimension $d_c = 4$.

At dimension $d = 2 + \epsilon$, we have $[c^2 u] = 2 - \epsilon$, which is relevant in the infrared scaling regime, and hence will tend to infinity under RG scale transformations near $d_{lc} = 2$. If instead we start near the upper critical dimension $d_c = 4$, setting $d = 4 - \epsilon$, the scaling dimension of the static expansion parameter u becomes $\epsilon - 2$, which is irrelevant in the infrared. Yet in the static nonlinear sigma model, information about the asymptotic infrared scaling behavior is extracted from an ultraviolet-stable RG fixed point that controls the short-distance divergences for $d > d_{lc} = 2$. For the static ultraviolet fixed point, near dimension $d_c = 4$, however, the parameter u becomes relevant. Thus, a standard, straightforward truncation over $\vec{\pi}^2 \propto u$ is improper as the corresponding perturbative expansion diverges near $d_c = 4$, and cannot be controlled at that static fixed point. In order to properly retrieve the scaling information near the ultraviolet RG fixed point near dimension $d_c = 4$, we would need to apply a resummation of all diagrams related to the $\vec{\pi}^2$ expansion, which appears to be unfeasible with currently available tools.

In conclusion, in stark contrast with its counterpart with purely relaxational kinetics, the dynamical critical behavior of the nonlinear sigma model with reversible mode-coupling terms cannot be simultaneously analyzed along with the static critical properties by means of a perturbative dimensional expansion either near $d_{lc} = 2$ or $d_c = 4$.

2.3.2 Scaling Behavior Near the Ordered Phase Coexistence Fixed Point

In the low-temperature phase with spontaneously broken rotational symmetry $O(n)$, the vectorial order parameter separates into an “Anderson–Higgs” mode σ and $n - 1$ massless Goldstone modes $\vec{\pi}$. We note, though, that the Higgs mode appears massive only in the mean-field (Gaussian) approximation, and below $d_c = 4$ is rendered massless too as a consequence of its coupling to the strong transverse fluctuations [68, 69, 70, 71, 72]. In an infinite system, the massless Goldstone modes induce universal static and dynamic scaling behavior that is distinct from the critical scaling properties. This coexistence limit is captured in the RG treatment by an infrared-stable zero-temperature coexistence fixed point. We thus anticipate novel universal scaling behavior for the massless Goldstone modes as well as the conserved magnetization density component that is dynamically coupled to the transverse order parameter fluctuations. In the following, we study the scaling behavior of the antiferromagnetic nonlinear sigma model with reversible mode couplings near this ordered phase

fixed point.

To reach the coexistence fixed point, we need to tune the effective temperature $u \rightarrow 0$ and work in a dimensional $\epsilon = 4 - d$ expansion near the upper critical dimension $d_c = 4$. However, since c^2 also scales as we approach the fixed point and the effective dynamical mode coupling parameter $g^2 = c^2 u$ becomes marginal near four dimensions, we need to keep g^2 fixed when we set $u = 0$. In this low-temperature coexistence regime, we define the multiplicative renormalization Z factors that are to absorb the ensuing ultraviolet divergences as follows,

$$D_R = Z_D D, \quad \lambda_R = Z_\lambda \lambda, \quad \Gamma_R = Z_\Gamma \Gamma, \quad g_R^2 = Z_g g^2 A_d \mu^{-\epsilon}, \quad c_R^2 = Z_c c^2 \mu^{-2}, \quad (2.21)$$

where μ labels an arbitrary momentum scale at which this renormalization is carried out, and $A_d = \Gamma(3 - d/2)/2^{d-1}\pi^{d/2}$ is a geometric factor. Our choice of the normalization point, which only must reside outside the infrared-singular region, lies at $\tilde{h} = 0$, $p = 0$, and $C(p, \omega)\sqrt{R(p, 0)\chi(p, 0)} = c\mu$ [67].

To one-loop order, the Z factors can then be inferred from the explicit expressions (2.19), which yields

$$\begin{aligned} Z_\lambda &= Z_g = Z_c = 1, \\ Z_\Gamma &= 1 + \frac{f}{2(1+w)} \frac{A_d \mu^{-\epsilon}}{\epsilon} \left[w + \left(1 + \frac{c^2}{D\lambda\mu^2} \right)^{-\epsilon/2} \right], \\ Z_D &= 1 + \frac{f}{1+v} \frac{A_d \mu^{-\epsilon}}{\epsilon} \left[1 + \frac{c^2}{(\Gamma + D)(\Gamma + \lambda)\mu^2} \right]^{-\epsilon/2}, \end{aligned} \quad (2.22)$$

where for convenience we have defined the dimensionless ratios of relaxation times w, v and the effective mode coupling strength f as

$$w = D/\lambda, \quad v = D/\Gamma, \quad f = g^2/D\Gamma. \quad (2.23)$$

The scale-dependent anomalous dimensions (Wilson's RG flow functions) thus follow

$$\begin{aligned} \zeta_\lambda &= \mu \frac{\partial}{\partial \mu} \bigg|_0 \ln \frac{\lambda_R}{\lambda} = \mu \frac{\partial}{\partial \mu} \bigg|_0 \ln Z_\lambda = 0, \\ \zeta_g &= \mu \frac{\partial}{\partial \mu} \bigg|_0 \ln \frac{g_R^2}{g^2} = -\epsilon + \mu \frac{\partial}{\partial \mu} \bigg|_0 \ln Z_g = -\epsilon, \\ \zeta_\Gamma &= \mu \frac{\partial}{\partial \mu} \bigg|_0 \ln \frac{\Gamma_R}{\Gamma} = \mu \frac{\partial}{\partial \mu} \bigg|_0 \ln Z_\Gamma = -\frac{f_R}{2(1+w_R)} \left[w_R + \left(1 + \frac{c_R^2}{D_R \lambda_R} \right)^{-(1+\epsilon/2)} \right], \\ \zeta_D &= \mu \frac{\partial}{\partial \mu} \bigg|_0 \ln \frac{D_R}{D} = \mu \frac{\partial}{\partial \mu} \bigg|_0 \ln Z_D = -\frac{f_R}{1+v_R} \left[1 + \frac{c_R^2}{(\Gamma_R + D_R)(\Gamma_R + \lambda_R)} \right]^{-(1+\epsilon/2)}. \end{aligned} \quad (2.24)$$

These anomalous dimensions enter the fundamental RG equations for the correlation and vertex functions as well as dynamical susceptibilities, which capture the behavior of the

model under the change of renormalization scales [50, 73, 74]. One may then invoke the method of characteristics to solve the RG partial differential equations. By introducing the flow parameter $\mu(l) = \mu l$, the RG equations can be separated into a set of coupled first-order differential flow equations. Though we seem to require many parameters, they are not completely independent from each other, and in the end we merely need the following four independent flow equations to describe the entire RG flow of the system,

$$\begin{aligned} l \frac{df(l)}{dl} &= \beta_f(l) = f(l) \left[\zeta_g(l) - \zeta_D(l) - \zeta_\Gamma(l) \right] , \\ l \frac{dc^2(l)}{dl} &= -2c^2(l) , \\ l \frac{dD(l)}{dl} &= D(l) \zeta_D(l) , \quad l \frac{d\Gamma(l)}{dl} = \Gamma(l) \zeta_\Gamma(l) , \end{aligned} \quad (2.25)$$

where the dependence of the RG zeta functions on the flow parameter l stems from the l -dependence of all the parameters on the r.h.s. of Eqs. (2.24). In terms of the anomalous dimensions, the scale-dependent effective dynamical exponents can be defined via

$$z_\lambda(l) = 2, \quad z_\Gamma(l) = 2 + \zeta_\Gamma(l), \quad z_D(l) = 2 + \zeta_D(l). \quad (2.26)$$

Since the transverse magnetization diffusivity λ acquires no fluctuation correction at one-loop order, the dynamic exponent for the perpendicular direction of the magnetization density retains its Gaussian value $z_\lambda = 2$, indicating standard diffusive relaxation.

The flow equation for the renormalized spin wave speed is immediately solved by $c(l) = c(1)/l$ with $c(1) = c_R$. Consequently, three distinct fixed points affect the RG flows: (i) The Gaussian fixed point $f_G^* = 0$ with mean-field dynamic scaling exponents $z_D = z_\lambda = z_\Gamma = 2$ is infrared-unstable (in the f direction) below the upper critical dimension $d_c = 4$, but governs the ultraviolet region for large $l > 100$.

(ii) Setting $c_R = 0$, we obtain the (quasi-)critical fixed point, albeit with the Anderson–Higgs mode “frozen”: In contrast with the Landau–Ginzburg–Wilson Hamiltonian, the nonlinear sigma model does not permit independent longitudinal fluctuations in the σ field. Eqs. (2.24) reduce to $\zeta_\Gamma = -f_R/2$, $\zeta_D = -f_R/(1 + v_R)$, and the existence of a nontrivial, finite mode coupling fixed point $0 < f^* < \infty$ requires the square bracket in the RG beta function β_f to vanish, which implies $-\zeta_\Gamma^* - \zeta_D^* = -\zeta_g^* = \epsilon$. The dimensionless relaxation time scale ratio v is governed by the beta function $\beta_v = v(\zeta_D - \zeta_\Gamma)$, implying for $v^* > 0$ strong dynamic scaling with $\zeta_D^* = \zeta_\Gamma^* = -\epsilon/2$. This leads to the one-loop fixed point values $v_c^* = 1$ and $f_c^* = \epsilon$, and $z_c = 2 - \epsilon/2 = d/2$. Note that these correspond to the critical fixed point of the n -component SSS model (with strong dynamic scaling) $v_c^* = 2n - 3$ and $f_c^* = \epsilon$ [49, 50, 56] for $n = 2$, i.e., effectively the planar model E [75], *not* the three-component model G applicable to the critical dynamics of isotropic Heisenberg antiferromagnets [51, 75, 76]. This reflects the suppressed longitudinal σ fluctuations; but since the dynamical critical exponent is in fact independent of n , the system appears to recover the correct critical scaling properties.

(iii) Finally for $c(1) = c_R > 0$, the RG flows asymptotically reach the coexistence fixed point as $l \rightarrow 0$, which governs the universal scaling behavior in the ordered phase at long wavelengths and low frequencies. With $c(l) = c(1)/l \rightarrow \infty$, we have $\zeta_\Gamma = -f_R w_R / [2(1 + w_R)]$ and $\zeta_D = 0$. Consequently $v_o^* = 0$, whereas w_R assumes a non-universal value that is determined by the initial conditions of the RG flow. A nontrivial RG fixed point value $0 < f_o^* < \infty$ now requires $-\zeta_\Gamma^* = \epsilon$, whence the modified effective mode-coupling strength $\tilde{f}_R = f_R w_R / (1 + w_R)$ must assume the universal fixed point value $\tilde{f}^* = 2\epsilon$. The original mode coupling strength f_R however approaches non-universal limiting values as $l \rightarrow 0$. For the associated effective dynamic scaling exponents, we obtain in the coexistence regime

$$z_D = 2, \quad z_\lambda = 2, \quad z_\Gamma = 2 - \epsilon = d - 2. \quad (2.27)$$

We remark that at the upper critical dimension $d_c = 4$, the longitudinal magnetization density would acquire mere logarithmic corrections to its mean-field diffusive relaxation. Near four dimensions, therefore, the crossover to the asymptotic scaling exponent becomes quite slow, as demonstrated in Fig. 2.11 in Appendix C.

For the relaxation coefficients $D(l)$, $\Gamma(l)$ and the associated effective dynamical exponents, we numerically solve the coupled set of flow equations (2.25) in three dimensions ($d = 3$, i.e., $\epsilon = 1$). (In Appendix C, for illustration we depict the RG flow at $d = 3.9$ or $\epsilon = 0.1$, where the perturbation expansion is more assuredly applicable.) The ensuing RG flow for the mode-coupling strength f with different initial values for $c(1)$ is shown in Fig. 2.1. Note that while the initial value was set to $f(1) = 1$, the RG flow was run both towards the ultraviolet regime (large l) as well as the here relevant infrared region $l \rightarrow 0$. We plot the resulting flows of the effective dynamic exponents $z_D(l)$ and $z_\Gamma(l)$ with different initial conditions in Figs. 2.2, 2.3, and 2.4. The RG flows with small initial values $c(1)$ depicted in Figs. 2.1, 2.2, and 2.3 indeed approach this (quasi-)critical fixed point at intermediate scales, but ultimately depart from it, since $c(l) = c(1)/l$ becomes large in the infrared regime $l < 1$.

The explicit numerical solutions of the coupled RG flow equations shown in the figures for $d = 3$ ($\epsilon = 1$) confirm the above stability and scaling analysis near the three distinct RG fixed points. For $l \rightarrow 0$, both scale-dependent effective dynamical exponents $z_D(l)$ (Fig. 2.2) and $z_\Gamma(l)$ (Fig. 2.3) flow to their ordered phase fixed point values $z_D = 2$ and $z_\Gamma = 1$. Thus, both dynamical exponents of the transverse components of the order parameter and magnetization density are $z_D = z_\lambda = 2$ in the coexistence limit, indicating purely diffusive behavior. In contrast, the dynamical scaling exponent of the longitudinal magnetization density z_Γ acquires nontrivial fluctuation corrections and anomalous, sub-diffusive relaxation: m_3 decouples from the perpendicular components of the magnetization density, but its coupling to the transverse order parameter fluctuations, i.e., the massless Goldstone modes, yields $z_\Gamma = d - 2$, implying linear scaling in three dimensions. These findings are consistent with the corresponding analysis of the SSS model in the ordered phase [67]. In addition, for small initial $c(1)$ values, the RG flows remarkably recover the correct critical dynamical exponent. Although we know that we cannot truly capture the critical regime of the nonlinear sigma

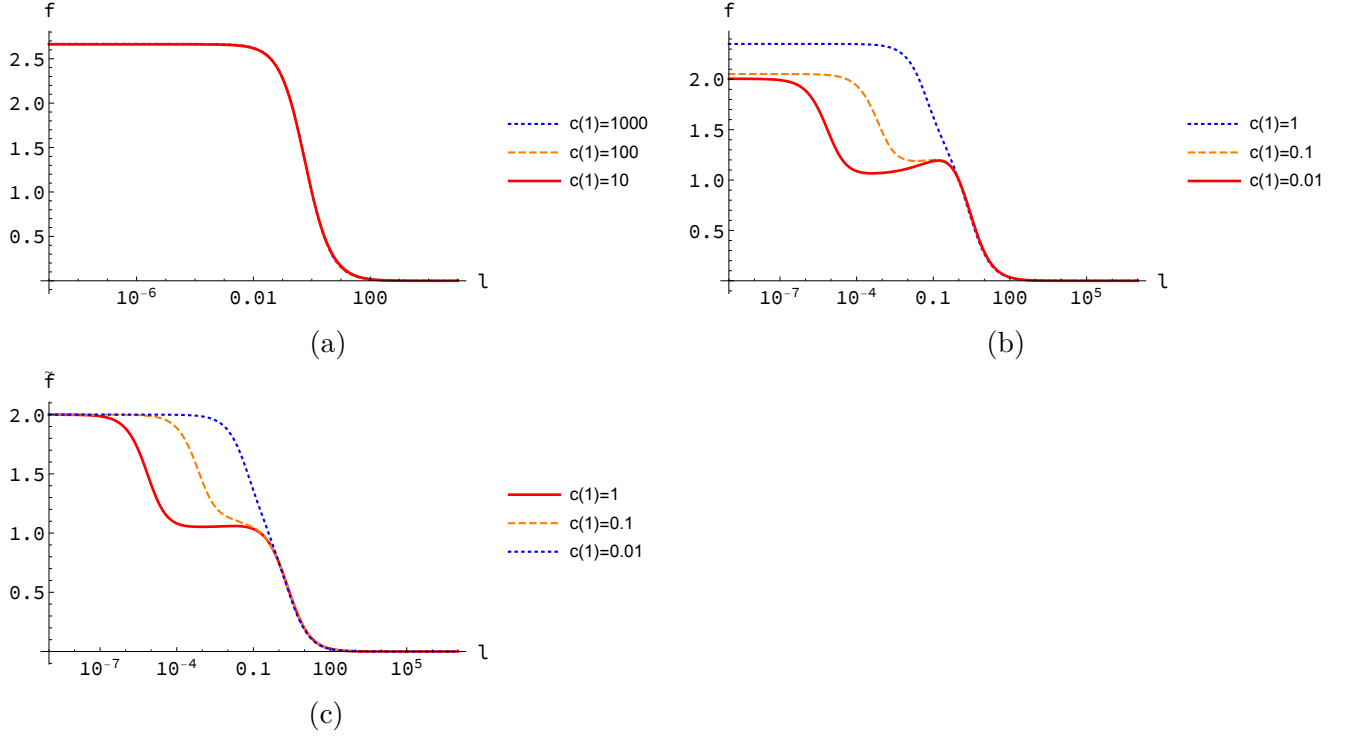


Figure 2.1: RG flow of the effective mode-coupling strength $f(l)$ with initial values $f(1) = 1$, $D(1) = 3$, $\Gamma(1) = 1$, $\lambda(1) = \lambda_R = 1$, and different initial values for $c(1)$ as indicated, in $d = 3$ dimensions, i.e., for $\epsilon = 1$. For large $c(1) \gg 1$ (a), one observes a direct crossover from the unstable Gaussian to the stable coexistence fixed point as $l \rightarrow 0$ (all three curves essentially coincide). For small $c(1) \leq 1$ (b), the RG flow first runs into the critical fixed point $f_c^* = \epsilon$, but eventually too approaches the asymptotic coexistence regime describing the scaling properties in the ordered phase. Whereas f approaches a non-universal value in the coexistence limit, the effective modified mode coupling $\tilde{f} = wf/(1+w) \rightarrow 2\epsilon$ universally for arbitrary initial flow conditions (c).

model within the $\epsilon = 4 - d$ expansion about the dynamical upper critical dimension, in both Figs. 2.2 and 2.3 we observe a brief crossover region towards the critical value $z_D = z_\Gamma = d/2$ for $c(1) < 1$. For RG flows initialized with larger $c(1) > 1$, Fig. 2.4 shows that the crossover to the (quasi-)critical regime diminishes gradually and finally disappears. For sufficiently large $c(1)$, the RG flow directly connects the ultraviolet-stable Gaussian fixed point to the infrared-stable ordered phase coexistence fixed point.

Even though the nonlinear sigma model and the SSS model are in the same universality class and acquire the same anomalous dynamical scaling behavior in the coexistence limit, we emphasize again that the underlying mechanisms differ. In the SSS model, the mass of the Anderson–Higgs mode σ flows to infinity under the RG transformations, and the longitudinal order parameter fluctuations hence ultimately become suppressed. In the nonlinear

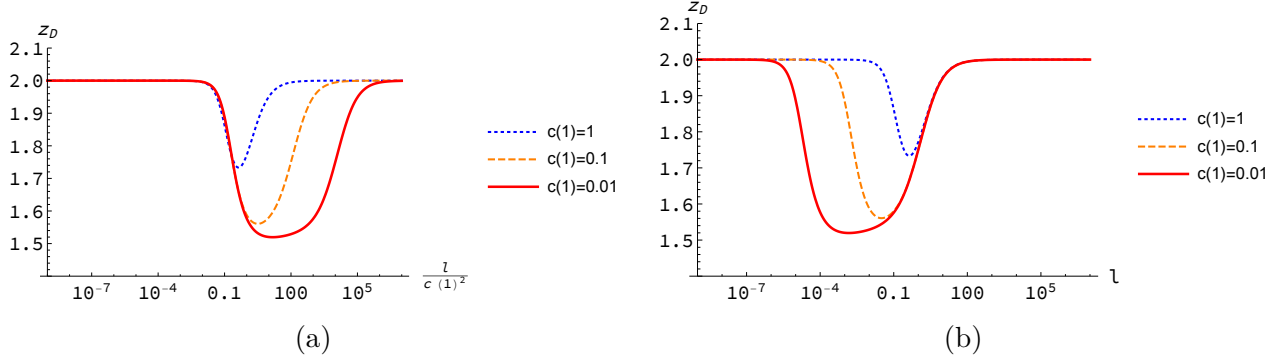


Figure 2.2: RG flow of the effective dynamical exponent $z_D(l)$ for the relaxation of the transverse order parameter components $\vec{\pi}$, with initial conditions $f(1) = 1$, $D(1) = 3$, $\Gamma(1) = 1$, $\lambda(1) = \lambda_R = 1$, and various (small) values of $c(1) = 1, 0.1, 0.01$, for $\epsilon = 1$ ($d = 3$). In (a), the flow parameter l has been rescaled by the initial value $c(1)^2$ to collapse the curves near their approach, as $l \rightarrow 0$, to the coexistence RG fixed point that governs the low-temperature ordered phase. In (b), in contrast the graphs for the same data collapse near the initial Gaussian RG fixed point. Both at the Gaussian and coexistence fixed points, $z_D = 2$; whereas at the critical RG fixed point, $z_D = d/2$.

sigma model, in contrast the magnitude of the order parameter is rigidly fixed. Thus, we can only consider the Goldstone mode $\vec{\pi}$ fluctuations, whereas longitudinal fluctuations are determined by the constraint. Near the ordered phase fixed point, the system is almost frozen and the nonlinear sigma model shows identical asymptotic scaling properties as the SSS model. Yet away from the coexistence fixed point, the RG flows for the various dynamical parameters of these two different models can be quite different.

We conclude this discussion with a schematic diagram of one possible scan across $|q|$ in the temperature–wavenumber space in Fig. 2.5, say in an appropriate (neutron) scattering experiment, which actually corresponds to the RG flow explored above. If we follow the vertical line in the figure, starting in the ordered region for $T < T_c$ with large momentum $|q|$ and subsequently decreasing the wavenumber, we first observe a crossover behavior from the short-distance Gaussian fixed point to critical scaling behavior in the region where $|q|\xi \approx 1$. Upon further decreasing $|q|$, one reaches the ordered phase coexistence scaling region and ultimately detects the crossover from the critical regime to the asymptotic coexistence fixed point. Deep in the antiferromagnetically ordered phase, and at long wavelengths $q \rightarrow 0$, after traversing the crossover region with nontrivial scaling behavior, the spin waves originating from the coupled transverse order parameter fields (Goldstone modes) and transverse magnetization components will be described asymptotically by the mean-field dispersion relation (2.20) with ballistic propagation $\sim c|q|$ and quadratic damping $D(q) \sim \lambda(q) \sim q^2$, albeit with renormalized amplitudes $c, D, \lambda \rightarrow c_R, D_R, \lambda_R$.

However, its nonlinear dynamical coupling to the Goldstone modes induces anomalous scal-

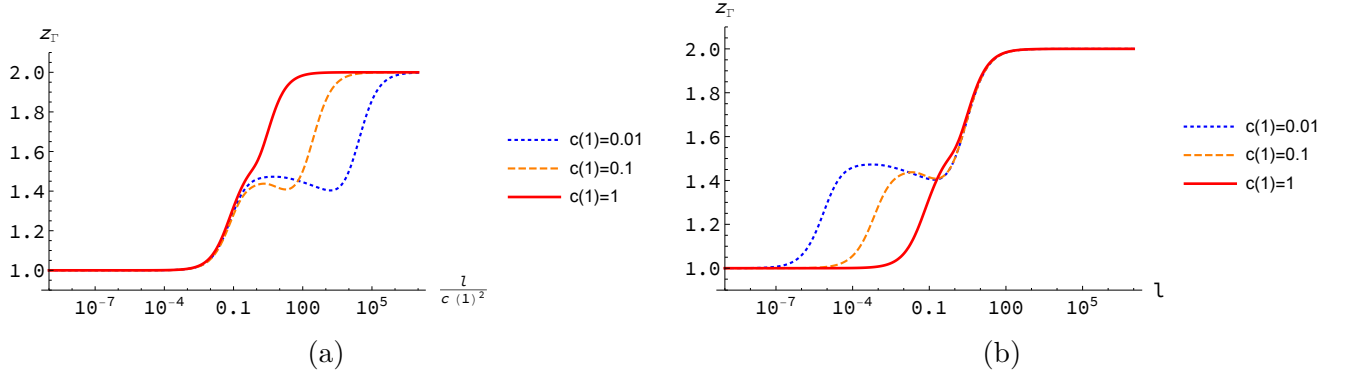


Figure 2.3: RG flow of the effective dynamical exponent $z_\Gamma(l)$ of the longitudinal component of the magnetization density m_3 in $d = 3$ dimensions, with initial values $f(1) = 1$, $D(1) = 3$, $\Gamma(1) = 1$, $\lambda(1) = \lambda_R = 1$, and $c(1)$ as indicated, plotted vs. the flow parameter $l/c(1)^2$ in (a), and vs. l in (b) to demonstrate data collapse in the vicinity of the coexistence and Gaussian fixed points, respectively. At the critical RG fixed point, $z_\Gamma = d/2$; in the ordered phase ($l \rightarrow 0$), the longitudinal magnetization relaxation acquires anomalous sub-diffusive scaling, described by $z_\Gamma = 2 - \epsilon = d - 2$.

ing properties for the longitudinal component m_3 of the conserved magnetization density field, namely the sub-diffusive wavevector dependence of the associated damping coefficient $\Gamma(q) \sim |q|^{z_\Gamma} = |q|^{d-2}$ in d spatial dimensions, i.e., $\Gamma(q) \sim |q|$ for $d = 3$, that replaces the corresponding diffusive mean-field behavior $\sim \Gamma q^2$. In a Lorentzian approximation for the associated dynamical susceptibility $R_\parallel(q, \omega)$ in (2.16), $\Lambda_\parallel(q, \omega) \approx \Gamma(q)$, this nontrivial wavevector scaling directly determines the linewidth of the longitudinal magnetization correlation function $C_\parallel(q, \omega) = (2k_B T / i\omega) \text{Im} R_\parallel(q, \omega)$. This quantity can be measured experimentally through polarized neutron scattering, although extracting the ultimate long-wavelength behavior may be challenging. Alternatively, spin-echo measurement techniques could provide access to the anomalous temporal decay of the longitudinal magnetization autocorrelations $C_\parallel(x=0, t) \sim t^{-d/z_\Gamma} = t^{-d/(d-2)} \sim t^{-3}$ in three dimensions, rather than the mean-field decay $C_\parallel(0, t) \sim t^{-d/2} = t^{-3/2}$ for $d = 3$.

2.4 Summary and Conclusion

In this chapter, we have investigated the critical dynamics of the antiferromagnetic nonlinear sigma model with conserved total magnetization. The Langevin dynamics then involves reversible, hydrodynamic mode-coupling terms. We have investigated the ensuing scaling properties by means of the perturbative field-theoretic RG approach, and computed dynamical response functions of both the order parameter and the magnetization densities to one-loop order. As expected near thermal equilibrium, the response functions show a separation of the dynamics from the statics. There emerges an explicit symmetry breaking between

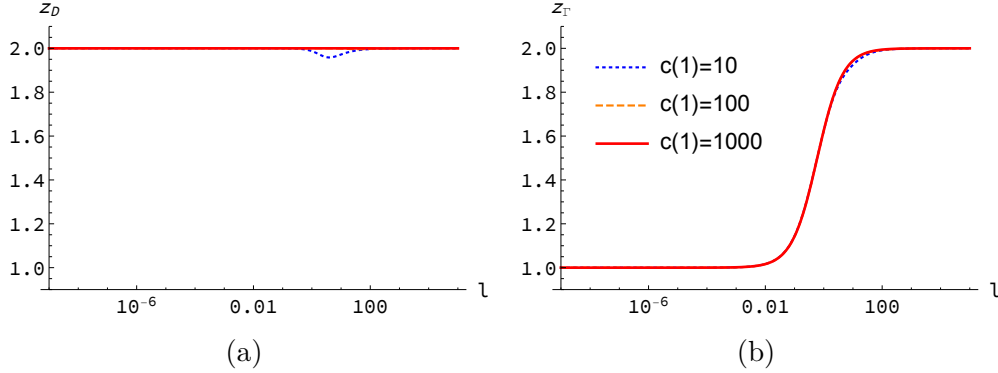


Figure 2.4: RG flow of the dynamic exponents $z_D(l)$ and $z_\Gamma(l)$ with initial conditions $f(1) = 1$, $D(1) = 3$, $\Gamma(1) = 1$, $\lambda(1) = \lambda_R = 1$, and large initial values $c(1) = 10, 100, 1000$. The RG flow is then set far away from the critical point, and bypasses the critical scaling regime entirely.

the response functions of the transverse and longitudinal components of the magnetization density, which suggests that the critical fixed point is no longer approachable in this dynamical nonlinear sigma model variant, since the rotational symmetry cannot be recovered. We have provided a detailed argument from the RG point of view why approaching the critical fixed point is not feasible, at least in this perturbative regime.

We have analyzed the dynamical scaling behavior near the ordered phase RG fixed point that describes the asymptotic coexistence limit via an $\epsilon = 4 - d$ expansion about the dynamical upper critical dimension $d_c = 4$. We find Goldstone-mode induced anomalous sub-diffusive scaling for the longitudinal component of the magnetization. The dynamic exponents at the coexistence ordered phase fixed point coincide with those for the SSS model which is based on a Landau–Ginzburg–Wilson Hamiltonian. We have numerically solved the RG flow equations, and observe that if initiated near the critical point, they display a brief crossover regime towards the critical region, even somewhat fortuitously recovering the correct dynamical critical exponent $z_c = d/2$, before ultimately reaching the coexistence limit with $z_D = z_\lambda = 2$ and $z_\Gamma = d - 2$. These relaxation predictions should be experimentally accessible through the dynamic scaling of neutron scattering linewidths or the temporal decay of the autocorrelation function for the longitudinal magnetization fluctuations.

2.5 Appendix

2.5.1 One-loop Results for Useful Correlation Functions

In this Appendix, we briefly provide more details and intermediate results for the explicit computation of various correlation functions, from which one may obtain the response func-

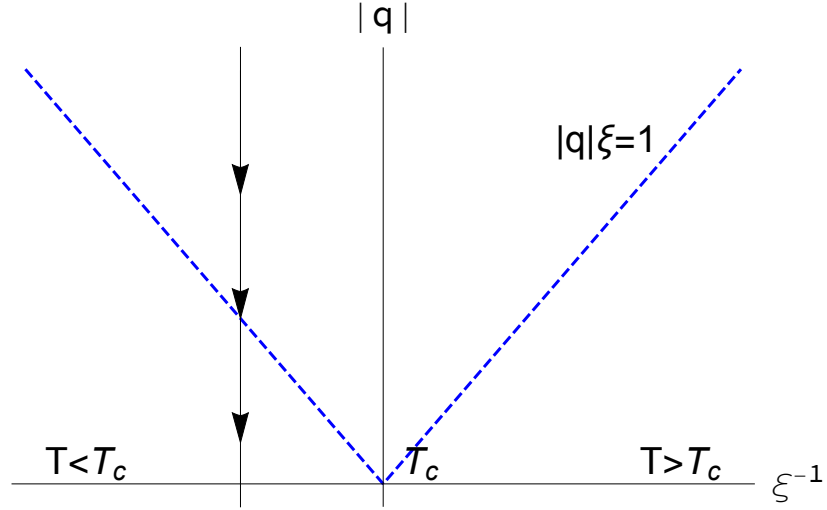


Figure 2.5: Schematic diagram of one RG flow in phase space, corresponding to a wavevector $|q|$ scan in a (neutron) scattering experiment at fixed temperature $T < T_c$.

tions, to one-loop order in the dynamical perturbation expansion. On the tree (mean-field) level, the non-vanishing propagators of the field theory read

$$\begin{aligned}
 \langle \pi_i \tilde{\pi}_j \rangle^{(0)}(p, \omega) &= \delta_{ij} \frac{i\omega - D(p^2 + \tilde{h})}{[\omega - \omega_+(p)][\omega - \omega_-(p)]} , \\
 \langle m_i \tilde{\pi}_j \rangle^{(0)}(p, \omega) &= \epsilon_{ij} \frac{-c(p^2 + \tilde{h})}{[\omega - \omega_+(p)][\omega - \omega_-(p)]} , \\
 \langle m_i \tilde{m}_j \rangle^{(0)}(p, \omega) &= \delta_{ij} \frac{i\omega - \lambda p^2}{[\omega - \omega_+(p)][\omega - \omega_-(p)]} , \\
 \langle \pi_i \tilde{m}_j \rangle^{(0)}(p, \omega) &= \epsilon_{ij} \frac{-c}{[\omega - \omega_+(p)][\omega - \omega_-(p)]} , \\
 \langle m_3 \tilde{m}_3 \rangle^{(0)}(p, \omega) &= \frac{1}{-i\omega + \Gamma p^2} ,
 \end{aligned} \tag{2.28}$$

where we have used the spin wave dispersions (2.20). In our convention, time and hence momentum always flow from right to left in Feynman diagrams.

All one-loop fluctuation corrections to the propagators of the order parameter $\vec{\pi}$ and the propagator of the parallel component of the magnetization density m_3 are plotted in Figs. 2.6 and 2.7. Here, the π , m , and m_3 fields are represented by solid, dashed, and wavy lines, respectively. The one-loop graphs for the propagator of the perpendicular components of the magnetization density m_1, m_2 and the mixed $\pi_i m_j$ propagators have the same loop structures, but just carry different external legs. The explicit results for the one-loop fluctuation corrections to the propagators read

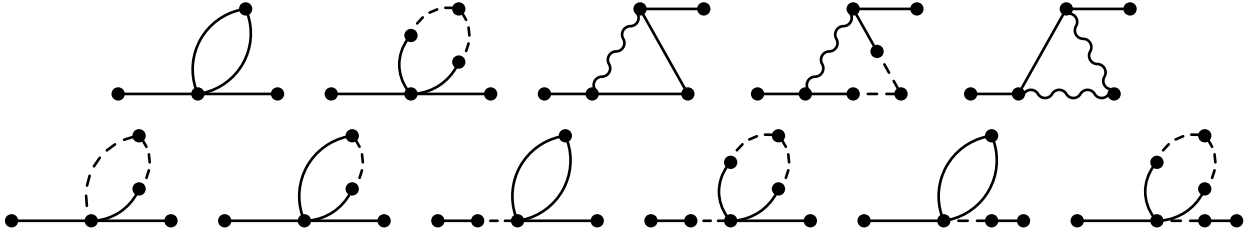


Figure 2.6: One-loop order contributions to $\langle \pi_i \tilde{\pi}_j \rangle$.

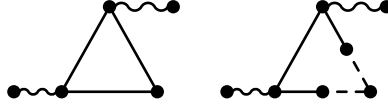


Figure 2.7: One-loop order contributions to $\langle m_3 \tilde{m}_3 \rangle$.

$$\begin{aligned}
 \langle m_i \tilde{m}_j \rangle^{(1)}(p, \omega) &= \delta_{ij} \frac{-c^2(p^2 + \tilde{h})}{[\omega - \omega_+(p)]^2 [\omega - \omega_-(p)]^2} \left[g^2(p^2 + \tilde{h})B(p, \omega) + (i\omega - Dp^2 - D\tilde{h})uA \right], \\
 \langle m_i \tilde{\pi}_j \rangle^{(1)}(p, \omega) &= \epsilon_{ij} \frac{-c(p^2 + \tilde{h})(i\omega - \lambda p^2)}{[\omega - \omega_+(p)]^2 [\omega - \omega_-(p)]^2} \left[g^2(p^2 + \tilde{h})B(p, \omega) + (i\omega - Dp^2 - D\tilde{h})uA \right], \\
 \langle \pi_i \tilde{\pi}_j \rangle^{(1)}(p, \omega) &= \delta_{ij} \frac{(i\omega - \lambda p^2)^2}{[\omega - \omega_+(p)]^2 [\omega - \omega_-(p)]^2} \left[g^2(p^2 + \tilde{h})B(p, \omega) + (i\omega - Dp^2 - D\tilde{h})uA \right], \\
 \langle \pi_i \tilde{m}_j \rangle^{(1)}(p, \omega) &= \epsilon_{ij} \frac{-c(i\omega - \lambda p^2)}{[\omega - \omega_+(p)]^2 [\omega - \omega_-(p)]^2} \left[g^2(p^2 + \tilde{h})B(p, \omega) + (i\omega - Dp^2 - D\tilde{h})uA \right], \\
 \langle m_3 \tilde{m}_3 \rangle^{(1)}(p, \omega) &= \frac{2g^2}{(-i\omega + \Gamma p^2)^2} E(p, \omega),
 \end{aligned} \tag{2.29}$$

where

$$\begin{aligned}
 A &= \int_k \frac{1}{k^2 + \tilde{h}}, \\
 B(p, \omega) &= \int_k \frac{i\omega - \Gamma(p-k)^2 - \lambda k^2}{(k^2 + \tilde{h})[-i\omega + i\omega_+(k) + \Gamma(p-k)^2][-i\omega + i\omega_-(k) + \Gamma(p-k)^2]}, \\
 E(p, \omega) &= - \int_k \frac{[k^2 - (p-k)^2][i\omega - \lambda k^2 - D(p-k)^2 - D\tilde{h}]}{[k^2 + \tilde{h}][(p-k)^2 - \tilde{h}][\omega - \omega_+(k) - \omega_+(p-k)]} \\
 &\quad \times \frac{\left([i\omega - \lambda(p-k)^2 - D\tilde{h}][i\omega - \lambda k^2 - \lambda(p-k)^2] + 2c^2(k^2 + \tilde{h}) \right)}{[\omega - \omega_-(k) - \omega_+(p-k)][\omega - \omega_-(k) - \omega_-(p-k)][\omega - \omega_+(k) - \omega_-(p-k)]}.
 \end{aligned} \tag{2.30}$$

The following relations are obtained by means of explicit calculation, and lead to immediate cancellations in the evaluation of response functions,

$$\begin{aligned}\langle m_i[\tilde{m}_j m_3] \rangle(p, \omega) &= \langle m_i[\tilde{m}_3 m_j] \rangle(p, \omega) , \\ \langle m_i[\tilde{\pi}_k \pi_k \pi_j] \rangle(p, \omega) &= \frac{1}{2} \langle m_i[\tilde{\pi}_j \vec{\pi}^2] \rangle(p, \omega) .\end{aligned}\tag{2.31}$$

The remaining one-loop results for other composite operator correlation functions that appear in the expressions for the dynamical response functions (2.16) are

$$\begin{aligned}\langle \pi_i[\tilde{m}_3 \pi_j] \rangle(p, \omega) &= \epsilon_{ij} u c \frac{i\omega - \lambda p^2}{[\omega - \omega_+(p)][\omega - \omega_-(p)]} B(p, \omega) , \\ \langle \pi_i[\tilde{m}_j \vec{\pi}^2] \rangle(p, \omega) &= \delta_{ij} \frac{2uc}{[\omega - \omega_+(p)][\omega - \omega_-(p)]} A , \\ \langle m_3[\tilde{\pi}_i \pi_j] \rangle(p, \omega) &= \epsilon_{ij} \frac{uc}{-i\omega + \Gamma p^2} E(p, \omega) ,\end{aligned}\tag{2.32}$$

and the associated Feynman diagrams are shown in Figs. 2.8, 2.9, and 2.10.

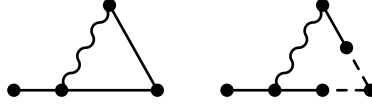


Figure 2.8: One-loop order contributions to $\langle \pi_i[\tilde{m}_3 \pi_j] \rangle$.

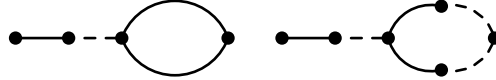


Figure 2.9: One-loop order contributions to $\langle \pi_i[\tilde{m}_j \vec{\pi}^2] \rangle$.

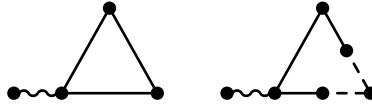


Figure 2.10: One-loop order contributions to $\langle m_3[\tilde{\pi}_i \pi_j] \rangle$.

At last, we may assemble these building blocks to construct the dynamical susceptibilities to one-loop order. The response function for the order parameter components becomes

$$\begin{aligned}\chi_{ij}(p, \omega) &= \delta_{ij} \frac{D(i\omega - \lambda p^2) - c^2}{[\omega - \omega_+(p)][\omega - \omega_-(p)]} \left[1 + \frac{(i\omega - \lambda p^2)(i\omega - Dp^2 - D\tilde{h})}{[\omega - \omega_+(p)][\omega - \omega_-(p)]} uA \right] \\ &+ \delta_{ij} \frac{uc^2}{[\omega - \omega_+(p)][\omega - \omega_-(p)]} \left[A + \frac{i\omega(i\omega - \lambda p^2)^2}{[\omega - \omega_+(p)][\omega - \omega_-(p)]} B(p, \omega) \right] ,\end{aligned}\tag{2.33}$$

while the response function for the perpendicular components of the magnetization density reads

$$R_{ij}(p, \omega) = \delta_{ij} \frac{-D\lambda p^2 (p^2 + \tilde{h}) - c^2 (p^2 + \tilde{h}) + i\omega\lambda p^2}{[\omega - \omega_+(p)][\omega - \omega_-(p)]} + \delta_{ij} \frac{-i\omega c^2 (p^2 + \tilde{h})}{[\omega - \omega_+(p)]^2 [\omega - \omega_-(p)]^2} \quad (2.34)$$

$$\times \left[(i\omega - Dp^2 - D\tilde{h}) uA + (p^2 + \tilde{h}) uc^2 B(p, \omega) \right] ,$$

and the response function for the parallel magnetization density component is

$$R_{\parallel}(p, \omega) = \frac{1}{-i\omega + \Gamma p^2} [\Gamma p^2 - 2g^2 E(p, \omega)] - \frac{2g^2 \Gamma p^2}{(-i\omega + \Gamma p^2)^2} E(p, \omega) . \quad (2.35)$$

Straightforward algebra then yields the expressions (2.17), (2.19) to first order in u .

2.5.2 Nonlinear Sigma Model: Other Dynamical Universality Classes

In this Appendix, we briefly analyze other standard dynamical critical universality classes in the context of the nonlinear sigma model [14, 49, 50]. We shall argue that in fact all other types of universal dynamics imposed on this system turn out either trivial or incompatible with the rigid nonlinear sigma model constraint.

Model C Dynamics

In model C dynamics, one allows for the static coupling of the conserved energy density $\mathcal{E}(x, t)$ to the order parameter. With the thermodynamics of a critical system captured by the Landau–Ginzburg–Wilson effective Hamiltonian, the energy density becomes directly coupled to the square of order parameter, whence the two-point correlation function for the energy density fluctuations $\langle \mathcal{E}\mathcal{E} \rangle$ is proportional to the specific heat C_V , as it should [14]. Yet in the nonlinear sigma model, one imposes the rigid constraint $\vec{n}^2 = 1$. Coupling the energy density to $\vec{n}^2$ in the Hamiltonian through a term $\frac{1}{2}\mathcal{E}(x, t)^2 + g\mathcal{E}(x, t)\vec{n}^2$ thus becomes trivial; the field $\mathcal{E}(x, t)$ may be readily integrated out without any effects on the order parameter fluctuations.

In the hope of incorporating nontrivial fluctuations of the energy density, we could instead consider the static coupling

$$H_C = \frac{1}{2} \int d^d x [\mathcal{E} - g(\nabla \vec{n})^2]^2 . \quad (2.36)$$

Note that this term is quadratic in $\mathcal{E}$ and can be integrated out to show that $\mathcal{E}$ is proportional to $\frac{1}{2}(\nabla \vec{n})^2$, i.e., the Hamiltonian density. However, a naive dimensional analysis then immediately yields that the resulting effective coupling $g^2 u$ has the negative scaling dimension $-d$ and is thus irrelevant in the RG sense. In consequence, near the critical point, the

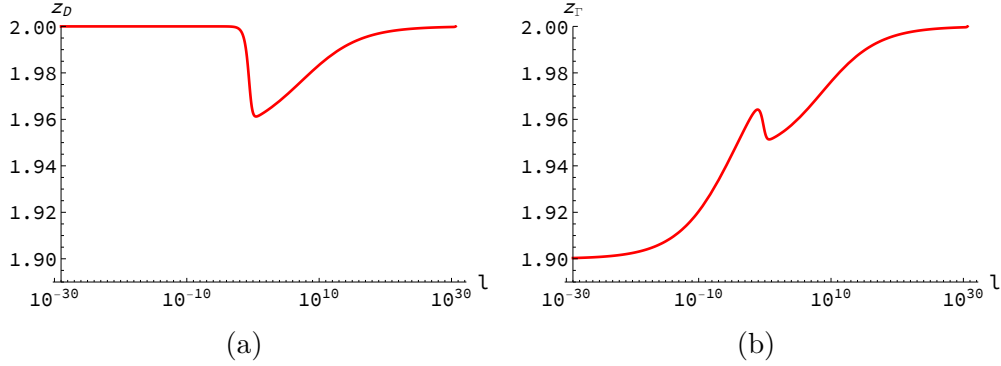


Figure 2.11: RG flow of the effective dynamic exponents $z_D(l)$ and $z_\Gamma(l)$ with the initial conditions $f(1) = 0.1$, $D(1) = 1.5$, $\Gamma(1) = 1$, $\lambda(1) = \lambda_R = 1$, and $c(1) = 1$, for $\epsilon = 0.1$ ($d = 3.9$). Asymptotically as $l \rightarrow 0$, $z_D = 2$ and $z_\Gamma = 2 - \epsilon$; the crossover for the latter to reach the coexistence scaling regime however requires extremely small flow parameter values $l < 10^{-20}$.

system decouples from the energy density. This suggests that the dynamic exponent of the order parameter assumes its model A value $z_n = 2 + c\eta$, while the dynamic scaling exponent for the conserved energy density retains its Gaussian value $z_\epsilon = 2$. This result is consistent with well-established findings from model C critical dynamics based on the $O(n)$ -symmetric Landau–Ginzburg–Wilson theory, namely that for negative specific heat exponent $\alpha < 0$ or vector order parameter component number $n \geq 2$, the energy density asymptotically decouples from the order parameter in any dimension $d > 2$, leading to model A critical scaling for the order parameter [14, 49, 50, 77].

Critical Dynamics with Conserved Order Parameter

In the standard dynamical critical universality classes with conserved total order parameter, i.e., models B, D and J, one requires the total order parameter in the system to be conserved [14]. In the absence of any nonlinear couplings (i.e., the Gaussian approximation), the order parameter field consequently relaxes diffusively. However, to implement the constraint of the nonlinear sigma model, one strictly fixes the σ component and considers only fluctuations of the transverse Goldstone modes $\vec{\pi}$. Yet to be consistent with the conservation law for the total order parameter, one would need to properly eliminate the zero-wavevector fluctuations for all modes, and at finite wavevectors allow diffusive couplings between the longitudinal σ and the transverse $\vec{\pi}$ sectors. Thus, the dynamical universality classes with conserved total order parameter appear inaccessible in the context of the nonlinear sigma model.

2.5.3 Scaling Behavior at $d = 3.9$

We numerically solved the coupled RG flow equations (2.25) for $\epsilon = 0.1$ and plot the ensuing flow of the effective dynamical exponents $z_D(l)$ and $z_\Gamma(l)$ in Fig. 2.11. While of course $d = 3.9$ is not a physically realizable spatial dimension, the ϵ expansion is on safer grounds in this case. However, we observe the same qualitative flow behavior as in three dimensions: Starting from the Gaussian fixed point values on the right, the effective exponents display a brief crossover to their critical values, and subsequently approach their asymptotic ordered-phase fixed point values. The order parameter $\vec{\pi}$ behaves purely diffusively, $z_D = 2$, but the longitudinal magnetization component m_3 acquires nontrivial corrections due to its coupling to the transverse Goldstone modes, and ultimately displays sub-diffusive scaling in the coexistence limit governed by $z_\Gamma = 2 - \epsilon$. Note that the crossover to this asymptotic coexistence scaling behavior happens exceedingly slowly for small values of ϵ , as becomes apparent by the huge range of flow parameters l required to capture the full crossover in Fig. 2.11(b). At $d_c = 4$, this slow power law approach would be replaced by logarithmic corrections to the mean-field diffusive relaxation for the longitudinal magnetization density.

Chapter 3

Coined Quantum Walks on the Line: Disorder, Entanglement and Localization

This chapter is adapted from our publication [78],

Louie Hong Yao and Sascha Wald, “Coined Quantum Walks on the Line: Disorder, Entanglement and Localization”, [arXiv: 2303.15978] (Submitted to Phys. Rev. E)

3.1 Introduction

Quantum walks have shown significant potential in quantum computing applications as a practical tool to build quantum algorithms [6, 79, 80, 81, 82, 83, 84, 85, 86, 87, 88, 89]. Even more so, quantum walks are computationally universal as Childs has shown in his seminal paper [90]. Long-standing results of quantum walks outperforming their classical counterparts, see, e.g., Refs. [84, 85, 91, 92, 93, 94, 95, 96], thus substantiate the promises of quantum technologies to revolutionize real-world applications in the near future, such as high-performance computing or secure communications [97, 98, 99, 100, 101, 102]. Despite continuous progress in quantum computing, arguably two of the most influential quantum algorithms have been developed decades ago, namely Shor’s factorizing algorithm [103] and Grover’s search algorithm [104]. It turns out that designing algorithms with quantum advantage is intricate [105] and thus it is important to properly understand the fundamental building blocks of these algorithms which can be formulated in terms of quantum walks. It is the purpose of this work to explore the influence of disorder on quantum walks. Disorder may arise naturally as undesirable error from faulty quantum operations but could potentially be used as a tailored resource to improve computational performance of quantum algorithms. It is well-established that disordered quantum media may lead to wave localization since the discovery of Anderson localization [15], see also Ref. [106] for a comprehensive overview. The localization phenomenon has been explored in a variety of setups [107, 108, 109, 110, 111, 112, 113, 114, 115], even without disorder [116]. In this work we will explore disorder induced localization in quantum walks and its implications on entanglement properties.

To this end, we are interested in coined quantum walks (CQWs) that are routinely described

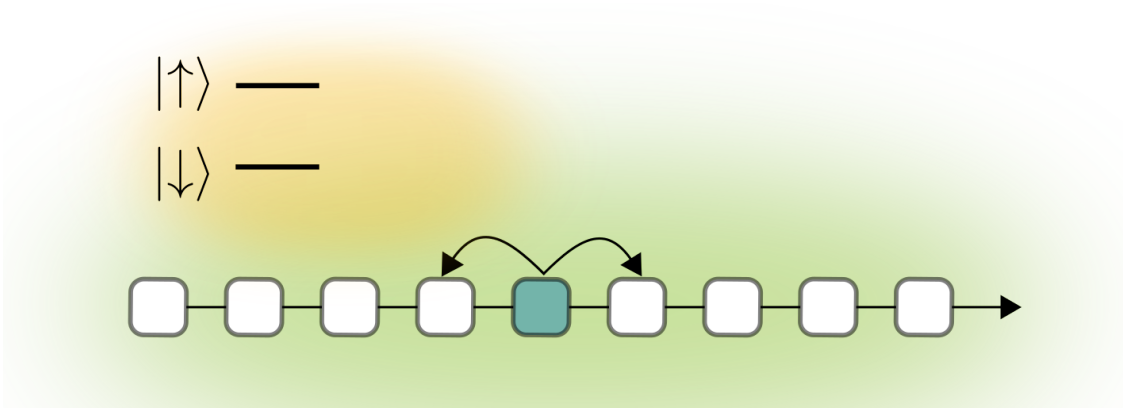


Figure 3.1: **Illustration coined quantum walk.** A CQW is a bipartite quantum system made up from a ‘walker’ and a ‘quantum coin’. The walker is described by a discrete position degree of freedom (green) and the coin is a two-level system (orange). The shading illustrates the wave function of each subsystem with the overlap indicating coin-walker entanglement.

as bipartite quantum system consisting of a ‘walker’ and a ‘quantum coin’, see Fig. 3.1. The walker may occupy sites on a certain geometry (line, circle, general graphs, etc.) and the coin is a two level system¹ whose state determines the walker propagation. Further details will be introduced in section 3.2. CQWs are generalizations of classical random walks to the quantum realm. Similar to a classical random walk on the line, where a coin toss decides whether a walker hops left or right, a quantum coin toss decides how the walker spreads over the lattice. Here we explore the effects of quenched disorder in the quantum coin toss such that the coin differs on different lattice sites.

In contrast to their classical counterparts, CQWs are generally deterministic since the underlying dynamics is unitary. Further differentiating factors are that CQWs occupy several sites simultaneously due to quantum superposition and the coin-walker interaction yields entanglement. It has been argued that the natural classical counterpart of CQWs are classical random walk with one-step memory [117]. This memory may yield faster spreading than a Markovian classical random walk. However, CQWs still spread asymptotically faster, due to quantum interference [117].

Beyond their computational universality, CQWs find applications in, e.g., neural networks to capture the structure of graphs [118, 119]. Here, feature-dependent coins are used at different nodes and CQWs can be used to classify graphs. Hence, varying coin features may be exploited to perform relevant tasks. Similarly, the coin may be used to bias CQWs [120].

¹For CQWs on graphs or higher dimensional geometries, quantum coins with more levels are necessary.

It is thus obvious that the coin operations and states play a fundamental role in the character of CQWs which further motivates our study of quenched coin disorder.

The manuscript is organized as follows. In section 3.2, we introduce CQWs starting from the Hadamard walk. We consider how the wave function of the composite system evolves in time and show the analytical solution of the Hadamard walk. We then introduce the coin disorder and discuss how averages over disorder realizations are taken. In section 3.3, we explore the effects of coin disorder on the quantum state of the bipartite system and the walker occupation probability. We find that the disorder significantly slows down the underlying dynamics and argue that our findings are consistent with a walker localization. We further support this in section 3.4 by considering the entanglement entropy and the entanglement negativity. Both these entanglement witnesses reveal features that substantiate the localization hypothesis. We contrast our results by considering different boundary conditions in section 3.5. In section 3.6, we summarize our results and discuss some interesting future directions. Appendix 3.7.1 follows Ref. [121] to detail how the Hadamard walk is solved in Fourier space.

3.2 The Model

CQWs are bipartite quantum systems made up from a walker and a quantum coin, see Fig. 3.1. Here, we consider arguably the simplest setup where the coin is a two-level system with corresponding coin Hilbert space $\mathcal{H}_c = \text{span}\{|\downarrow\rangle, |\uparrow\rangle\} = \mathbb{C}^2$ and the walker propagates on the infinite line (alterations are readily introduced). Thus, the position x of the walker can take on discrete values $x \in \mathbb{Z}$ and the walker Hilbert space is $\mathcal{H}_w = \text{span}\{|x\rangle \mid x \in \mathbb{Z}\}$. The composite system is described by quantum states residing in the Hilbert space $\mathcal{H} = \mathcal{H}_w \otimes \mathcal{H}_c$. This bipartite system undergoes a two-step discrete-time dynamics as follows. Given a quantum state $|\psi(t)\rangle \in \mathcal{H}$ at time t , first a quantum coin operator C is applied. C is such that, although it acts on the full Hilbert space, the walker occupation probability, i.e.,

$$p_x = |\langle x \uparrow | \psi(t) \rangle|^2 + |\langle x \downarrow | \psi(t) \rangle|^2 \quad (3.1)$$

remain unchanged. Subsequently, a shift operator S is applied that propagates the walker along the line depending of the state of the two-level system, i.e., $|\psi(t+1)\rangle = SC|\psi(t)\rangle$. Time-evolved states are thus deduced from the initial state as

$$|\psi(t)\rangle = (SC)^t |\psi(0)\rangle. \quad (3.2)$$

Arguably the most studied CQW is the Hadamard walk which is defined by the following operators

$$C = \mathbb{1}_w \otimes H = \mathbb{1}_w \otimes \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}, \quad (3.3)$$

$$S = \sum_{x \in \mathbb{Z}} |x+1\rangle \langle x| \otimes |\uparrow\rangle \langle \uparrow| + |x-1\rangle \langle x| \otimes |\downarrow\rangle \langle \downarrow|. \quad (3.4)$$

For the Hadamard walk, each site is equivalent and a ‘fair’ coin toss propagates the walker. The initial coin configuration yields the potential for an underlying drift in the Hadamard walk since the time evolution is unitary. This is usually circumvented by considering

$$|\psi(0)\rangle = |0\rangle \otimes \frac{1}{\sqrt{2}} (|\downarrow\rangle + i|\uparrow\rangle). \quad (3.5)$$

as initial state. The initial coin state is an eigenstate of the Y gate. Since the Hadamard gate is a superposition of the X and the Z gate, this initial coin state ensures that there is no drift and the dynamics is symmetric.

The Hadamard walk and its applications have been extensively studied, see, e.g., Refs. [121, 122, 123, 124, 125] to name a few. Due to the spatial homogeneity of the coin operator, the time-evolved wave function can even be analytically derived [121]. In App. 3.7.1 we recall how to solve the Hadamard walk, following Ref. [121]. For the initial state (3.5) we find

$$\begin{aligned} \langle x \downarrow | \psi(t) \rangle &= \frac{1 + (-1)^{t+x}}{2^{(t+3)/2}} \int_{-\pi}^{\pi} \frac{dk}{2\pi} e^{-ikx} \left(\sqrt{1 + \cos^2 k} - i \sin k \right)^t \\ &\quad \times \left(1 + \frac{\cos k}{\sqrt{1 + \cos^2 k}} + i \frac{e^{-ik}}{\sqrt{1 + \cos^2 k}} \right), \end{aligned} \quad (3.6)$$

$$\begin{aligned} \langle x \uparrow | \psi(t) \rangle &= \frac{1 + (-1)^{t+x}}{2^{(t+3)/2}} \int_{-\pi}^{\pi} \frac{dk}{2\pi} e^{-ikx} \left(\sqrt{1 + \cos^2 k} - i \sin k \right)^t \\ &\quad \times \left(i \left[1 - \frac{\cos k}{\sqrt{1 + \cos^2 k}} \right] + \frac{e^{ik}}{\sqrt{1 + \cos^2 k}} \right). \end{aligned} \quad (3.7)$$

The most salient feature of the walker occupation probability for the Hadamard walk consists of two ballistically propagating peaks emerging from the origin, see Fig. 3.2.

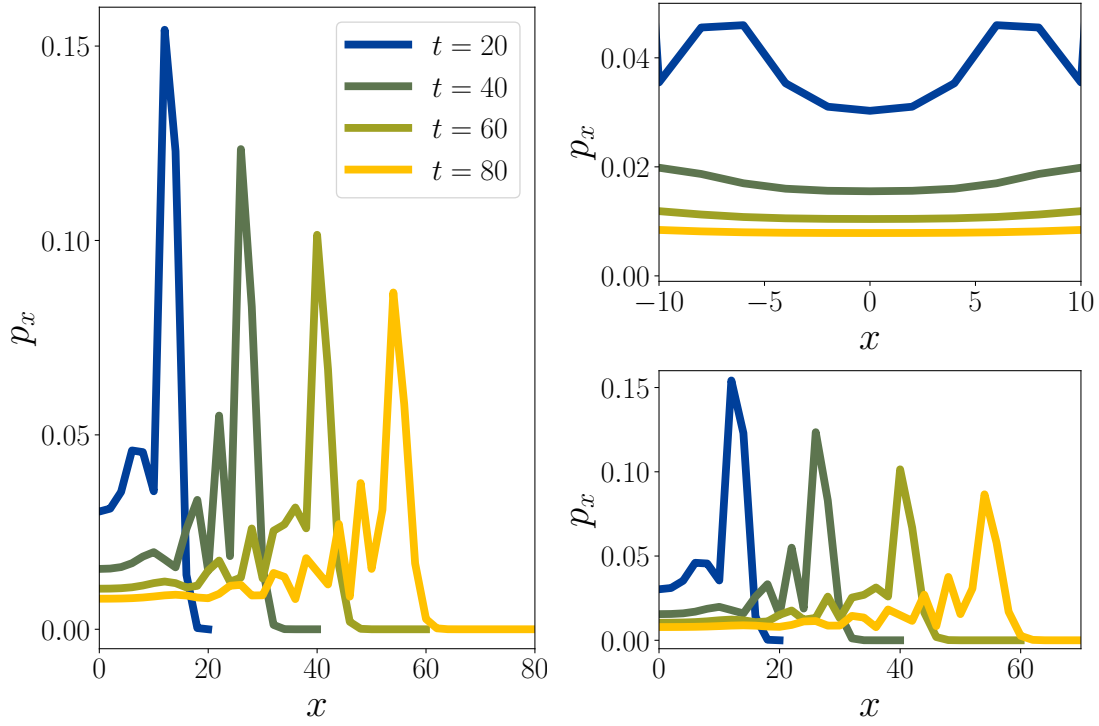


Figure 3.2: **Walker distribution of the Hadamard walk.** The left panel shows the occupation probability p_x for different times $t = 20, 40, 60, 80$ for a Hadamard walk with the initial state (3.5). The upper right panel illustrates the vanishing center probability p_0 and how the distribution flattens with time. The lower right panel shows the travelling peaks. These results are obtained from the simulation of Eq. (3.2).

The width of these peaks scales asymptotically as $O(t^{1/3})$ and between the peaks the wave function is essentially uniformly distributed [121]. Over time, coin and walker become entangled. This entanglement can be quantified by the entanglement entropy (EE), viz.,

$$S = -\text{tr} \rho_c \ln \rho_c. \quad (3.8)$$

Here, $\rho_c = \text{tr}_w \rho$ is the reduced density matrix of the coin obtained by tracing out the walker degrees of freedom from the full density matrix ρ . For the Hadamard walk, the EE settles to a constant value around 0.605 [125].²

Certain aspects of disorder in quantum walks have been studied in the past, see, e.g., Refs. [126, 127, 128, 129, 130]. Here, we are interested in the effects of disorder in the

²We considered the natural logarithm to estimate this absolute value which is therefore distinct from the value reported in Ref. [125].

coin operator on the properties of CQWs. We consider the gate

$$G(r) = \begin{pmatrix} \sqrt{r} & \sqrt{1-r} \\ \sqrt{1-r} & -\sqrt{r} \end{pmatrix} \quad (3.9)$$

with $r \in [0, 1]$. For certain values of r the gate G reduces to common gates, viz.,

$$G(0) = X, \quad G(1/2) = H, \quad G(1) = Z. \quad (3.10)$$

We shall consider CQWs in which the lattice site x has an assigned random number r_x and an associated gate $G(r_x)$. The coin operator is then altered as follows

$$C(\{r_x\}) = \sum_{x \in \mathbb{Z}} |x\rangle \langle x| \otimes G(r_x). \quad (3.11)$$

$G(r_x)$ is still composed of an X and a Z gate, viz., $G(r_x) = \sqrt{r_x}Z + \sqrt{1-r_x}X$ such that the initial state in Eq. (3.5) still yields a symmetric propagation.

Although the coin operator is still in block diagonal form, it does not trivially factorize anymore into a product of two operators acting on $\mathcal{H}_w$ and $\mathcal{H}_c$ separately. We introduce a parameter W that controls the disorder strength, i.e.,

$$r_x = \frac{1}{2} (1 + W\xi_x). \quad (3.12)$$

Here, $\xi_x \in [-1, 1]$ are uniformly distributed random numbers. This choice readily recovers the Hadamard walk for $W = 0$ and a completely disordered walk for $W = 1$.

To analyze the influence of the quenched coin disorder on CQWs, we study different disorder realizations. We write $\{\xi_x^{(i)}\}$ where $i = 1, 2, \dots$ labels the realization. Each realization i yields a quantum state $\rho_i(t) = |\psi^{(i)}(t)\rangle \langle \psi^{(i)}(t)|$. Any system quantity f can be evaluated in two distinct ways. Either we first evaluate the density matrix of the ensemble of realizations

$$\overline{\rho_i} = \frac{1}{N} \sum_{i=1}^N |\psi^{(i)}\rangle \langle \psi^{(i)}| \quad (3.13)$$

and then evaluate the ensemble average $f(\overline{\rho_i})$ or we first evaluate f for a certain realization and then compute the realization average

$$\overline{f(\rho_i)} = \frac{1}{N} \sum_{i=1}^N f(|\psi^{(i)}\rangle \langle \psi^{(i)}|). \quad (3.14)$$

For linear observables, both averages are equivalent, and the expectation values of an operator O can be defined uniquely as $\langle O \rangle = \text{Tr}(O\overline{\rho_i})$. Hence, the walker occupation probability $p_x = \text{tr}(|x\rangle \langle x| \overline{\rho_i})$ is directly obtained as

$$p_x(t) = \frac{1}{N} \sum_{i=1}^N |\langle x \uparrow | \psi^{(i)}(t) \rangle|^2 + |\langle x \downarrow | \psi^{(i)}(t) \rangle|^2. \quad (3.15)$$

However, for nonlinear f such as entanglement entropy which we will consider in section 3.4, the two averages differ.

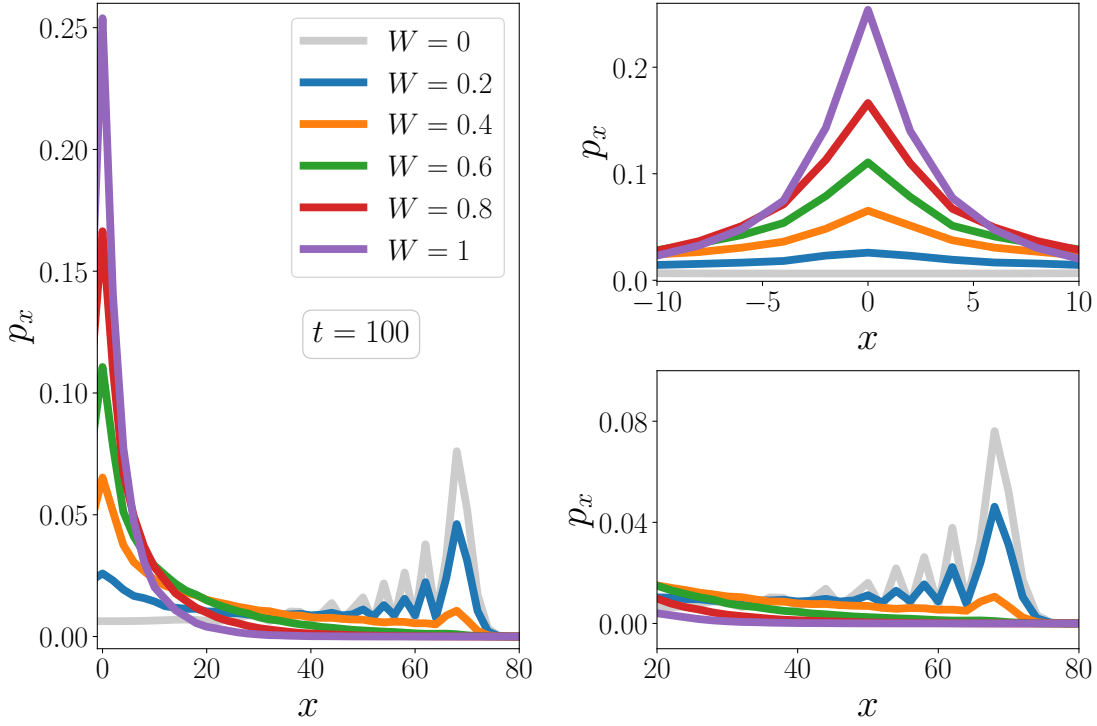


Figure 3.3: **Walker distribution of the disordered CQW.** The left panel shows the occupation probability p_x at $t = 100$ for a CQW with a disordered coin operator, see Eq. (3.11), starting in the initial state (3.5) for different disorder strengths W . The upper right panel shows that the center peak does not vanish in the disordered case and the lower right panel shows that the traveling peaks are suppressed with increasing disorder. These results are obtained by averaging over 1000 independent coin operator initialization.

3.3 Walker Occupation Probability

In Fig. 3.3 we illustrate the walker occupation probability of a CQW (see Eq. (3.15)) on the infinite line after 100 time steps for different disorder strengths W . For $W = 0$, i.e., the Hadamard walk, we again observe the characteristic peaks from Fig. 3.2. For small to moderate disorder strengths ($W = 0.2, 0.4$) these peaks persist but also a third, central peak appears which is qualitatively different from the Hadamard walk. For larger disorder strengths, we observe that the central peak becomes the dominating feature of the probability distribution indicating that the walker is effectively trapped with at most a very slow underlying dynamics. This behavior is indicative of an Anderson localization in the disordered CQW. To analyze this localization further, we study properties of the probability distribution and the corresponding quantum wave function. Our results are illustrated in Fig. 3.4. The emergent central peak can be quantified by the return probability p_0 of finding the walker on its initial site $x = 0$. For the Hadamard walk it is known that p_0 decays

algebraically as $\sim 1/t$.

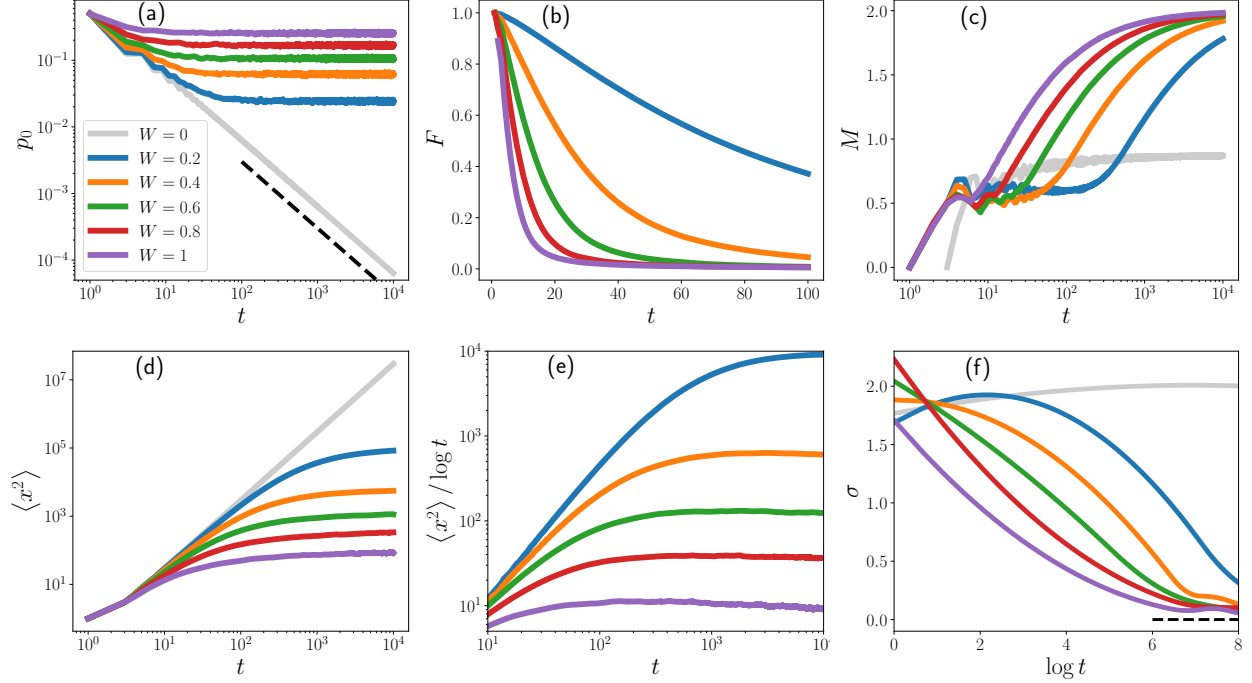


Figure 3.4: Influence of disordered coin operators on walker distribution. We consider different properties of the walker distribution and the quantum state for different disorder strengths $W = 0$ (gray), $W = 0.2$ (blue), $W = 0.4$ (orange), $W = 0.6$ (green), $W = 0.8$ (red), $W = 1$ (purple). Panel (a) shows the return probability p_0 . For $W = 0$ we observe an algebraic decay as $p_0 \sim t^{-1}$ (as indicated by the black dashed line). Conversely, for $W > 0$ we see that $p_0 > 0$ at all times with the plateau value increasing for stronger disorder. In panel (b) we compare the quantum state for $W > 0$ to that of the Hadamard walk ($W = 0$) using the state fidelity, see Eq. (3.16). The quantum state quickly deviates from that of the Hadamard walk, even for small W . Panel (c) shows the mixing ratio, see Eq. (3.18). At intermediate times, coin disorder ($W > 0$) improves the mixing properties of the walk. Conversely at late times we see that the occupation probability of the disordered walker deviate significantly from the flat distribution. In panel (d) we show the mean squared displacement. For $W = 0$ we find the expected algebraic growth. For $W > 0$ we observe a significantly slowed down dynamics. This is further analyzed in panel (e) where we compare $\langle x^2 \rangle$ to $\log t$. We see that eventually $\langle x^2 \rangle$ grows sublogarithmically. In panel (f) this is confirmed by analyzing the growth exponent σ , see Eq. (3.20). While the Hadamard walk shows $\sigma = 2$, for $W > 0$ we consistently find $\sigma \rightarrow 0$. All results are averaged over 1000 independent disorder realizations.

In Fig. 3.4(a), we see this algebraic decay for $W = 0$ (note the logarithmic scales). For different disorder strengths $W > 0$, we see that the central peak does not vanish. Instead we

observe a finite return probability for $W > 0$ and the corresponding plateau value increases with increasing W . Hence, the character of the probability distribution is significantly altered.

To gather further insights into the nature of the dynamics of the disordered CQW, we consider in Fig. 3.4(b) the state fidelity. We compare the quantum state $|\psi_i\rangle$ of the disordered composite system with that of the Hadamard walk $|\varphi\rangle$ at the same time, viz.,

$$F = \frac{1}{N} \sum_{i=1}^N |\langle \psi^{(i)} | \varphi \rangle|^2. \quad (3.16)$$

We see that even for small W , the state deviates significantly from that of the Hadamard walk. The larger the disorder strength the faster the state deviates.

In Fig. 3.4(c) we analyze the influence of disorder on the mixing properties of the CQW. To this end, we compare the walker occupation probability distributions with the flat distribution. To ensure a meaningful flat state for the infinite system, we must consider that our initial system state implies that at even (odd) times only even (odd) sites can be occupied. Hence, we must consider the flat state restricted to the sites that correspond to the parity of the current time step and that lay within the physical light cone of the dynamics. Thus, we refer to the following probability distribution

$$p_{\text{flat}}(x, t) = \begin{cases} 1/(t+1), & |x| \leq t \wedge (t-x) \text{ even} \\ 0, & \text{else} \end{cases} \quad (3.17)$$

as the flat distribution at time t for the system on the infinite line. The mixing ratio M is then defined by the 1-norm of the distance

$$M = \|p_x - p_{\text{flat}}\|_1. \quad (3.18)$$

As we observe from Fig. 3.4(c), a small amount of disorder W initially increases the mixing of the quantum walk (e.g., for $W = 0.2$) which is probably related to the appearance of the central peak. Interestingly, eventually $M \rightarrow 2$ for $W > 0$ in all cases we considered. From Eq. (3.18) it is obvious that the mixing ratio satisfies $M \leq 2$. The fact that all walks tend toward the maximum mixing ratio implies that the two distributions that are being compared do not have significant overlap. This means that the walker spreads *significantly slower* than the physical light cone. In turn, the Hadamard walk ($W = 0$) keeps up with the light cone and the mixing ratio does not reach $M = 2$.

In Fig. 3.4(d) we further characterize the slow dynamics considering the mean squared displacement of the quantum walker, viz.,

$$\langle x^2 \rangle = \sum_{x \in \mathbb{Z}} p_x x^2. \quad (3.19)$$

For the Hadamard walk we see that, as expected, $\langle x^2 \rangle$ grows quadratically, indicating a ballistic dynamics (note again the logarithmic scale in Fig. 3.4(d)). The coin-disorder yet again significantly alters this behavior. For $W > 0$, we see that the mean squared displacement deviates from that of the Hadamard walk on a finite time scale that decreases with increasing disorder strength and eventually always becomes subdiffusive.

In Fig. 3.4(e) we reconsider the mean squared displacement with the Hadamard walk removed and rescaled by $\log t$. We see that $\langle x^2 \rangle$ grows at most sublogarithmically, see, e.g., $W = 0.8, 1$. To further analyze the growth behavior, we assume that it may be characterized by a power-law, i.e., $\langle x^2 \rangle \sim t^\sigma$. This allows to extract the growth exponent σ as

$$\frac{d \log \langle x^2 \rangle}{d \log t} = \sigma. \quad (3.20)$$

In Fig. 3.4(f) we extract this exponent numerically by interpolating the data using smoothed cubic splines and evaluating the numerical derivative. For a ballistic spreading ($W = 0$), we find $\sigma = 2$. Conversely, a diffusive dynamics would yield $\sigma = 1$. When $\sigma = 0$, there is no spreading and instead a localization phenomenon takes place [131]. For any $W > 0$, we see from Fig. 3.4(f) that $\sigma \rightarrow 0$. Hence, we find strong numerical evidence that the CQW with coin disorder localizes on the length- and time-scales we explored.

3.4 Entanglement Properties

Since the coin disorder significantly alters the dynamics of the quantum walk, it is interesting to explore the effects of disorder on the entanglement between coin and walker. The initial state given in Eq. (3.5) is a pure product state and thus, walker and coin are initially not entangled. Without disorder, the system remains at all times in a pure state and therefore the EE (see Eq. (3.8)) is a good entanglement quantifier. As we have explained in section 3.2, in the presence of coin disorder we may consider either the ensemble average or the realization average. The ensemble average describes the statistical state of the system but is generally not pure and thus the EE is not a faithful entanglement witness. Conversely, every realization stays in a pure state at all times and thus the EE is a good entanglement witness for each individual run. Hence, to quantify the effects of disorder on the EE we consider the EE for each realization individually and average the resulting EEs afterwards. In Fig. 3.5 we show the resulting EE. First, we see that we recover the well-known result for the Hadamard walk for $W = 0$ [125]. Further, we observe that the average entanglement of the CQW with coin disorder is lower than that of the Hadamard walk, indicating that the disorder effectively decreases the entanglement between walker and coin. With increasing W , we also observe that fluctuations are introduced to the entanglement entropy. Interestingly, these fluctuations do not vanish upon increasing the number of disorder realizations. We may understand these oscillations as further indicator for a localization phenomenon taking place. This is because the quantum state cannot be immobile since only those sites can

be occupied that coincide with the time parity (even, odd). Hence, even a state that we consider localized will alter between even and odd time steps. The stronger the disorder, the faster the localization occurs such that even and odd states may be picked from the initial transient regime and thus show a significantly distinct entanglement character. Hence, the EE for even (odd) steps is rather constant (see inset in Fig. 3.5) but the localization prevents further approaching a unique EE as it is the case for the Hadamard walk.

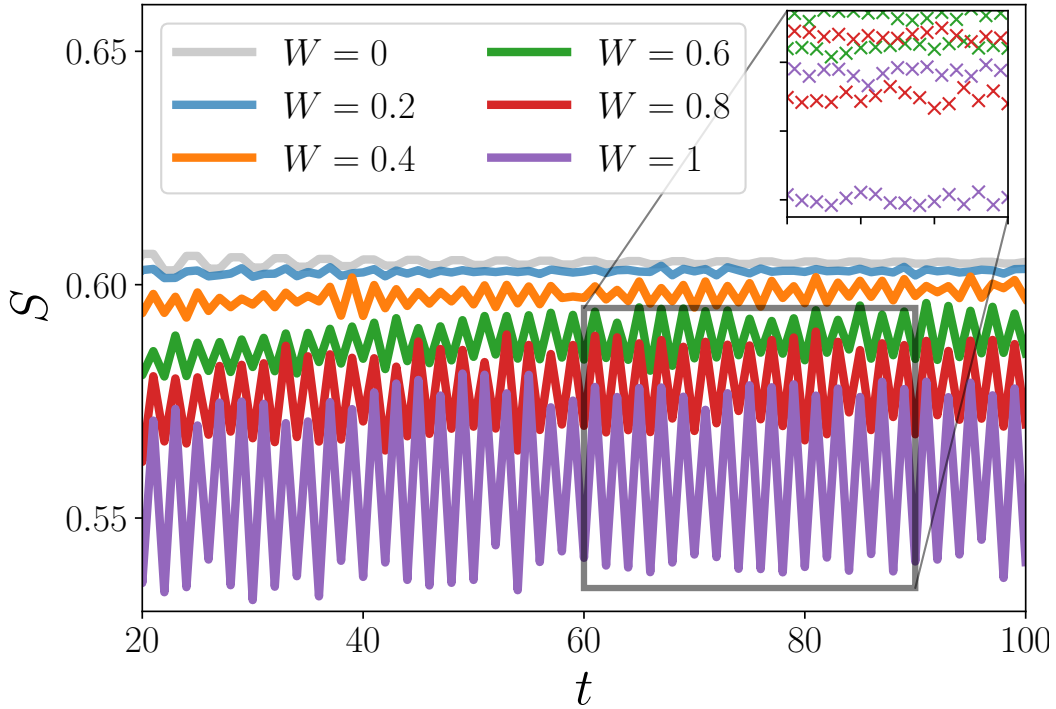


Figure 3.5: **Entanglement entropy.** For $W > 0$, we trace out the walker degrees of freedom for each disorder realization and evaluate the resulting EE. The results are averaged over 1000 independent disorder realizations. With increasing W oscillations emerge that further support the localization hypothesis. The inset shows that the EE is rather constant for even (odd) time steps.

To further investigate the entanglement properties of the CQW with coin disorder, we consider the ensemble of realizations. The resulting mixed state ρ is the accurate description of the bipartite quantum system and not pure. An entanglement witness for such mixed states is the entanglement negativity which is defined as [132]

$$\mathcal{N} = -\frac{1}{2} \left(1 - \sum_i |\lambda'_i| \right). \quad (3.21)$$

Here, λ'_i are the eigenvalues of the partial transpose ρ' of the density matrix ρ , viz.,

$$\rho'_{x\sigma, x'\sigma'} = \rho_{x\sigma', x'\sigma} \quad (3.22)$$

with $x, x' \in \mathbb{Z}$ and $\sigma, \sigma' \in \{\uparrow, \downarrow\}$. Naturally, if ρ can be written as a sum of product states of individual subsystem density matrices so can ρ' . The normalization $\text{tr } \rho = 1$ is carried over to ρ' such that $\sum_i \lambda'_i = 1$. Thus, in the case that ρ' is a sum of product states all $\lambda'_i \geq 0$ such that $\sum_i |\lambda'_i| = 1$ and consequently $\mathcal{N} = 0$. Any negative eigenvalue will indicate a non-separable quantum state and thus the presence of entanglement. In this case $\sum_i |\lambda'_i| > 1$ and thus $\mathcal{N} > 0$.

In Fig. 3.6 we show our results for the entanglement negativity for the CQW with coin disorder. For the Hadamard walk, we recover the established behavior of the negativity [133]:

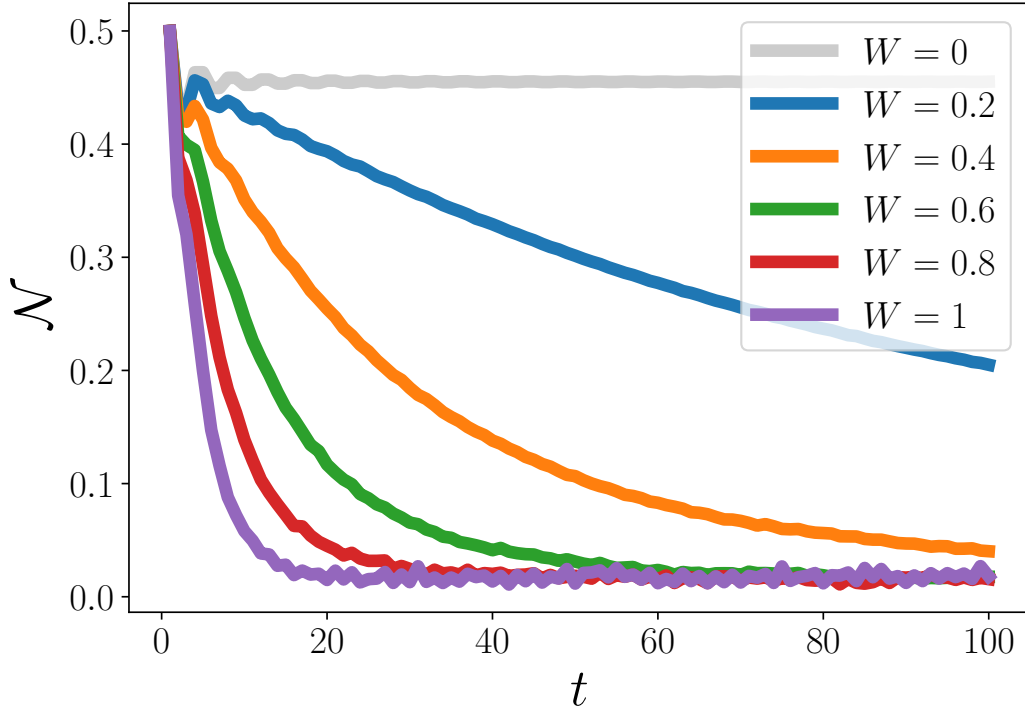


Figure 3.6: **Entanglement negativity.** For different values of the coin disorder W , we depict the entanglement negativity between coin and quantum walker. For $W = 0$, we observe $\mathcal{N} \simeq 0.45$ for large times clearly indicating an entangled quantum state. Conversely, for $W > 0$ we see $\mathcal{N} \rightarrow 0$. We consider 1000 independent disorder realizations.

following an initial transient regime, $\mathcal{N}$ settles to a constant value and remains finite. For $W > 0$ we observe that the negativity decays over time hinting at an absence of entanglement in the ensemble of initializations. We stress that this does not mean that the quantum state is not entangled but we may understand the vanishing of $\mathcal{N}$ as an indication that the

quantum state is ‘more separable’. This again supports the argument that the quantum walker undergoes localization: if the state was separable, then the walker state is unaffected by coin state yielding an effectively frozen walker.

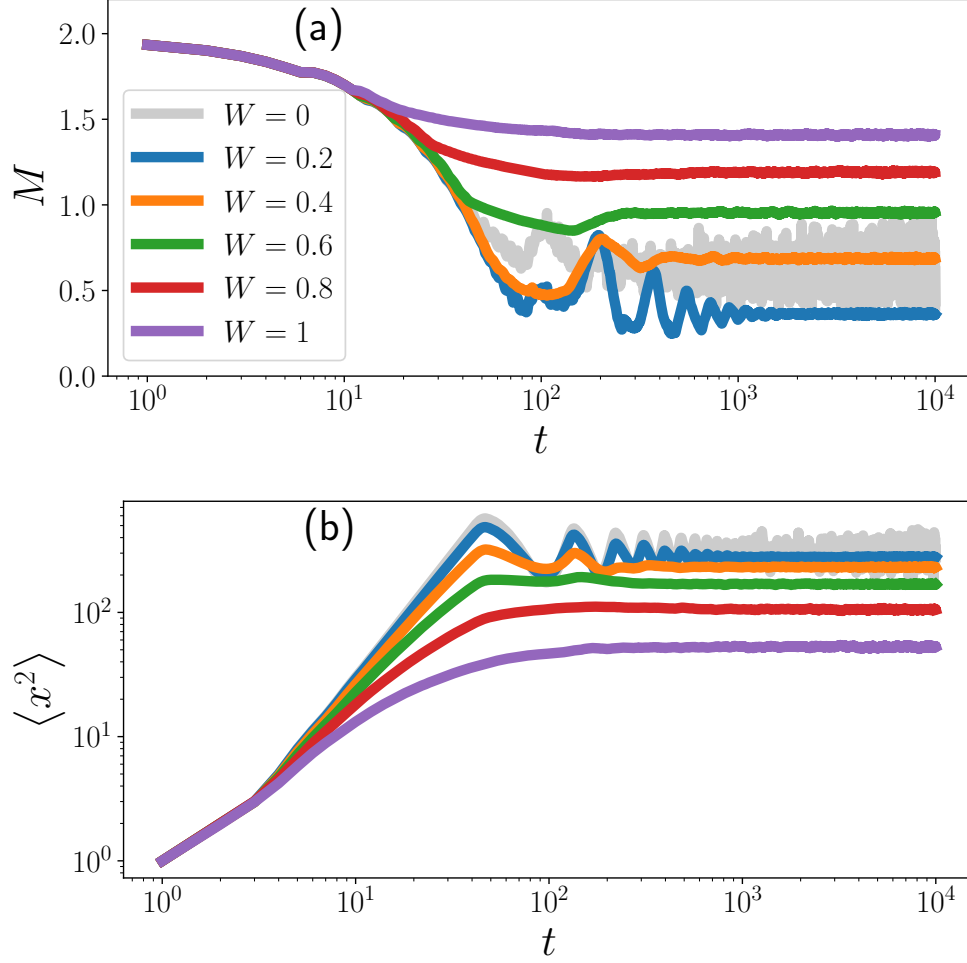


Figure 3.7: **Periodic boundary conditions.** We consider the CQW with quenched coin disorder and periodic boundary conditions. To this end we consider a circle with a total of 61 sites and average over 1000 independent disorder realizations.

3.5 Alternative Boundary Conditions

For late times, the linear spreading of the light cone makes computational advances increasingly challenging since the Hilbert space dimension increases rapidly. Alternative boundary conditions such as periodic or reflective boundary conditions naturally limit the Hilbert space dimension and allow more straightforward computational approaches. Here we complement

our analysis by considering some properties of the CQW with coin disorder for periodic and reflective boundary conditions.

Periodic boundary conditions. In Fig. 3.7 we show the mixing ratio as well as the mean squared displacement for a system of 61 sites (30 sites in positive and negative direction respectively). First, we note that the definition of the flat distribution must be altered to evaluate meaningful mixing ratios. This is because the periodic boundary conditions break the even - odd parity of the CQW due to the boundary hopping which corresponds to an even - even transition. Hence, we compare the walker probability distribution with $p_{\text{flat}}^{(r)}(x) = 1/L$ where L is the total number of sites. For the Hadamard walk ($W = 0$), the initial state (see Eq. (3.5)) is far away from $p_{\text{flat}}^{(r)}$ and mixing occurs rather fast. Around $t \approx 100 = \mathcal{O}(L)$ the mixing ratio peaks since the two ballistic peaks meet and interfere constructively. The spreading of the peaks with time eventually yields rather constant oscillations and a rather strong mixing. For small disorder strengths (e.g., $W = 0.2$), we see that the CQW mixes better and oscillations are notably absent again hinting at a localized state. Upon increasing W , we observe that states become less mixed as we would expect since a single, prominent peak is forming. This is supported by the results for the mean squared displacement. For this finite system, there is a natural upper bound and for each disorder strength $W > 0$, $\langle x^2 \rangle$ saturates at a level below that of the Hadamard walk.

Reflective boundary conditions. In Fig. 3.8 we show the analogous results to Fig. 3.7 but with reflective boundary conditions. Importantly, reflective boundary conditions again preserve the even - odd parity of the CQW but as for the periodic boundary conditions we do not rely on a light cone distribution since the system is finite. Qualitatively, the results for reflective boundary conditions coincide with those of periodic boundary conditions although the absolute values of mixing and mean squared displacement vary slightly.

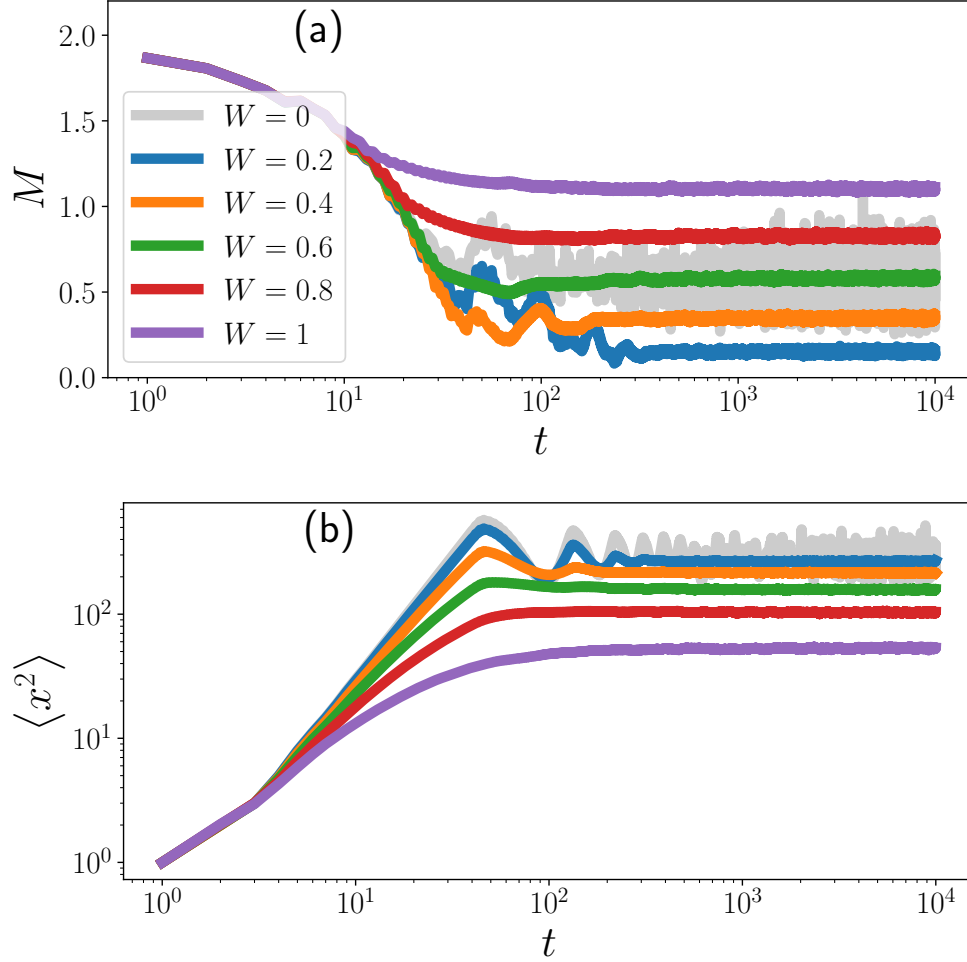


Figure 3.8: **Reflective boundary conditions.** We consider the CQW with coin disorder and reflective boundary conditions. To this end we consider a line with a total of 61 sites and average over 1000 independent disorder realizations.

3.6 Conclusion & Outlook

The Hadamard walk - often referred to as quantum analogue of the classical random walk - is a well-studied system that has been considered in a variety of different setups. Here, we addressed the question how quenched disorder in the coin operations influences CQWs. First, we observed clear differences in the quantum walker occupation probability: While for the Hadamard walk the occupation probability is characterized by two ballistically traveling peaks, the coin disorder hinders this ballistic spreading. Instead we observed dynamics that is significantly slowed down as evidenced by the mixing ratio and the state fidelity. In particular, we see that a new central peak emerges that becomes the asymptotically domi-

nating feature of the occupation probability signaling walker localization. This is supported by an analysis of the mean squared displacement that reveals a sublogarithmic growth as opposed to a quadratic growth for the Hadamard walk or a linear growth for classical diffusion. Hence, the underlying dynamics is extremely slow and since the leading behavior of $\langle x^2 \rangle$ is not algebraic we contemplate that the walker localizes.

Next, we considered the entanglement behavior between the quantum coin and the walker. Here, we presented two separate approaches the results of which point in the same direction. First, we studied the EE. We considered individual realizations of the CQW and averaged the EE of each realizations. We found that the disorder lowers the average EE per run with increasing disorder. Interestingly we also observed that, with increasing disorder strength W , the EE shows oscillations that do not decrease upon increasing the number of disorder realizations. Rather these oscillations are a further indicator of localization in the CQW in the following sense. For $W > 0$, the walker state is frozen and the larger W the faster this happens. But the walker state cannot be equal at all times since the system as we have set it up has an underlying even - odd parity. Hence, the system alternates between two distinct states and these states differ in their entanglement properties yielding increasing oscillations for increasing W as the localization happens earlier in the transient regime.

Conversely, to quantify the entanglement properties of the ensemble of realizations, we considered the entanglement negativity. The negativity $\mathcal{N}$ is a faithful entanglement quantifier for mixed states but from $\mathcal{N} = 0$ one cannot automatically deduce that there is no entanglement present in the system. The negativity for the standard Hadamard walk quickly converges to a finite value $\mathcal{N} > 0$ indicating that the state of the composite quantum system at late times is strongly entangled. Upon introducing coin disorder, we observed that the negativity quickly decays to zero hinting at a quantum state for the composite system that might be separable or for which entanglement is at least not a dominating feature. This would imply that the quantum coin state does not significantly influence the walker state. Hence, since the coin induces the walker dynamics, we may interpret this as a further indicator for a walker localization.

Despite the apparent simplicity of CQWs, there are a variety of directions with interesting research avenues to explore. For example, it would be interesting to further explore the interplay between disorder and coin-walker entanglement in the current setup. One might, e.g., consider different initial conditions that are entangled to varying degrees and see how the disorder affects the entanglement over time. Along these lines, one might as well consider a stochastic resetting [134, 135]. This could potentially allow to inject entanglement back in the system and might yield a more entangled steady state whose localization properties need to be explored carefully. It would also be interesting to study quenched coin disorder for different topologies. Here, one might consider higher dimensional regular lattices or complex networks with higher connectivity. In these more complicated setups, it might be that localization requires a minimal amount of disorder $W > 0$. In this context, it would be also interesting to explore connections between disordered CQWs and quantum Hall systems. This could be done by linking CQWs with the Chalker-Coddington model [136] and studying

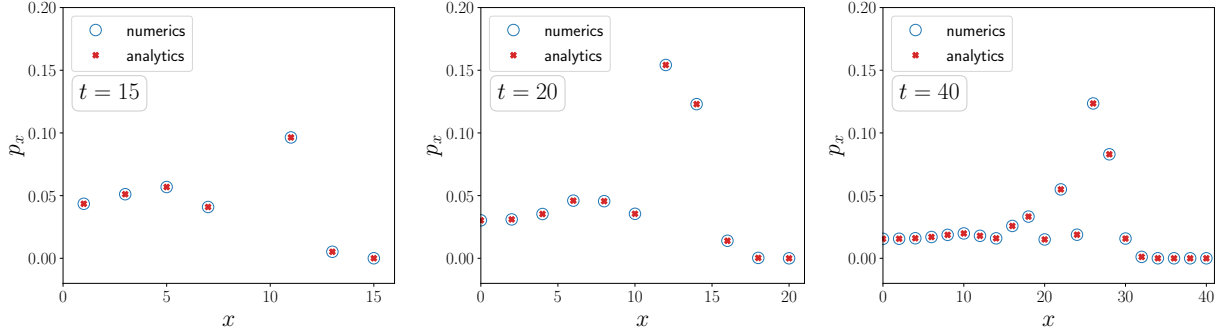


Figure 3.9: **Occupation probability Hadamard walk.** We compare the walker occupation probability p_x resulting from the analytical solution of the Hadamard walk (see Eqs. (3.33)) to that obtained from the numerical evaluation by iteratively applying the coin and shift operator (see Eqs. (3.3, 3.4)) to the initial state (3.5).

renormalization group approaches to CQWs that have been previously used in quantum Hall systems, see, e.g., Ref. [137].

3.7 Appendix

3.7.1 Solution of the Hadamard Walk

Here, we briefly outline the analytical solution of the Hadamard walk, following Ref. [121]. We write

$$|\psi\rangle = \sum_x (\psi_{x,\downarrow} |\downarrow\rangle + \psi_{x,\uparrow} |\uparrow\rangle) |x\rangle = \sum_x |\vec{\psi}_x\rangle |x\rangle \quad (3.23)$$

with the two component vectors $|\vec{\psi}_x\rangle = (\psi_{x,\downarrow}, \psi_{x,\uparrow})$. This allows us to decompose the Hadamard gate into its row components and deduce the recursion relation

$$|\vec{\psi}_x(t+1)\rangle = J_+ |\vec{\psi}_{x-1}(t)\rangle + J_- |\vec{\psi}_{x+1}(t)\rangle, \quad (3.24)$$

with the matrices

$$J_+ = \begin{pmatrix} 0 & 0 \\ \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} \end{pmatrix}, \quad J_- = \begin{pmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ 0 & 0 \end{pmatrix}, \quad (3.25)$$

such that $H = J_+ + J_-$. Apparently the Hadamard walk is translation-invariant such that we may transform the recursion relation into Fourier space, viz.,

$$|\tilde{\vec{\psi}}_k(t)\rangle = \sum_x |\vec{\psi}_x(t)\rangle e^{ikx}. \quad (3.26)$$

This yields the recursion relation in Fourier space

$$|\tilde{\psi}_k(t+1)\rangle = \mathcal{J}_k |\tilde{\psi}_k(t)\rangle. \quad (3.27)$$

Thus, $\mathcal{J}_k \equiv J_+ e^{ik} + J_- e^{-ik}$ generates the discrete time evolution of the corresponding Fourier component such that $|\tilde{\psi}_k(t)\rangle = \mathcal{J}_k^t |\tilde{\psi}_k(0)\rangle$. In order to fully determine the dynamics of the Fourier modes it suffices to diagonalize the 2×2 matrix $\mathcal{J}_k$. The eigenvalues are readily found, viz.,

$$\lambda_{\pm} = \frac{1}{\sqrt{2}} \left(\pm \sqrt{1 + \cos^2(k)} - i \sin(k) \right). \quad (3.28)$$

Since $\mathcal{J}_k$ is unitary, $\lambda_{\pm}$ lay on the unit circle in the complex plane and we further observe $\lambda_+ = -\lambda_-^*$. Hence we may write $\lambda_+ = e^{-i\omega_k}$ and $\lambda_- = e^{i(\pi+\omega_k)}$ with $\sin \omega_k = \sin(k)/\sqrt{2}$. The corresponding eigenvectors $|\pm\rangle$ can be found from a straightforward but lengthy calculation, viz.,

$$|\pm\rangle = \sqrt{\frac{1}{2} \pm \frac{\cos k}{2\sqrt{1 + \cos^2 k}}} \begin{pmatrix} e^{-ik} \\ \pm \sqrt{2} e^{\mp i\omega} - e^{-ik} \end{pmatrix}, \quad (3.29)$$

Hence, we may write $\mathcal{J}_k = \sum_{\sigma=\pm} \lambda_{\sigma} |\sigma\rangle \langle\sigma|$ and the time evolution can be explicitly recovered as

$$|\vec{\psi}_k(t)\rangle = \lambda_+^t |+\rangle \langle + | \vec{\psi}_k(0)\rangle + \lambda_-^t |-\rangle \langle - | \vec{\psi}_k(0)\rangle. \quad (3.30)$$

For an arbitrary initial coin state $|\tilde{\Psi}_k(0)\rangle = (a, b)$ we may then write the time evolved state explicitly in Fourier space as

$$\begin{aligned} \tilde{\psi}_k^{\downarrow}(t) = \frac{a}{2} & \left[\left(1 + \frac{\cos k}{\sqrt{1 + \cos^2 k}} \right) e^{-i\omega_k t} + (-1)^t \left(1 - \frac{\cos k}{\sqrt{1 + \cos^2 k}} \right) e^{i\omega_k t} \right] \\ & + \frac{b}{2} e^{-ik} \frac{e^{-i\omega_k t} - (-1)^t e^{i\omega_k t}}{\sqrt{1 + \cos^2 k}}, \end{aligned} \quad (3.31)$$

$$\begin{aligned} \tilde{\psi}_k^{\uparrow}(t) = \frac{b}{2} & \left[\left(1 - \frac{\cos k}{\sqrt{1 + \cos^2 k}} \right) e^{-i\omega_k t} + (-1)^t \left(1 + \frac{\cos k}{\sqrt{1 + \cos^2 k}} \right) e^{i\omega_k t} \right] \\ & + \frac{a}{2} e^{ik} \frac{e^{-i\omega_k t} - (-1)^t e^{i\omega_k t}}{\sqrt{1 + \cos^2 k}}. \end{aligned} \quad (3.32)$$

These Fourier expressions can be readily translated into real space in order to obtain the walker probability distribution and deduce related quantities such as the mixing ratio. We find

$$\psi_x^\downarrow = (1 + (-1)^{t+n}) \left[\frac{a}{2} \int_{-\pi}^{\pi} \frac{dk}{2\pi} \left(1 + \frac{\cos k}{\sqrt{1 + \cos^2 k}} \right) e^{-i(kx + \omega_k t)} + \frac{b}{2} \int_{-\pi}^{\pi} \frac{dk}{2\pi} \frac{e^{-ik}}{\sqrt{1 + \cos^2 k}} e^{-i(kx + \omega_k t)} \right], \quad (3.33a)$$

$$\psi_x^\uparrow = (1 + (-1)^{t+n}) \left[\frac{a}{2} \int_{-\pi}^{\pi} \frac{dk}{2\pi} \frac{e^{ik}}{\sqrt{1 + \cos^2 k}} e^{-i(kx + \omega_k t)} + \frac{b}{2} \int_{-\pi}^{\pi} \frac{dk}{2\pi} \left(1 - \frac{\cos k}{\sqrt{1 + \cos^2 k}} \right) e^{-i(kx + \omega_k t)} \right]. \quad (3.33b)$$

In Fig. 3.9 we compare the occupation probability of the walker obtained from the analytical solution to that of the numerical solution for different time steps and we observe perfect agreement.

Chapter 4

Perturbative Field-Theoretical Analysis of Three-Species Cyclic Predator-Prey Models

This chapter is adapted from our publication [138],

Louie Hong Yao, Mohamed Swailem, Ulrich Dobramysl and Uwe C. Täuber, “Perturbative Field-Theoretical Analysis of Three-Species Cyclic Predator-Prey Models”, J. Phys. A: Math. Theor. (2023) 56, 225001

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My contributions to this publication include independently performing all calculations and preparing the first draft of the manuscript.

4.1 Introduction

Population dynamics has been and continues to be an extremely active field of research since about forty years [139, 140, 141, 142, 143, 144, 145]. Steady progress in the development of mathematical and computational tools as well as the application of methods from statistical physics have allowed qualitative and quantitative insight into the behavior of interacting species. Various simplified models have been invoked to address prototypical situations in real ecosystems: The paradigmatic two-species Lotka–Volterra (LV) predator-prey model [146, 147] was originally introduced to study fish population oscillations in the Adriatic sea, as well as to explain auto-catalytic chemical reaction cycles. The Rock-Paper-Scissors (RPS) model [142, 148, 149, 150, 151, 152] addresses the case of three cyclically interacting species with a conserved total number of individuals, whereas the May–Leonard (ML) model [139, 153, 154, 155, 156, 157, 158] describes a more general, non-conserved situation. These models are obviously and necessarily rather simplified and lack many of the details of ecological neighborhoods. However, recent efforts aim at the realization and experimental implementation of such systems [159, 160, 161, 162, 163, 164]. Furthermore, it is reasonable to assume that simplified constructs such as the LV, ML, and RPS systems should be useful as elementary motifs and building blocks of models for more extended ecosystems. It is there-

fore imperative to investigate which of their features are qualitatively and/or quantitatively robust and remain important when multiple interacting species are coupled to environments with richer structures.

Traditionally, species dynamics in ecosystems are modelled via coupled non-linear ordinary differential equations. In the case of spatially extended systems, this approach is generalized by using partial differential equations that represent species dispersion through simple diffusion, i.e., coupled reaction-diffusion equations. However, this mean-field or mass action approach fails to take into account the inherent randomness and stochastic nature of the underlying processes stemming from fluctuations in the discrete number of individuals, and neglects spatio-temporal correlations. Yet fluctuations and correlations can lead to dramatically different behavior than predicted by mean-field theory [165]. For example, the classical LV mean-field rate equations predict neutral cycles and hence non-linear oscillations around a marginal fixed point, while stochastic computer simulations of this system yield decaying oscillations towards a (quasi-)stable state [166, 167, 168]. This stationary state exhibits large and erratic excursions triggered by fluctuations in the species concentrations in zero-dimensional [169] as well as spatially extended systems [170]. Spatially extended stochastic LV model variants also show intriguing spatial patterns and moving activity fronts [167, 171, 172]. Crucially, stochastic variants of the LV model exhibit a large susceptibility to randomness in the predator-prey interaction rates [173, 174].

Spatially extended cyclic models such as the RPS or ML systems are influenced by internal reaction noise and exhibit differences in species extinction times and resulting spiral pattern wavelengths compared to the mean-field approximation [151, 156, 175]. In one dimension, ‘superdomains’ may form in these cyclic models [176]. Although both models are cyclic in nature, they exhibit different sensitivity to stochastic fluctuations. The RPS model, a generalization of the LV model to three cyclically competing species, displays comparatively weak fluctuation renormalizations in the quasi-stable coexistence state and minimal modifications due to randomized reaction rates [152]. In contrast, the ML model features a stronger renormalization of the oscillation frequency in the unstable region where spiral structures form spontaneously, but appears to have an insignificant response to randomized reaction rates [155]. These observations from Monte Carlo simulations raise the intriguing question: Under what conditions will fluctuations significantly alter the system’s properties and cause marked deviations from simple mean-field predictions?

To at least partially answer this question, a field-theoretical perturbation analysis was applied to the stochastic spatially extended LV model in Ref. [177]. To one-loop order, this semi-quantitative analysis confirms that i) the fluctuation-induced damping renders the system unstable against spatio-temporal structures, and ii) fluctuations significantly renormalize the oscillation frequency in the two-species co-existence phases, especially below three dimensions. Aiming to better understand the fluctuations in spatially extended RPS [Fig. 4.1(a,b)] and ML models [Fig. 4.1(c,d)], we utilize a similar Doi–Peliti field theory representation for their associated stochastic reaction processes. To study the impact of intrinsic fluctuations on system parameters, a one-loop calculation is carried out in the perturbative regime, where

the reaction rates are small as compared with the diffusivity, and a thorough comparison between the RPS, ML, and LV systems is conducted. In contrast to earlier observations in numerical simulations, the RPS model exhibits noticeable fluctuation-induced corrections in the perturbative regime, similar to the LV model. We believe that, as the dissipation becomes non-negligible in the non-perturbative regime, the associated infra-red (IR) divergence is regularized, and thus substantial renormalizations become effectively suppressed. We note that in all investigated systems, the field-theoretic loop expansion technically only applies to the stable regions with spatially homogeneous ground states. Our results demonstrate that, at least in the stable region, the dynamical features of the ML model conversely do not receive significant modifications from fluctuations. Based on these explicit calculation results, we also provide pertinent arguments that explain the absence of spontaneous spatio-temporal patterns in the RPS model with conserved total population number, as opposed to the ML model, which for sufficiently large system sizes develops spiral oscillatory patterns, as depicted in Fig. 4.1(c,d).

The chapter is organized as follows: Detailed perturbative field-theoretical analyses for the cyclic and symmetric RPS and ML models are performed in sections 4.2 and 4.3, respectively, where we establish the Doi–Peliti functionals for both models and state their corresponding generalized Langevin equations. Renormalized damping coefficients, oscillation frequencies, as well as diffusivities are calculated up to one-loop order in the perturbative fluctuation expansion. In section 4.4, a comprehensive comparison between the LV, RPS, and ML models is provided, and pertinent distinctions between these paradigmatic systems are highlighted. Specifically, we discuss the influence of fluctuations and the stability of spatio-temporal structures, and also briefly address the effect of quenched disorder in the reaction rates. We conclude with a brief summary and outlook. Finally, Appendix 4.6.1 presents a succinct review of the Doi–Peliti field theory approach and also provides a brief analysis of the asymmetric RPS model, demonstrating its effective two-species limit for strong asymmetry at the mean-field level. The remaining appendices list additional technical and computational details for the symmetric ML model.

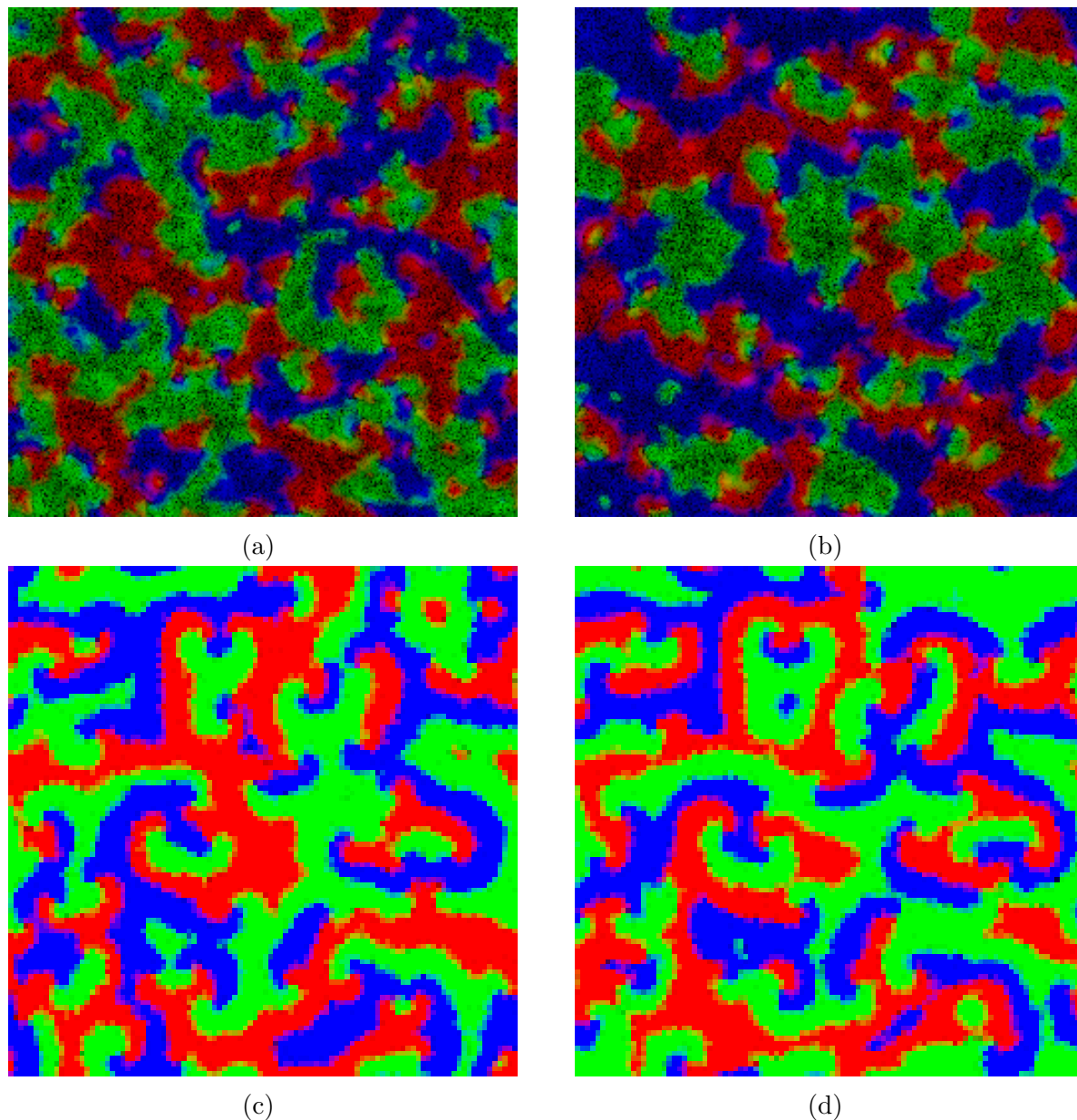


Figure 4.1: Snapshots of the spatial particle distribution in cyclic three-species RPS and ML models for single stochastic simulation runs (system size 100×100 lattice sites): Each lattice pixel is assigned an RGB value such that each color value is proportional to the number of individuals of a specific species. A color value 0 represents the absence of the species corresponding to that assigned color; therefore, black pixels indicate empty sites. Top: RPS model with reaction rate parameter $\lambda' = 0.5$ at (a) $t = 300$ Monte Carlo Steps (MCS) and (b) $t = 400$ MCS; bottom: ML model with predation rate $\sigma' = 0.5$ and reproduction rate $\mu = 0.5$ at (c) $t = 300$ MCS and (d) $t = 400$ MCS, respectively. The red species predaes on the blue species, the blue species on the green species, and the green species on the red species in both models.

4.2 Stochastic Rock-Paper-Scissors (RPS) Model

4.2.1 RPS Model and Mean-Field Rate Equations

The RPS model consists of three particle species, subject to the cyclically coupled stochastic competition reactions



In this chapter, we consider the cyclic-symmetric case, such that $\lambda'_1 = \lambda'_2 = \lambda'_3 = \lambda'$. In this limit, the system displays a discrete S_3 symmetry among the three species. A brief analysis of the general asymmetric case is presented in Appendix A. We note that every species interacts via a standard non-linear Lotka–Volterra predation reaction with the subsequent species in the cycle, consuming a “prey” particle and reproducing at the same instant. The total number of individuals is unchanged by all reactions, hence particle number conservation holds globally and locally (except for hops to neighboring lattice sites, see below).

We consider a model wherein particles from all three species perform random walks on a d -dimensional hyper-cubic lattice with L^d sites and lattice constant c . We do not restrict the number of particles per lattice site, hence we do not consider finite local carrying capacities here (the total number of particles is fixed). The rate at which particles hop between sites is given by D/c^2 , where D denotes a macroscopic diffusion constant. The reactions (4.1) occur on-site, and only if two particles of differing species are present. Reaction products are put on the same lattice point as the reactants.

In the limit of large diffusivities (relative to the reaction rates λ') the system can be considered well-mixed. Hence, the RPS rules can be approximated by the three coupled mean-field rate equations for the homogenized species concentrations and with the volume reactivities $\lambda = c^{-d}\lambda'$:

$$\begin{aligned} \frac{da_1(t)}{dt} &= \lambda a_1(t) [a_2(t) - a_3(t)] , \\ \frac{da_2(t)}{dt} &= \lambda a_2(t) [a_3(t) - a_1(t)] , \\ \frac{da_3(t)}{dt} &= \lambda a_3(t) [a_1(t) - a_2(t)] . \end{aligned} \tag{4.2}$$

This system of ordinary differential equations yields non-linear oscillations around a neutral fixed-line which is determined by the initial conditions. The fixed-line steady-state concentrations can be obtained by setting the time derivatives to zero, resulting in

$$a_i^\infty = \frac{\rho}{3} , \quad \forall i \in \{1, 2, 3\} , \tag{4.3}$$

with the conserved total population density $\rho = a_1 + a_2 + a_3 = \text{const}$, parameterizing the fixed line. Linearization about this three-species coexistence fixed-line yields the stability matrix

$$S_{\text{RPS}} = \frac{\lambda\rho}{3} \begin{pmatrix} 0 & +1 & -1 \\ -1 & 0 & +1 \\ +1 & -1 & 0 \end{pmatrix}, \quad (4.4)$$

with eigenvalues $\{0, -i\omega_0, i\omega_0\}$. Since the non-zero eigenvalues are purely imaginary, the mean-field RPS system performs perpetual non-linear oscillations around the coexistence fixed point with frequency (in the linearized approximation) $\omega_0 = \rho\lambda/\sqrt{3}$.

4.2.2 Doi–Peliti Field Theory and Generalized Langevin Equations

The bulk part of the Doi–Peliti action for the stochastic spatially extended RPS model follows directly from the reactions (4.1) and reads ¹

$$\mathcal{A}^{\text{RPS}} = \sum_{i=1,2,3} \int dt d^d x \hat{a}_i (\partial_t - D\nabla^2) a_i + \lambda \sum_{i=1,2,3} \int dt d^d x \hat{a}_i (\hat{a}_{i+1} - \hat{a}_i) a_i a_{i+1}. \quad (4.5)$$

For convenience, here we drop all position and time indices $(\vec{x}, t)$ on the fields and identify $a_4 = a_1$. The first term describes the random nearest-neighbor hopping of the particles in the system, while the second contribution originates from the nonlinear reactions (4.1). As the auxiliary field $\hat{a}_i(\vec{x}, t)$ corresponds to a projection dual state, with average $\langle \hat{a}_i(\vec{x}, t) \rangle = 1$, a Doi shift $\tilde{a}_i(\vec{x}, t) = \hat{a}_i(\vec{x}, t) - 1$ is conveniently applied to have the new field averaged to $\langle \tilde{a}_i(\vec{x}, t) \rangle = 0$. After the Doi shift and ignoring boundary terms, the action becomes

$$\mathcal{A}^{\text{RPS}} = \sum_{i=1,2,3} \int dt d^d x \tilde{a}_i (\partial_t - D\nabla^2) a_i + \lambda \sum_{i=1,2,3} \int dt d^d x (\tilde{a}_i + 1) (\tilde{a}_{i+1} - \tilde{a}_i) a_i a_{i+1}. \quad (4.6)$$

This shifted action may now be viewed as a Janssen–De Dominicis response functional [11, 12] that represents the stochastic dynamics in terms of generalized Langevin equations. The $\tilde{a}_i$ fields play the role of response fields and their coupling to the particle densities, shown in the terms that are second order in these fields, entails the presence of multiplicative noise terms. This comparison leads to the formulation of equivalent Langevin stochastic differential equations encoded in the action (4.6),

$$\partial_t a_i = D\nabla^2 a_i + \lambda a_i (a_{i+1} - a_{i-1}) + \zeta_i, \quad (4.7)$$

where $\zeta_i(\vec{x}, t)$ are the components of multiplicative noise in the system with vanishing means and correlations

$$\langle \zeta_i(\vec{x}_1, t_1) \zeta_j(\vec{x}_2, t_2) \rangle = 2Z_{ij} \delta^{(d)}(\vec{x}_1 - \vec{x}_2) \delta(t_1 - t_2), \quad (4.8)$$

¹A brief introduction of the Doi–Peliti field theory representation is presented in Appendix A. We refer interested readers to Refs. [50, 178] for more details.

with the noise correlation matrix

$$Z = \lambda \begin{pmatrix} a_1 a_2 & -\frac{1}{2} a_1 a_2 & -\frac{1}{2} a_1 a_3 \\ -\frac{1}{2} a_1 a_2 & a_2 a_3 & -\frac{1}{2} a_2 a_3 \\ -\frac{1}{2} a_1 a_3 & -\frac{1}{2} a_2 a_3 & a_1 a_3 \end{pmatrix} . \quad (4.9)$$

Note that the noise auto-correlations Z_{ii} are always determined by the concentration of the predator species A_i and its respective prey A_{i+1} , and the scale is set by the predation rate λ . Hence the noise directly associated with a given species is solely determined by its role as predator.

4.2.3 Particle Number Conservation and Noether's Theorem

Before we proceed with the perturbation theory analysis, we quickly comment on the conserved Noether current associated with the total particle number preservation in the stochastic reaction processes (4.1). This conservation law corresponds to a global $U(1)$ symmetry in the Doi–Peliti action (4.5) for the RPS model, namely it remains invariant under the $U(1)$ gauge transformation

$$\hat{a}'_i = e^{-i\theta} \hat{a}_i , \quad a'_i = e^{i\theta} a_i , \quad (4.10)$$

where θ is an arbitrary phase angle. The conservation law follows from the action (4.5) and the symmetry transformation (4.10) and assumes the usual form of a continuity equation

$$\partial_t j_0 + \nabla \cdot \vec{j} = 0 , \quad (4.11)$$

with

$$j_0 = \sum_i \hat{a}_i a_i , \quad \vec{j} = -D \sum_i (\hat{a}_i \nabla a_i - a_i \nabla \hat{a}_i) . \quad (4.12)$$

When choosing the Doi field $\hat{a}_i = 1$, a_i represents the density of particle species A_i and Eq. (4.12) turns into the diffusion equation for the conserved total particle number density,

$$\partial_t \sum_{i=1,2,3} a_i = D \nabla^2 \sum_{i=1,2,3} a_i . \quad (4.13)$$

We note that the symmetry (4.10) corresponds to the freedom of choosing the phases of the probability state a_i and its dual projected state $\hat{a}_i$.

4.2.4 Diagonalization of the Harmonic Action

To start, we transform the fields to describe the fluctuations around the stationary fixed-point species concentrations. To this end we employ the linear transformation

$$c_i(\vec{x}, t) = a_i(\vec{x}, t) - \frac{\rho}{3} , \quad \tilde{c}_i(\vec{x}, t) = \tilde{a}_i(\vec{x}, t) , \quad (4.14)$$

which implies $\langle c_i \rangle = 0$. In the symmetric RPS model, there is both total particle number conservation and cyclic permutation symmetry among the three distinct species. These two symmetries combined imply vanishing additive counterterms to the stationary concentrations due to fluctuations. The action for these new fluctuating fields now reads

$$\begin{aligned} \mathcal{A}^{\text{RPS}} = \int dt d^d x \sum_i \left[\tilde{c}_i (\partial_t - D \nabla^2) c_i - \frac{\lambda \rho^2}{3} \tilde{c}_i (\tilde{c}_i - \tilde{c}_{i+1}) - \frac{\lambda \rho}{3} \tilde{c}_i (\tilde{c}_{i+1} - \tilde{c}_{i+2}) \right. \\ \left. - \frac{\lambda \rho}{3} \tilde{c}_i^2 (c_i + c_{i+1}) + \frac{\lambda \rho}{3} \tilde{c}_i \tilde{c}_{i+1} (c_i + c_{i+1}) - \lambda \tilde{c}_i c_i (c_{i+1} - c_{i+1}) - \lambda \tilde{c}_i^2 c_i c_{i+1} + \lambda \tilde{c}_i \tilde{c}_{i+1} c_i c_{i+1} \right], \end{aligned} \quad (4.15)$$

where we again identify $c_4 = c_1$ and $c_5 = c_2$ for convenience. The quadratic part in the above action can be diagonalized by means of the following linear transformation

$$\begin{pmatrix} c_1 \\ c_2 \\ c_3 \end{pmatrix} = \frac{1}{\sqrt{3}} \begin{pmatrix} 1 & -\frac{1+i\sqrt{3}}{2} & -\frac{1-i\sqrt{3}}{2} \\ 1 & -\frac{1-i\sqrt{3}}{2} & -\frac{1+i\sqrt{3}}{2} \\ 1 & 1 & 1 \end{pmatrix} \begin{pmatrix} \phi_o \\ \phi_+ \\ \phi_- \end{pmatrix}, \quad (4.16)$$

and

$$\begin{pmatrix} \tilde{c}_1 \\ \tilde{c}_2 \\ \tilde{c}_3 \end{pmatrix} = \frac{1}{\sqrt{3}} \begin{pmatrix} 1 & -\frac{1-i\sqrt{3}}{2} & -\frac{1+i\sqrt{3}}{2} \\ 1 & -\frac{1+i\sqrt{3}}{2} & -\frac{1-i\sqrt{3}}{2} \\ 1 & 1 & 1 \end{pmatrix} \begin{pmatrix} \tilde{\phi}_o \\ \tilde{\phi}_+ \\ \tilde{\phi}_- \end{pmatrix}. \quad (4.17)$$

The resulting action becomes $\mathcal{A}^{\text{RPS}} = \mathcal{A}_0^{\text{RPS}} + \mathcal{A}_{\text{int}}^{\text{RPS}}$, with the Gaussian part

$$\mathcal{A}_0^{\text{RPS}} = \int dt d^d x \left[\tilde{\phi}_+ (\partial_t - D \nabla^2 + i\omega_0) \phi_+ + \tilde{\phi}_o (\partial_t - D \nabla^2) \phi_o + \tilde{\phi}_- (\partial_t - D \nabla^2 - i\omega_0) \phi_- \right], \quad (4.18)$$

and the nonlinear contributions (vertices)

$$\begin{aligned} \mathcal{A}_{\text{int}}^{\text{RPS}} = \int dt d^d x \left[-\lambda \rho^2 \tilde{\phi}_+ \tilde{\phi}_- + i \frac{\lambda \rho}{3} \tilde{\phi}_o (\tilde{\phi}_+ \phi_+ - \tilde{\phi}_- \phi_-) - \frac{2\lambda \rho}{\sqrt{3}} \tilde{\phi}_+ \tilde{\phi}_- \phi_o \right. \\ \left. - i\lambda (\tilde{\phi}_+ \phi_-^2 - \tilde{\phi}_- \phi_+^2 - \tilde{\phi}_+ \phi_+ \phi_o + \tilde{\phi}_- \phi_- \phi_o) \right. \\ \left. - i \frac{\lambda \rho}{6} \left[(1 - i\sqrt{3}) \tilde{\phi}_+^2 \phi_- - (1 + i\sqrt{3}) \tilde{\phi}_-^2 \phi_+ \right] + \text{four-point vertices} \right]. \end{aligned} \quad (4.19)$$

Here, $\omega_0 = \lambda \rho / \sqrt{3}$ denotes the zeroth-order oscillation frequency of the $\phi_{+/-}$ modes. $\mathcal{A}_0^{\text{RPS}}$ is the diagonalized harmonic part of the action, while $\mathcal{A}_{\text{int}}^{\text{RPS}}$ represents the “interaction” contributions for the perturbative expansion. We omit the explicit expressions for the four-point vertices as they will not contribute to the dispersion relations at one-loop order, which shall be clear in the calculation below. It is manifest that $\phi_o = (a_1 + a_2 + a_3 - \rho) / \sqrt{3}$ represents the fluctuation of the total particle number density. Due to the conservation law (4.13), the ϕ_o mode is purely diffusive, and its exact dispersion relation in the harmonic part of the action acquires no fluctuation corrections. The ϕ_+ and ϕ_- modes may be viewed as the left- and right-rotating waves in the system. At tree level, they are purely oscillating modes without dissipation, i.e., the real part of the mass term vanishes.

4.2.5 One-loop Fluctuation Corrections

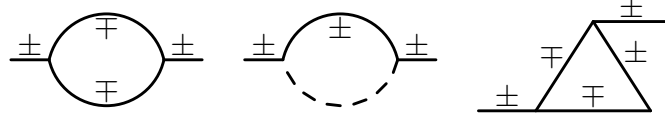


Figure 4.2: One-loop fluctuation contributions to the two-point vertex function $\Gamma_{\tilde{\phi}_{\pm}\phi_{\pm}}^{(1,1)}$ in RPS model. The solid lines represent the ϕ_+ and ϕ_- modes, whereas the dashed lines represent the purely diffusive ϕ_o mode.

We have applied a field-theoretical perturbation theory to one-loop order and calculated the renormalized diffusion constant D_r , damping constant γ_r , and oscillation frequency ω_r ². To all orders in the fluctuation expansion extending beyond the mean-field approximation, there should be no correction to the two-point vertex function $\Gamma_{\tilde{\phi}_o\phi_o}^{(1,1)}$ or propagator self-energy for the ϕ_o mode, whence it retains its tree-level purely diffusive dispersion relation as dictated by the conservation law. For the $\phi_{\pm}$ modes, the one-loop Feynman diagrams for the two-point vertex functions $\Gamma_{\tilde{\phi}_{\pm}\phi_{\pm}}^{(1,1)}$ are displayed in Fig. 4.2. The solid lines represent the ϕ_+ and ϕ_- propagators, while the dashed lines indicate the diffusive mode ϕ_o . In our convention, time and hence momentum always flow from right to left in the Feynman diagrams. The analytic expression for the two-point vertex function $\Gamma_{\tilde{\phi}_{\pm}\phi_{\pm}}^{(1,1)}$ reads

$$\begin{aligned} \Gamma_{\tilde{\phi}_{\pm}\phi_{\pm}}^{(1,1)}(p, \omega) = & i\omega + Dp^2 + u_0 \pm i\omega_0 + \frac{\sqrt{3}\lambda\omega_0}{6D} \int_k I\left(\frac{u_0 \pm i\omega_0}{2D}\right) \\ & - \frac{\sqrt{3}\lambda\omega_0}{6D} (1 \pm i\sqrt{3}) \int_k I\left(\frac{u_0 \mp i\omega_0}{D}\right) - \frac{\lambda\omega_0^2}{D^2} \int_k \frac{1}{k^2 + \frac{u_0}{D}} I\left(\frac{u_0 \mp i\omega_0}{D}\right), \end{aligned} \quad (4.20)$$

where $\int_k$ is short-hand for the d -dimensional wavevector integral $\int d^d k / (2\pi)^d$, and the function I is defined as

$$I(m^2) = \frac{1}{k^2 + m^2 + \frac{i\omega + Dp^2}{2D} + p \cdot k}. \quad (4.21)$$

The damping constant u_0 in Eq. (4.20) is introduced to regularize the infrared (IR) singularities that emerge in later calculations. A nonzero renormalized u_r will be generated by the fluctuations, but it is of higher order in the perturbation expansion; thus, we need to take $u_0 \rightarrow 0$ at the end. This two-point function can also be expressed with the renormalized parameters as

$$\Gamma_{\tilde{\phi}_{\pm}\phi_{\pm}}^{(1,1)}(p, \omega) = Z_{\phi_{\pm}} (i\omega + D_r p^2 + u_r \pm i\omega_r), \quad (4.22)$$

where $Z_{\phi_{\pm}}$ absorbs all related wave function renormalizations (ultraviolet / UV divergences) in (4.20). The renormalized diffusivity D_r , damping u_r , and oscillation frequency ω_r can

²For more details on the perturbation expansion and Feynman graph representations, we refer to Refs. [50, 74, 177].

be inferred accordingly from the explicit one-loop result (4.20) and (4.22). We obtain the following formal expressions for D_r , u_r , and ω_r ,

$$\begin{aligned}
D_r = & D + \frac{\sqrt{3}\lambda\omega_0}{6dD} \int_k \frac{k^2}{(k^2 \pm \frac{i\omega_0}{2D})^3} - \frac{\sqrt{3}\lambda\omega_0}{6dD} (1 \pm i\sqrt{3}) \int_k \frac{k^2}{(k^2 \mp \frac{i\omega_0}{D})^3} \\
& - \frac{\lambda\omega_0^2}{dD^2} \int_k \frac{1}{(k^2 \mp \frac{i\omega_0}{D})^3}, \\
u_r \pm i\omega_r = & \pm i\omega_0 \left[1 - \frac{\lambda}{2D} \int_k \frac{1}{k^2 + \frac{u_0}{D}} \pm \frac{i\sqrt{3}\lambda}{6D} \int_k \left(\frac{1}{k^2 \mp \frac{i\omega_0}{D}} - \frac{1}{k^2 \pm \frac{i\omega_0}{2D}} \right) \right. \\
& \left. + \frac{\sqrt{3}\lambda\omega_0}{12D^2} \int_k \frac{1}{(k^2 \pm \frac{i\omega_0}{2D})^2} - \frac{\sqrt{3}\lambda\omega_0}{12D^2} (1 \mp i\sqrt{3}) \int_k \frac{1}{(k^2 \pm \frac{i\omega_0}{2D})^2} \right].
\end{aligned} \tag{4.23}$$

Hence we indeed see that a non-zero damping u_r is generated at one-loop order from the fluctuations, in agreement with Monte Carlo simulation data [152]. The infra-red (IR) divergence at one-loop order that appears when in the renormalized oscillation frequency ω_r in low dimensions $d \leq 2$ is caused by the contribution of the massless ϕ_o mode as u_0 is set to zero. The infra-red (IR) divergence at one-loop order that appears in the renormalized oscillation frequency ω_r in low dimensions $d \leq 2$ is caused by the superposition of ϕ_+ and ϕ_- modes as u_0 is set to zero. Our analysis of the one-loop results shows that the $\phi_{\pm}$ modes are inherently massive, as they acquire non-zero damping u_r . Thus, the IR divergence can be resolved simply by maintaining a finite value for u_0 . For dimensions $d \geq 2$, there are also UV divergences present. Nevertheless, all systems of interest have a natural cutoff in the UV limit, which is defined by the lattice constant c . The renormalized variables in different physically accessible dimensions are presented below.

$d = 1$:

In one dimension, the renormalized parameters are

$$\begin{aligned}
\text{Re}D_r = & D + \lambda\sqrt{\frac{D}{\omega_0}} \left(\frac{7\sqrt{2}}{64} + \frac{\sqrt{6}}{192} - \frac{\sqrt{3}}{48} \right), \\
\omega_r = & \omega_0 \left[1 - \frac{\lambda}{4D} \sqrt{\frac{D}{u_0}} - \frac{\lambda}{D} \sqrt{\frac{D}{\omega_0}} \left(\frac{\sqrt{3}}{8} + \frac{\sqrt{6}}{32} + \frac{\sqrt{2}}{32} \right) \right], \\
u_r = & \frac{\lambda\omega_0}{D} \sqrt{\frac{D}{\omega_0}} \left(\frac{\sqrt{3}}{8} - \frac{\sqrt{6}}{32} + \frac{\sqrt{2}}{32} \right);
\end{aligned} \tag{4.24}$$

some numerical results are depicted in Fig. 4.3. We observe that the renormalized frequency ω_r diverges when $u_0 \rightarrow 0$. This IR divergence indicates strong fluctuation corrections to the oscillation frequency in the perturbative regime where reaction rates are small, and

$u_0 \rightarrow u_r \sim \lambda$ is of first order in the reactivity. However, numerical simulations are invariably performed outside this regime for the sake of computational efficiency, as large reaction rates are used to avoid long relaxation times. Thus, no strong fluctuation-induced renormalization have been encountered in the simulations. To one-loop order, $u_r > 0$, which indicates the stability of the system's spatially homogeneous ground state with respect to fluctuations.

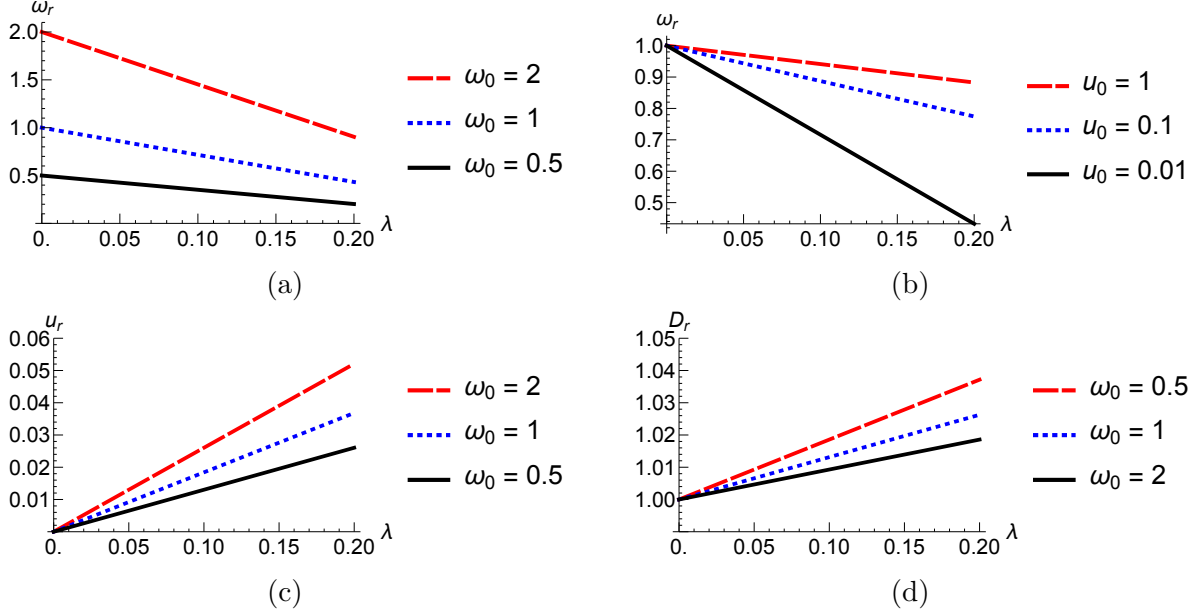


Figure 4.3: Renormalized parameters in one dimension ($d = 1$) in the RPS model: (a) Renormalized frequency ω_r as a function of the reactivity parameter λ , with $D = 1$, $u_0 = 0.01$, and for different bare frequencies ω_0 . (b) Renormalized frequency ω_r as a function of the parameter λ , with $\omega_0 = 1$, $D = 1$, and different bare damping coefficients u_0 . (c) Renormalized u_r as a function of the parameter λ with $D = 1$ and different bare frequencies ω_0 . (d) Renormalized diffusion constant D_r as a function of the parameter λ with $D = 1$ and different bare frequencies ω_0 .

$d = 2$:

In two dimensions, the renormalized variables read

$$\begin{aligned}
 \text{Re}D_r &= D + \frac{3\lambda}{32\pi}, \\
 \omega_r &= \omega_0 \left[1 - \frac{\lambda}{8D\pi} \ln \left(\frac{D\Lambda^2}{u_0} \right) - \frac{\lambda}{D\pi} \left(\frac{1}{16} + \frac{\sqrt{3}\pi}{24} \right) \right], \\
 u_r &= \frac{\sqrt{3}\lambda\omega_0}{48D\pi} (3 + 2 \ln 2).
 \end{aligned} \tag{4.25}$$

Note that we have explicitly introduced the cutoff $\Lambda \sim \pi/c$ to regularize the UV divergence for the renormalized oscillation frequency. We plot ω_r and the damping parameter u_r in Fig. 4.4. The renormalized diffusion constant D_r only linearly depends on the parameter λ . As in the one-dimensional case, the oscillation frequency ω_r diverges as $u_0 \rightarrow 0$. We note that the damping constant u_r is also positive at $d = 2$.

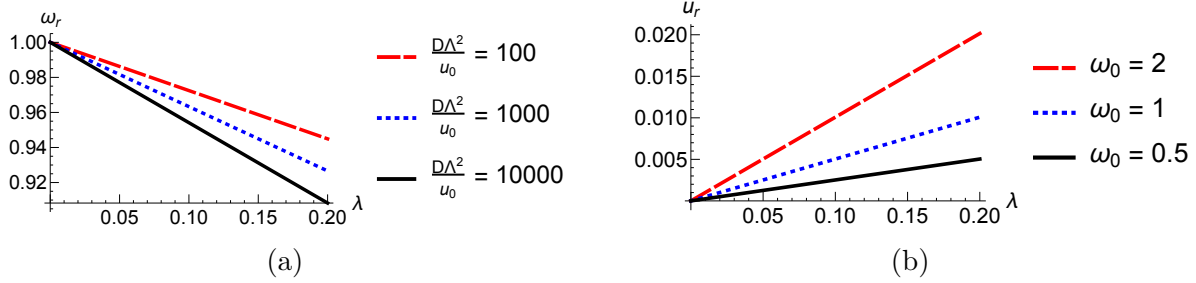


Figure 4.4: Renormalized parameters in two dimensions ($d = 2$) in the RPS model: (a) Renormalized frequency ω_r as a function of the reactivity parameter λ with $D = 1$ and different ratios $D\Delta^2/u_0$. (b) Renormalized damping u_r as a function of the parameter λ with $D = 1$ and different bare frequencies ω_0 .

$d = 3$:

In three dimensions, we may safely set $u_0 = 0$ and the renormalized system parameters follow as

$$\begin{aligned} \text{Re}D_r &= D + \frac{\lambda}{\pi} \sqrt{\frac{\omega_0}{D}} \left(\frac{\sqrt{3}}{192} - \frac{\sqrt{6} - 5\sqrt{2}}{384} \right), \\ \omega_r &= \omega_0 \left[1 - \frac{\lambda}{D\pi} \sqrt{\frac{\omega_0}{D}} \left(\frac{\sqrt{3}}{96} + \frac{5\sqrt{6}}{192} + \frac{\sqrt{2}}{64} \right) \right], \\ u_r &= \frac{\lambda\omega_0}{D\pi} \sqrt{\frac{\omega_0}{D}} \left(-\frac{\sqrt{3}}{96} + \frac{5\sqrt{6}}{192} - \frac{\sqrt{2}}{64} \right). \end{aligned} \quad (4.26)$$

We notice that for $d > 2$ the IR divergences disappear and fluctuation effects become generally weak. u_r is also positive for $d = 3$, as displayed in Fig. 4.5.

We have found that in dimensions $d = 1, 2$, and 3 , the diffusivity D experiences an upward shift, indicating that fluctuations enhance the diffusion. Our results, depicted in Fig. 4.3, 4.4, and 4.5, show that as the reaction rate increases, the characteristic frequency ω_r shifts to smaller values, as the reactions drive the system towards a spatially more homogeneous distribution, leading to slower oscillations. The decline in the characteristic frequencies is in accordance with the numerical simulation data in Ref. [152]. In contrast with the LV model, Monte Carlo simulations of the RPS system do not appear to show strong renormalization

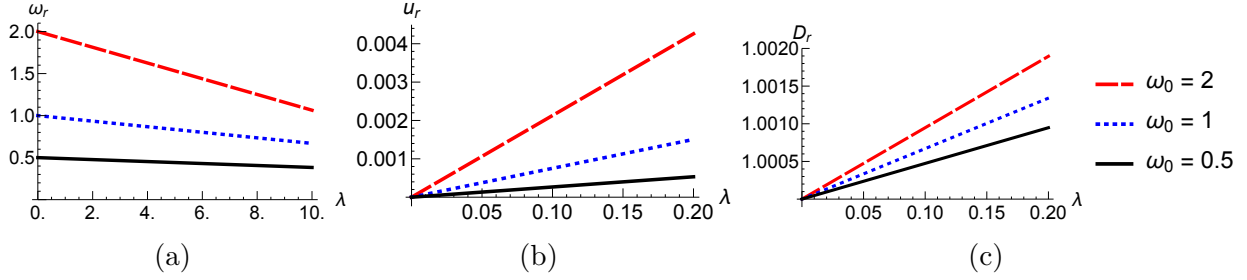


Figure 4.5: Renormalized parameters in three dimensions ($d = 3$) in the RPS model: (a) Renormalized frequency ω_r as a function of the reactivity parameter λ with $D = 1$ and different ratios $D\Lambda^2/u_0$. (b) Renormalized damping u_r as a function of the parameter λ with $D = 1$ and different bare frequencies ω_0 . (c) Renormalized diffusion constant D_r as a function of the parameter λ with $D = 1$ and different bare frequencies ω_0 .

effects [152], although both models feature a logarithmic divergence in two dimensions. The IR divergence in the RPS model appears as a consequence of the fact that the corrections are built using the Gaussian theory which has zero damping, precisely as in the LV model. The positive fluctuation-induced damping μ_r , in contrast to the possibly negative one in the LV model, indicates that the system remains stable against the spontaneous emergence of spatio-temporal structures.

4.3 Stochastic May–Leonard (ML) Model

4.3.1 ML Model and Mean-Field Rate Equations

The following discussion of the mean-field theory, Doi-Peliti action, and Langevin representation for the spatially extended stochastic ML model was laid out in detail in Ref. [158]. Here we summarize the pertinent points needed for our comparison with the RPS model and the computation of the fluctuation corrections to one-loop order. Following the conventions in Ref. [158], the reactions in the ML model read



where $i = 1, 2, 3$ denotes the three competing species, and we identify $B_4 = B_1$ as before. In contrast to the RPS system, the reactions in the ML model do not conserve the total particle number. The first two reactions implement predation and reproduction independently, while the third reaction implements “soft” site occupation constraint to effectively represent a finite carrying capacity. As in the RPS model, we consider a model wherein particles from all three

species perform random walks on a d -dimensional hyper-cubic lattice with L^d sites and lattice constant c . In the large diffusivity limit, the dynamics is governed by the mean-field rate equations

$$\begin{aligned}\frac{db_1(t)}{dt} &= b_1(t) \left(-\sigma b_3(t) + \mu - \kappa b_1(t) \right) , \\ \frac{db_2(t)}{dt} &= b_2(t) \left(-\sigma b_1(t) + \mu - \kappa b_2(t) \right) , \\ \frac{db_3(t)}{dt} &= b_3(t) \left(-\sigma b_2(t) + \mu - \kappa b_3(t) \right) ,\end{aligned}\tag{4.28}$$

where $\sigma = c^d \sigma'$ and $\kappa = c^d \kappa'$ are the volume reaction rates. Instead of a fixed line defined by the initial condition, the ML system displays a unique fixed point at mean-field level. By setting the time derivatives to be 0, the steady-state concentrations are found to be

$$b_i^\infty = \frac{\mu}{\sigma + \kappa} , \quad \forall i \in \{1, 2, 3\} ,\tag{4.29}$$

and the associated stability matrix reads

$$S_{\text{ML}} = -\frac{\mu}{\sigma + \kappa} \begin{pmatrix} \kappa & 0 & \sigma \\ \sigma & \kappa & 0 \\ 0 & \sigma & \kappa \end{pmatrix} .\tag{4.30}$$

Its eigenvalues at the coexistence fixed point are $\{-\mu, -\mu(2\kappa - \sigma \pm i\sqrt{3}\sigma)/2(\sigma + \kappa)\}$. The first eigenvalue $-\mu$ is always negative which implies the stability of the corresponding eigenmode, namely the exponential decay of the total particle number, see below. The imaginary part of the two complex conjugate eigenvalues, $\pm\sqrt{3}\mu\sigma/2(\sigma + \kappa)$, represents the frequency of temporal oscillations for the associate modes, whose amplitudes are either exponentially damped or growing. When $2\kappa > \sigma$, the real part of the complex eigenvalues is negative and the limit circles are stable. Otherwise, for $2\kappa < \sigma$, the limit circles are unstable and one observes the spontaneous formation of spiral structures in the system. In the vicinity of the Hopf bifurcation at $2\kappa = \sigma$, the time evolution of the two modes corresponding to the complex conjugate eigenvalues becomes much slower than the fast relaxing mode, which introduces a natural time scale separation. As a consequence of the critical slowing down near the Hopf bifurcation, the fast relaxing mode can be integrated out and the system is effectively governed by the complex time-dependent Ginzburg–Landau equation [158].

4.3.2 Doi–Peliti Field Theory and Generalized Langevin Equations

The Doi-Peliti action follows from the reactions of the ML model and reads

$$\mathcal{A}^{\text{ML}} = \sum_{i=1,2,3} \int dt d^d x \left[\hat{b}_i (\partial_t - D\nabla^2) b_i + \mu \hat{b}_i b_i (1 - \hat{b}_i) + \kappa \hat{b}_i b_i^2 (\hat{b}_i - 1) \right. \\ \left. + \sigma \hat{b}_i b_i b_{i+1} (\hat{b}_{i+1} - 1) \right]. \quad (4.31)$$

This action does not obey the $U(1)$ global symmetry present in the RPS model; indeed, the total particle number is not conserved under the ML reactions (4.27). Following the Doi shift to the fluctuating auxiliary fields $\tilde{b}_i(\vec{x}, t) = \hat{b}_i(\vec{x}, t) - 1$, the action becomes

$$\mathcal{A}^{\text{ML}} = \sum_{i=1,2,3} \int dt d^d x \left[\tilde{b}_i (\partial_t - D\nabla^2 - \mu) b_i - \mu \tilde{b}_i^2 b_i + \kappa \tilde{b}_i b_i^2 (\tilde{b}_i + 1) \right. \\ \left. + \sigma \tilde{b}_{i+1} b_i b_{i+1} (\tilde{b}_i + 1) \right]. \quad (4.32)$$

As in the RPS model above, we may now view this shifted action as a Janssen–De Dominicis functional which is equivalent to the corresponding generalized Langevin equations

$$\partial_t b_i = D\nabla^2 b_i + \mu b_i - \kappa b_i^2 - \sigma b_i b_{i+2} + \xi_i, \quad (4.33)$$

where $\xi_i(\vec{x}, t)$ represent the multiplicative noise components with correlators

$$\langle \xi_i(\vec{x}_1, t_1) \xi_j(\vec{x}_2, t_2) \rangle = 2\Xi_{ij} \delta^{(d)}(\vec{x}_1 - \vec{x}_2) \delta(t_1 - t_2), \quad (4.34)$$

with

$$\Xi = \begin{pmatrix} \mu b_1 - \kappa b_1^2 & -\frac{\sigma}{2} b_1 b_2 & -\frac{\sigma}{2} b_1 b_3 \\ -\frac{\sigma}{2} b_1 b_2 & \mu b_2 - \lambda b_2^2 & -\frac{\sigma}{2} b_2 b_3 \\ -\frac{\sigma}{2} b_1 b_3 & -\frac{\sigma}{2} b_2 b_3 & \mu b_3 - \lambda b_3^2 \end{pmatrix}. \quad (4.35)$$

4.3.3 Diagonalization of the Harmonic Action

Before diagonalizing the quadratic action, we first shift to fluctuating fields, $\tilde{d}_i(\vec{x}, t) = \tilde{b}_i(\vec{x}, t)$ and $d_i(\vec{x}, t) = b_i(\vec{x}, t) - \frac{\mu}{\sigma + \kappa} - C$. Here C is a counterterm which encodes the fluctuation corrections to the average concentrations. Owing to the cyclic symmetry among the three different species, we only need to introduce a single counterterm. The harmonic part of the action in terms of the new fields $\tilde{d}_i$ and d_i reads

$$\mathcal{A}_0^{\text{ML}} = \sum_i \int dt d^d x \left[\tilde{d}_i \left(\partial_t - D\nabla^2 + \frac{\kappa\mu}{\kappa + \sigma} + (2\kappa + \sigma)C \right) d_i + \left(\frac{\sigma\mu}{\kappa + \sigma} + \sigma C \right) \tilde{d}_i d_{i+1} \right]. \quad (4.36)$$

Since the counterterm C is of first order in the perturbative expansion parameters, up to zeroth order the harmonic part of the action can be diagonalized by the following linear transformation

$$\begin{pmatrix} \tilde{d}_1 \\ \tilde{d}_2 \\ \tilde{d}_3 \end{pmatrix} = \frac{1}{\sqrt{3}} \begin{pmatrix} 1 & -\frac{1-i\sqrt{3}}{2} & -\frac{1+i\sqrt{3}}{2} \\ 1 & -\frac{1+i\sqrt{3}}{2} & -\frac{1-i\sqrt{3}}{2} \\ 1 & 1 & 1 \end{pmatrix} \begin{pmatrix} \tilde{\psi}_o \\ \tilde{\psi}_+ \\ \tilde{\psi}_- \end{pmatrix}, \quad (4.37)$$

and

$$\begin{pmatrix} d_1 \\ d_2 \\ d_3 \end{pmatrix} = \frac{1}{\sqrt{3}} \begin{pmatrix} 1 & -\frac{1+i\sqrt{3}}{2} & -\frac{1-i\sqrt{3}}{2} \\ 1 & -\frac{1-i\sqrt{3}}{2} & -\frac{1+i\sqrt{3}}{2} \\ 1 & 1 & 1 \end{pmatrix} \begin{pmatrix} \psi_o \\ \psi_+ \\ \psi_- \end{pmatrix}. \quad (4.38)$$

After applying this linear transformation, the action can be expressed as $\mathcal{A}^{\text{ML}} = \mathcal{A}_0^{\text{ML}} + \mathcal{A}_s^{\text{ML}} + \mathcal{A}_{\text{int}}^{\text{ML}}$, representing, respectively, the harmonic, source, and non-linear interaction terms. Again, we omit the four-point vertices, since they will not contribute to the dispersion relation renormalizations at one-loop order. The other terms are

$$\begin{aligned} \mathcal{A}_0^{\text{ML}} = \int dt d^d x & \left[\tilde{\psi}_o (\partial_t - D\nabla^2 + \mu + 2(\sigma + \kappa)C) \psi_o + \tilde{\psi}_+ (\partial_t - D\nabla^2 + \gamma_0 + i\nu_0) \psi_+ \right. \\ & + \tilde{\psi}_- (\partial_t - D\nabla^2 + \gamma_0 - i\nu_0) \psi_- \\ & \left. + \frac{1}{2} (\sigma + 4\kappa + i\sqrt{3}\sigma) C \tilde{\psi}_+ \psi_+ + \frac{1}{2} (\sigma + 4\kappa - i\sqrt{3}\sigma) C \tilde{\psi}_- \psi_- \right], \end{aligned} \quad (4.39)$$

$$\begin{aligned} \mathcal{A}_s^{\text{ML}} = \int dt d^d x & \left[(\mu C + (\kappa + \sigma)C^2) (\sqrt{3}\tilde{\psi}_o + \tilde{\psi}_o^2) \right. \\ & \left. + \left(-\frac{3\mu^2\sigma}{(\kappa + \sigma)^2} + 2\mu\frac{\kappa - 2\sigma}{\kappa + \sigma} C + (2\kappa - \sigma)C^2 \right) \tilde{\psi}_+ \tilde{\psi}_- \right], \end{aligned} \quad (4.40)$$

$$\begin{aligned} \mathcal{A}_{\text{int}}^{\text{ML}} = \int dt d^d x & \left[\left(\frac{\mu(\kappa - 2\sigma)}{\sqrt{3}(\kappa + \sigma)} + \frac{2\kappa - \sigma}{\sqrt{3}} C \right) (\tilde{\psi}_+^2 \psi_- + \tilde{\psi}_-^2 \psi_+) + \frac{\kappa + \sigma}{\sqrt{3}} \tilde{\psi}_o \psi_o^2 \right. \\ & + \left(\frac{\mu}{\sqrt{3}} + \frac{2(\kappa + \sigma)}{\sqrt{3}} C \right) \tilde{\psi}_o^2 \psi_o + \left(\frac{\mu(2\kappa - \sigma)}{\sqrt{3}(\kappa + \sigma)} + \frac{4\kappa + \sigma}{\sqrt{3}} C \right) (\tilde{\psi}_o \tilde{\psi}_+ \psi_+ + \tilde{\psi}_o \tilde{\psi}_- \psi_-) \\ & + \frac{\sqrt{3}}{6} (2\kappa - \sigma + \sqrt{3}i\sigma) \tilde{\psi}_- \psi_+^2 + \frac{\sqrt{3}}{6} (2\kappa - \sigma - \sqrt{3}i\sigma) \tilde{\psi}_+ \psi_-^2 + \frac{2\kappa - \sigma}{\sqrt{3}} \tilde{\psi}_o \psi_+ \psi_- \\ & \left. + \frac{\sqrt{3}}{6} (4\kappa + \sigma - \sqrt{3}i\sigma) \tilde{\psi}_- \psi_o \psi_- + \frac{\sqrt{3}}{6} (4\kappa + \sigma + \sqrt{3}i\sigma) \tilde{\psi}_+ \psi_o \psi_+ + \text{four-point vertices} \right], \end{aligned} \quad (4.41)$$

where $\gamma_0 = \mu(2\kappa - \sigma)/2(\sigma + \kappa)$ and $\nu_0 = \sqrt{3}\mu\sigma/2(\sigma + \kappa)$. The ψ_o mode corresponds to the fluctuation of the total particle density and decays exponentially at tree level. In contrast to the RPS model, the ML $\psi_{\pm}$ modes display non-vanishing dissipation γ_0 already on the mean-field level. As mentioned above, a Hopf bifurcation occurs at $2\kappa = \sigma$; when $2\kappa < \sigma$, the system is unstable and spiral structures are spontaneously generated. In the

perturbative regime, the assumed tiny fluctuation corrections should not change the overall stability features, but will only shift the Hopf bifurcation point by a small amount.

4.3.4 One-loop Fluctuation Corrections



Figure 4.6: Contributions to $\langle\psi_o\rangle$ in the ML model up to one-loop order. The solid lines represent the $\psi_{\pm}$ modes as indicated, while the dashed lines denotes the ψ_o mode.

Prior to calculating the renormalized quantities, we need to determine the counterterm C by requiring the average fluctuation of the total density to be zero, $\langle\psi_o\rangle = 0$. Up to one-loop order, the contributions to $\langle\psi_o\rangle$ are shown in Fig. 4.6. We note that the second diagram in Fig. 4.6 is of second order and thus can be dropped. The corresponding analytic expression results in

$$C = -\frac{\mu\sigma(2\kappa - \sigma)}{2D(\kappa + \sigma)^2} \int_k \frac{1}{k^2 + \frac{\gamma_0}{D}}. \quad (4.42)$$

We may now proceed to the fluctuation renormalization of the two-point vertex functions $\Gamma_{\tilde{\psi}_o\psi_o}^{(1,1)}$ and $\Gamma_{\tilde{\psi}_{\pm}\psi_{\pm}}^{(1,1)}$, which encode the self-energies entering the dispersion relation of the ψ_o and $\psi_{\pm}$ modes. As the total particle number is not conserved in the ML model, the dispersion relation acquires non-trivial corrections from the perturbation expansion. The one-loop diagrams that contribute to the vertex function $\Gamma_{\tilde{\psi}_o\psi_o}^{(1,1)}$ are pictured in Fig. 4.7. The last diagram is of higher order and thus can be omitted; this results in

$$\begin{aligned} \Gamma_{\tilde{\psi}_o\psi_o}^{(1,1)}(p, \omega) = & i\omega + Dp^2 + \mu + 2(\kappa + \sigma)C - \frac{\mu(\kappa + \sigma)}{3D} \int_k I\left(\frac{\mu}{D}\right) \\ & - \frac{2(\sigma + \kappa)\gamma_0}{3D\mu} (\gamma_0 - \sqrt{3}\nu_0) \int_k I\left(\frac{\gamma_0}{D}\right) - \frac{2\sqrt{3}(\sigma + \kappa)\gamma_0\nu_0}{3D^2\mu} (\gamma_0 + \mu) \int_k \frac{1}{k^2 + \frac{\gamma_0}{D}} I\left(\frac{\gamma_0}{D}\right). \end{aligned} \quad (4.43)$$

Provided $\gamma_0 > 0$, all corrections at one-loop level are real, and no imaginary part appears in the mass term of the ψ_o mode, hence there are no total particle number oscillations. However, for $\gamma_0 < 0$ the system exhibits emergent oscillations of the total particle number, indicating the spontaneous formation of spatio-temporal structures. As the renormalized two-point vertex function can also be written as

$$\Gamma_{\tilde{\psi}_o\psi_o}^{(1,1)}(p, \omega) = Z_{\phi_o} (i\omega + D_r^o p^2 + \mu_r), \quad (4.44)$$

the renormalized diffusivity D_r^o and mass parameter μ_r can be calculated accordingly. Here, Z_{ϕ_o} absorbs all wave function renormalizations. Since the rotating wave modes $\psi_{\pm}$ acquires

a different diffusivity renormalization from the o mode, we carefully distinguish the renormalized quantities $D_r^\pm$ and D_r^o .

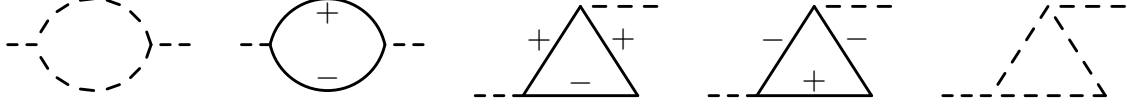


Figure 4.7: One-loop fluctuation contributions to the two-point vertex function $\Gamma_{\tilde{\psi}_o\psi_o}^{(1,1)}$ in the ML model.

The explicit expressions for D_r^o and μ_r read

$$\begin{aligned} \mu_r &= \mu \left[1 - \frac{2(\sigma + \kappa)}{3D} \frac{\gamma_0}{\mu} \int_k \frac{1}{k^2 + \frac{\gamma_0}{D}} - \frac{\sigma + \kappa}{3D} \int_k \frac{1}{k^2 + \frac{\mu}{D}} - \frac{\mu(\sigma + \kappa)}{6D^2} \int_k \frac{1}{(k^2 + \frac{\mu}{D})^2} \right. \\ &\quad \left. - \frac{(\sigma + \kappa)\gamma_0}{3D^2} \left(1 + \frac{2\sqrt{3}\nu_0\gamma_0}{\mu^2} \right) \int_k \frac{1}{(k^2 + \frac{\gamma_0}{D})^2} - \frac{\sqrt{3}(\sigma + \kappa)}{3D^3} \frac{\nu_0\gamma_0(\gamma_0 + \mu)}{\mu} \int_k \frac{1}{(k^2 + \frac{\gamma_0}{D})^3} \right], \\ D_r^o &= D - \frac{\mu(\sigma + \kappa)}{3dD} \int_k \frac{k^2}{(k^2 + \frac{\mu}{D})^3} - \frac{2(\sigma + \kappa)}{3dD} \frac{\gamma_0}{\mu} (\gamma_0 - \sqrt{3}\nu_0) \int_k \frac{k^2}{(k^2 + \frac{\gamma_0}{D})^3} \\ &\quad - \frac{2\sqrt{3}(\sigma + \kappa)}{3dD^2} \frac{\nu_0\gamma_0}{\mu} (\gamma_0 + \mu) \int_k \frac{k^2}{(k^2 + \frac{\gamma_0}{D})^4}. \end{aligned} \quad (4.45)$$

After evaluating the integrals one arrives at

$$\begin{aligned} \mu_r &= 1 - \frac{\Gamma(1 - d/2)}{2^d \pi^{d/2}} \left(\frac{\sigma + \kappa}{3D} \left(\frac{\mu}{D} \right)^{d/2-1} + \frac{2(\sigma + \kappa)\gamma_0}{3D\mu} \left(\frac{\gamma_0}{D} \right)^{d/2-1} \right) \\ &\quad - \frac{\Gamma(2 - d/2)}{2^d \pi^{d/2}} \left[\frac{\mu(\sigma + \kappa)}{6D^2} \left(\frac{\mu}{D} \right)^{d/2-2} + \frac{(\sigma + \kappa)\gamma_0}{3D^2} \left(1 + \frac{2\sqrt{3}\nu_0\gamma_0}{\mu^2} \right) \left(\frac{\gamma_0}{D} \right)^{d/2-2} \right] \\ &\quad - \frac{\Gamma(3 - d/2)}{2^d \pi^{d/2}} \frac{\sqrt{3}(\sigma + \kappa)\nu_0\gamma_0}{3D^3\mu} (\gamma_0 + \mu) \left(\frac{\gamma_0}{D} \right)^{d/2-3}, \\ D_r^o &= D - \frac{\Gamma(2 - d/2)}{2^{d+2} \pi^{d/2}} \left[\frac{\mu(\sigma + \kappa)}{3D} \left(\frac{\mu}{D} \right)^{d/2-2} + \frac{2(\sigma + \kappa)\gamma_0}{3D\mu} (\gamma_0 - \sqrt{3}\nu_0) \left(\frac{\gamma_0}{D} \right)^{d/2-2} \right] \\ &\quad - \frac{\Gamma(3 - d/2)}{3 \cdot 2^{d+2} \pi^{d/2}} \frac{2\sqrt{3}(\sigma + \kappa)}{3D^2\mu} \nu_0\gamma_0(\gamma_0 + \mu) \left(\frac{\gamma_0}{D} \right)^{d/2-3}. \end{aligned} \quad (4.46)$$

For $d \geq 2$, UV divergences in μ_r are manifest; but since the lattice constant c serves as a natural UV cutoff in lattice models, we will not discuss these UV divergences further.

The renormalized vertex function $\Gamma_{\tilde{\psi}_\pm\psi_\pm}^{(1,1)}$ can also be calculated according to the one-loop

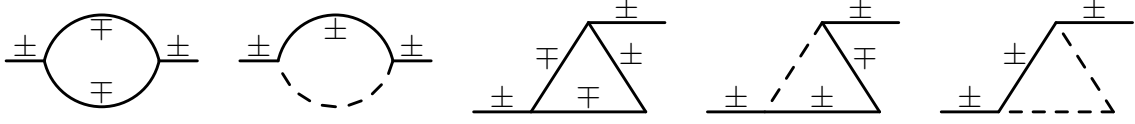


Figure 4.8: One-loop fluctuation contributions to the two-point vertex functions $\Gamma_{\tilde{\psi}_{\pm}\psi_{\pm}}^{(1,1)}$ in the ML model.

diagrams in Fig. 4.8, resulting in

$$\begin{aligned}
 \Gamma_{\tilde{\psi}_{\pm}\psi_{\pm}}^{(1,1)}(p, \omega) = & i\omega + Dp^2 + \gamma_0 \pm i\nu_0 + \frac{\sigma + \kappa}{\mu} (\gamma_0 + \mu \pm i\nu_0) C \\
 & - \frac{(\kappa + \sigma)(\gamma_0 - \sqrt{3}\nu_0)}{3D\mu} (\gamma_0 \mp i\nu_0) \int_k I\left(\frac{\gamma_0 \mp i\nu_0}{D}\right) \\
 & - \frac{(\sigma + \kappa)\gamma_0}{3D\mu} (\gamma_0 + \mu \pm i\nu_0) \int_k I\left(\frac{\gamma_0 + \mu \pm i\nu_0}{2D}\right) \\
 & - \frac{2\sqrt{3}(\sigma + \kappa)\nu_0}{3D^2\mu} (\gamma_0^2 + \nu_0^2) \int_k \frac{1}{k^2 + \frac{\gamma_0}{D}} I\left(\frac{\gamma_0 \mp i\nu_0}{D}\right) \\
 & - \frac{\sqrt{3}(\sigma + \kappa)\gamma_0\nu_0}{3D^2\mu} (\gamma_0 + \mu \pm i\nu_0) \int_k \frac{1}{k^2 + \frac{\gamma_0}{D}} I\left(\frac{\gamma_0 + \mu \pm i\nu_0}{2D}\right).
 \end{aligned} \tag{4.47}$$

Upon invoking the relation with renormalized quantities

$$\Gamma_{\tilde{\psi}_{\pm}\psi_{\pm}}^{(1,1)}(p, \omega) = Z_{\phi_{\pm}} (i\omega + D_r^{\pm} p^2 + \gamma_r \pm i\nu_r), \tag{4.48}$$

the expressions for the renormalized parameters γ_r and ν_r are readily inferred,

$$\begin{aligned}
 \gamma_r \pm i\nu_r = & \gamma_0 \pm i\nu_0 + (\sigma + \kappa) \left[M_1^{(\pm)} \frac{\Gamma(1 - d/2)}{2^d \pi^{d/2}} \left(\frac{\gamma_0}{D}\right)^{d/2-1} \right. \\
 & + M_2^{(\pm)} \frac{\Gamma(1 - d/2)}{2^d \pi^{d/2}} \left(\frac{\gamma_0^2 + \nu_0^2}{D^2}\right)^{(d-2)/4} \exp\left(\mp i \frac{d-2}{2} \theta\right) \\
 & + M_3^{(\pm)} \frac{\Gamma(1 - d/2)}{2^d \pi^{d/2}} \left(\frac{(\mu + \gamma_0)^2 + \nu_0^2}{4D^2}\right)^{(d-2)/4} \exp\left(\pm i \frac{d-2}{2} \eta\right) \\
 & + M_4^{(\pm)} \frac{\Gamma(2 - d/2)}{2^d \pi^{d/2}} \left(\frac{\gamma_0^2 + \nu_0^2}{D^2}\right)^{(d-4)/4} \exp\left(\mp i \frac{d-4}{2} \theta\right) \\
 & \left. + M_5^{(\pm)} \frac{\Gamma(2 - d/2)}{2^d \pi^{d/2}} \left(\frac{(\mu + \gamma_0)^2 + \nu_0^2}{4D^2}\right)^{(d-4)/4} \exp\left(\pm i \frac{d-4}{2} \eta\right) \right],
 \end{aligned} \tag{4.49}$$

where the coefficients $M_i^{(\pm)}$ are defined in Eq. (4.91) in the appendix, and the angles θ and η are given by $\tan \theta = \nu_0/\gamma_0$ and $\tan \eta = \nu_0/(\gamma_0 + \mu)$. We note that at odd dimensions d , the first term in the bracket in Eq. (4.49) switches from real to imaginary as γ_0 changes its sign;

however, at even dimensions, this term is always real. Finally, the renormalized diffusivity reads

$$\begin{aligned}
D_r^\pm = D - \frac{\kappa + \sigma}{d 2^d \pi^{d/2}} & \left[\Gamma(1 - d/2) P_1^{(\pm)} \left(\frac{\gamma_0^2 + \nu_0^2}{D^2} \right)^{(d-2)/4} \exp\left(\mp i \frac{d-2}{2} \theta\right) \right. \\
& + \Gamma(2 - d/2) P_2^{(\pm)} \left(\frac{\gamma_0^2 + \nu_0^2}{D^2} \right)^{(d-4)/4} \exp\left(\mp i \frac{d-4}{2} \theta\right) \\
& + \frac{\Gamma(3 - d/2)}{2} P_3^{(\pm)} \left(\frac{\gamma_0^2 + \nu_0^2}{D^2} \right)^{(d-6)/4} \exp\left(\mp i \frac{d-6}{2} \theta\right) \\
& + \Gamma(1 - d/2) Q_1^{(\pm)} \left(\frac{(\mu + \gamma_0)^2 + \nu_0^2}{4D^2} \right)^{(d-2)/4} \exp\left(\pm i \frac{d-2}{2} \eta\right) \\
& + \Gamma(2 - d/2) Q_2^{(\pm)} \left(\frac{(\mu + \gamma_0)^2 + \nu_0^2}{4D^2} \right)^{(d-4)/4} \exp\left(\pm i \frac{d-4}{2} \eta\right) \\
& + \frac{\Gamma(3 - d/2)}{2} Q_3^{(\pm)} \left(\frac{(\mu + \gamma_0)^2 + \nu_0^2}{4D^2} \right)^{(d-6)/4} \exp\left(\pm i \frac{d-6}{2} \eta\right) \\
& \left. - \Gamma(1 - d/2) \left(P_1^{(\pm)} + Q_1^{(\pm)} \right) \left(\frac{\gamma_0}{D} \right)^{(d-2)/2} \right]. \tag{4.50}
\end{aligned}$$

In the appendices, we provide additional details and the definitions of the various coefficients, as well as explicit evaluations for $d = 1, 2, 3$. Here, we focus on the behavior of the damping parameter μ_r across different dimensions. It is important to note that μ_r is generally a complex number: Its imaginary part conveys information about spatial oscillations, while its real part represents either exponential decay or growth of the average particle density.

$d = 1$:

In one dimension, the renormalized damping parameter μ_r reads

$$\mu_r = \mu \left[1 - \frac{5(\sigma + \kappa)}{24D} \sqrt{\frac{D}{\mu}} - \frac{\sigma + \kappa}{D} \sqrt{\frac{D}{\gamma_0}} \left(\frac{1}{12} + \frac{\gamma_0}{3\mu} + \frac{\sqrt{3}\nu_0}{16\mu} + \frac{\sqrt{3}\nu_0}{16\gamma_0} + \frac{\sqrt{3}\nu_0\gamma_0}{6\mu^2} \right) \right]. \tag{4.51}$$

For $\gamma_0 < 0$, μ_r acquires an imaginary part, indicating oscillatory behavior. However, if $\gamma_0 > 0$, there is only damping. We display different scenarios in Fig. 4.9.

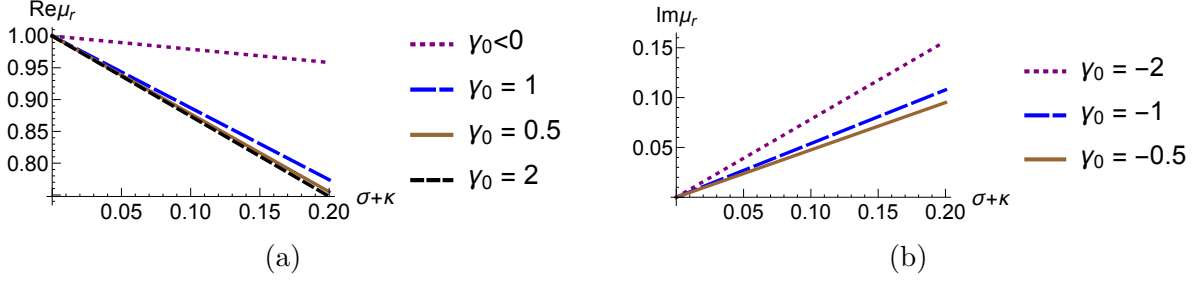


Figure 4.9: Renormalized μ_r in one dimension ($d = 1$): (a) Real part of μ_r as a function of $\sigma + \kappa$ with $D = 1$, $\mu = 1$, $\nu_0 = 1$, and different values of γ_0 . (b) Imaginary part of u_r as a function of λ with $D = 1$, $\mu = 1$, $\nu_0 = 1$, and different $\gamma_0 < 0$.

$d = 2$:

At two dimensions, we need to introduce the UV cutoff $\Lambda \sim \pi/c$; the damping parameter becomes

$$\mu_r = \mu \left[1 - \frac{\sigma + \kappa}{6D\pi} \frac{\gamma_0}{\mu} \ln \frac{D\Lambda^2}{\gamma_0} - \frac{\sigma + \kappa}{12D\pi} \ln \frac{D\Lambda^2}{\mu} - \frac{\sigma + \kappa}{24D\pi} - \frac{\sigma + \kappa}{12D\pi} \left(1 + \frac{\sqrt{3}\nu_0}{2\mu} + \frac{\sqrt{3}\nu_0}{2\gamma_0} + \frac{2\sqrt{3}\nu_0\gamma_0}{\mu^2} \right) \right]. \quad (4.52)$$

As in the one-dimensional case, when $\gamma_0 > 0$, we have pure damping, whereas the system displays population oscillations if $\gamma_0 < 0$. The damping coefficients μ_r at $d = 2$ for different bare parameters are plotted in Fig. 4.10.

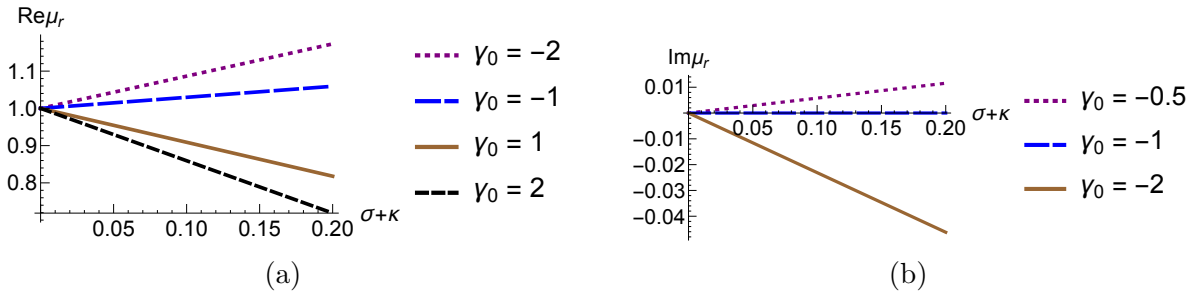


Figure 4.10: Renormalized μ_r at two dimensions ($d = 2$) with cutoff $\Lambda^2 = 10000$: (a) Real part of μ_r as a function of $\sigma + \kappa$ with $D = 1$, $\mu = 1$, $\nu_0 = 1$, and different values of γ_0 . (b) Imaginary part of u_r as a function of λ with $D = 1$, $\mu = 1$, $\nu_0 = 1$, and different $\gamma_0 < 0$.

$d = 3$:

In three dimensions, the damping parameter reads

$$\mu_r = \mu \left[1 + \frac{\sigma + \kappa}{16D\pi} \sqrt{\frac{\mu}{D}} + \frac{\sigma + \kappa}{6D\pi} \sqrt{\frac{\gamma_0}{D}} \left(-\frac{1}{4} + \frac{\gamma_0}{\mu} - \frac{\sqrt{3}\nu_0}{16\mu} - \frac{\sqrt{3}\nu_0}{16\gamma_0} - \frac{\sqrt{3}\nu_0\gamma_0}{2\mu^2} \right) \right]. \quad (4.53)$$

Again, oscillations emerge in the region where $\gamma_0 < 0$. The real and imaginary parts of the damping parameter μ are depicted in Fig. 4.11.

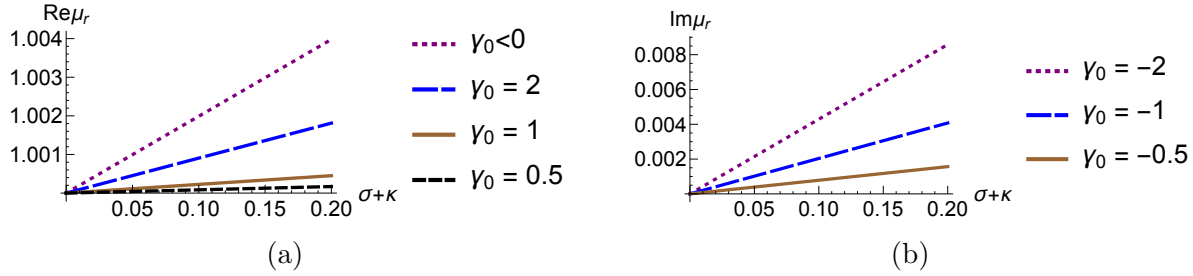


Figure 4.11: Renormalized μ_r at three dimensions ($d = 3$): (a) Real part of μ_r as a function of $\sigma + \kappa$ with $D = 1$, $\mu = 1$, $\nu_0 = 1$, and different values of γ_0 . (b) Imaginary part of u_r as a function of λ with $D = 1$, $\mu = 1$, $\nu_0 = 1$, and different $\gamma_0 < 0$.

For $\nu_0 = 1$, the damping μ_r decreases in one and two dimensions, but increases in three dimensions in the stable region where $\gamma_0 > 0$, as shown in Figs. 4.9, 4.10, and 4.11. This indicates that the reactions effectively slow down the relaxation processes in one and two dimensions, but speed them up in three dimensions. However, due to the highly nonlinear dependence on the parameters μ_0 , γ_0 , and ν_0 , a more general conclusion cannot be made. It is worth noting that in the unstable region, an imaginary part of μ_r is generated, formally resulting from the subtraction of an inadequate homogeneous steady state. Yet these emergent oscillations manifestly indicate the instability with respect to spontaneous formation of spatio-temporal patterns in this regime. We emphasize again that the one-loop fluctuation corrections should merely induce small quantitative corrections, and cannot induce qualitative changes in the region where perturbation theory is applicable. The ML system thus maintains a bifurcation point, below which the homogeneous ground state is rendered unstable and spiral structures emerge.

4.4 Comparison between the RPS, ML, and LV Models

In this section, we present a thorough comparison between the spatically extended stochastic LV, RPS, and ML models. We specifically discuss the spontaneous formation of spatio-temporal structures and the stability of the homogeneous state up to perturbative one-loop

order in the fluctuation corrections. We also briefly address the influence of quenched spatial disorder in the reaction rates in the perturbative regime.

4.4.1 Spiral Formation from a Single Lattice Site Point of View

It is well-established that in sufficiently large spatial systems, the ML model displays spontaneously emerging dynamic spiral structures in individual simulation runs (these are of course averaged out in ensemble averages). Here, we propose that one crucial necessary condition for the formation of such persistent spatio-temporal patterns is the existence of a stable and uniform oscillation frequency at the local lattice site level, which then allows spatially extended coherent oscillatory features.

Each site in a lattice subject to stochastic reactions and spreading processes can be regarded as a separate system that is coupled to a particle reservoir (in the thermodynamic limit). In the ML model, at the (linearized) mean-field level, the local oscillation frequency is uniquely determined by the reaction rates, as is also apparent in the diagonalized ML Doi–Peliti action (4.39) at tree level. A similar definition of the oscillation frequency at linearized mean field level can also be obtained in the LV model [177]. However, in the RPS model at tree level, the oscillation frequency is set by the global conserved particle number ρ . As the particle number at each site is changing all the time owing to its coupling to the environment that serves as a nonlocal reservoir, there does not exist a unique characteristic oscillation frequency for each site during any single run stochastic realization. Ultimately, these nonlocal effects originate from the long-range correlations introduced by the global particle number conservation law, whose relevance in the context of pattern formation was demonstrated in Ref. [149]. The average of the oscillation frequency with a fixed total particle number is given by the expression in the diagonalized RPS Doi–Peliti action (4.18).

These straightforward tree-level arguments are readily generalized to all (loop) orders in the perturbation expansion. In the ML model, no nonlinear terms that depend on the total particle density (or any other global quantity) are present in the action, and thus the renormalized frequency will also be independent of the particle number density. This is not the case for the RPS model, where ρ manifestly enters the vertices. A perhaps more straightforward way to understand this distinction invokes the fixed points (stationary species densities) of the systems. In the RPS system, there exists a fixed line that is parameterized by the conserved total particle number. For each lattice site in the RPS model, the population oscillations wander along this fixed line with a mean that corresponds to the averaged local total particle number at this specific site. In contrast, the ML and LV models have unique fixed points, independent of any global constraints that originate from conservation laws, and consequently all lattice sites are governed by identical oscillation frequencies determined by these fixed points.

To illustrate these points, we plot the time evolution of the population density of a single species at two randomly chosen lattice sites in a single simulation run for the RPS and ML

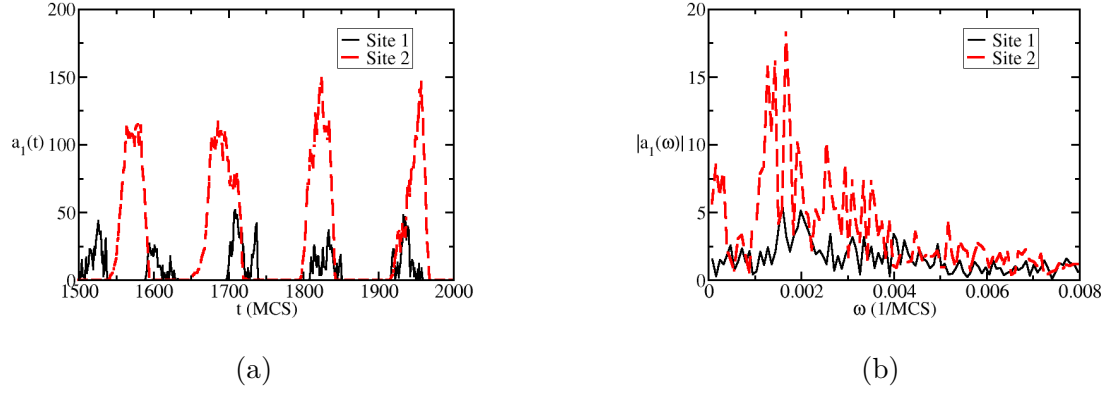


Figure 4.12: (a) Time evolution of the density of species A_1 in the RPS model on two randomly chosen sites; (b) frequency spectrum of the time series in (a) obtained through a Fourier transform. The simulation was run with a reaction rate 0.5 and on a lattice with 100×100 sites. The reactions in the simulation take place off-site and no additional hopping processes are incorporated.

models in Figs. 4.12 and 4.13, respectively. For the RPS species density, the time intervals separating different peaks are not regularly spaced for the two lattice sites. Correspondingly, its Fourier transform displays multiple peaks with almost equal intensities, and no well-defined characteristic frequency is discernible. In contrast, the peaks in the ML species density time evolution are evenly separated, and hence a dominant Fourier peak emerges. These numerical observations support our analysis that the frequency in a single run in the ML model is well-defined, while that is clearly not the case for the RPS system. Yet a well-defined oscillation frequency clearly constitutes a necessary condition to form spatio-temporal patterns.

Although the arguments in this section are formulated in the framework of individual sites in a regular lattice, they are readily extended to an effective unit cell that is similar in size to the characteristic diffusion length scale, or to models defined on a continuum which require a finite reaction range. As long as the system size is much larger than any of these small length scales (that provide suitable ultraviolet cutoffs for the continuum field theory), the specific microscopic details implemented in numerical simulations are not expected to have a significant impact on our conclusions.

4.4.2 Stability of the Homogeneous Ground States against Fluctuations (to One-Loop Order)

While we posit above that a stable oscillation frequency at each lattice site is a necessary requirement to form oscillatory spatio-temporal patterns such as spirals, this is not a sufficient

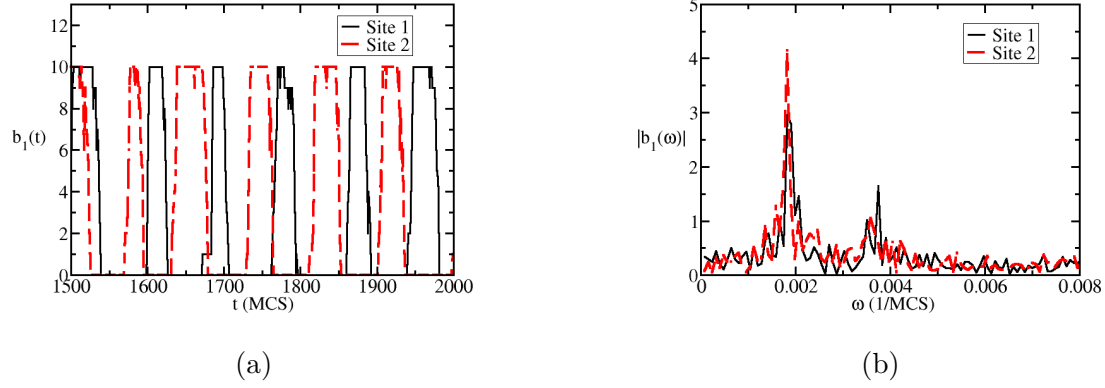


Figure 4.13: (a) Time evolution of the density of species B_1 in the ML model on two randomly chosen sites; (b) frequency spectrum of the time series in (a) obtained through a Fourier transform. In the simulation, the predation and reproduction rates are both set to 0.5 and the system size is 100×100 lattice sites. The reactions in the simulation take place off-site, and no additional hopping processes are incorporated.

condition. Another crucial ingredient is of course that the spatially homogeneous stationary state is rendered unstable; fluctuations of a certain wavevector range will then spontaneously generate spatial patterns. [179, 180]

In the stochastic spatially extended LV model [177], in the absence of site restrictions, the population oscillation damping vanishes in the Gaussian approximation. To one-loop order, a negative damping frequency is generated which indicates an instability of the spatially uniform system, inducing nontrivial particle transport that in turn drives the formation of expanding evasion-pursuit activity waves. In the ML model, the damping coefficient is already nonzero in the Gaussian approximation. As stated above, when $2\kappa < \sigma$, the limit cycles of the ML model become unstable and spiral structures emerge. Yet within the realm of a perturbative approach, any fluctuation corrections will only shift the Hopf bifurcation point, but cannot qualitatively change the system's overall features. In contrast, the RPS system behaves similarly to the LV system, as we encounter a vanishing damping coefficient in the Gaussian approximation. However, at one-loop level, the generated mass term is positive indicating merely a generated finite damping constant, as opposed to its negative counterpart in the LV model. Hence the RPS model remains inert against spontaneous pattern formation. Higher-order terms in the fluctuation expansion should not overturn the sign of the one-loop results within the perturbative regime, which renders this argument perturbatively robust.

4.4.3 Influence of Quenched Spatially Disordered Reaction Rates

In this part, we briefly investigate the effect of spatially disordered, uniformly distributed quenched reaction probabilities on the fluctuation corrections. We start with the Doi–Peliti action

$$\mathcal{A} = \int dt d^d x [\mathcal{L}_0(\hat{a}_i, a_i) + \mathcal{L}'(\hat{a}_i, a_i)], \quad (4.54)$$

where $\mathcal{L}_0$ and $\mathcal{L}'$ are (usually polynomial) functions of the fields $\{\hat{a}_i\}$ and $\{a_i\}$. We introduce spatial disorder to $\mathcal{L}'$, which we take to represent stochastic reactions while $\mathcal{L}_0$ encodes particle diffusions. The action with quenched spatial disorder is then given by

$$\mathcal{A}_D = \int dt d^d x \mathcal{L}_0 + \int d^d x \eta(\vec{x}) \int d\mathcal{L}'; \quad (4.55)$$

here, we assume $\eta(\vec{x})$ to be uniformly distributed in the interval $[0, 2]$ with mean $\bar{\eta} = 1$. Note that the reaction rates are only spatially disordered and remain fixed in time. The average of any observables follows from Eq. (4.68) through

$$\overline{\langle O(t) \rangle} \propto \prod_{\vec{x}} \int_0^2 \frac{d\eta(\vec{x})}{2} \int \prod_i \mathcal{D}[\hat{a}_i] \mathcal{D}[a_i] O(\{\hat{a}_i, a_i\}) e^{-\mathcal{A}_D}, \quad (4.56)$$

where the overline denotes the quenched disorder average. We can readily integrate out the disorder $\eta(\vec{x})$ first, since the observable O is independent of the random variables η , and arrive at

$$\overline{\langle O(t) \rangle} \propto \int \prod_i \mathcal{D}[\hat{a}_i] \mathcal{D}[a_i] O(\{\hat{a}_i, a_i\}) e^{-\mathcal{A}'_D}, \quad (4.57)$$

with

$$\mathcal{A}'_D = \mathcal{A} + \int d^d x \ln \left[\frac{\sinh(\int dt \mathcal{L}')}{\int dt \mathcal{L}'} \right]. \quad (4.58)$$

Incorporating disorder in the original Doi–Peliti action (4.54) thus effectively leads to an additional term that is nonlocal in the time domain, owing to the temporally fixed reaction rates. However, in the perturbative regime where $\mathcal{L}'$ is small, this extra term can be expanded near $\mathcal{L}' = 0$:

$$\ln \left[\frac{\sinh(\int dt \mathcal{L}')}{\int dt \mathcal{L}'} \right] = \frac{1}{3} \int dt dt' \mathcal{L}'_t \mathcal{L}'_{t'} + \mathcal{O}(\mathcal{L}'^3), \quad (4.59)$$

where the labels t and t' distinguish the different time dependences. It is evident from this expansion that the extra temporally nonlocal term “entangles” different replicas of the system. However, as the first term is already second-order in $\mathcal{L}'$, it is of higher order than the original action $\mathcal{A}$, and should not markedly affect the system’s fluctuation corrections in the naive perturbation regime, at least to low loop orders. This observation may account for the insensitivity of the RPS and ML models to quenched randomness in the reaction rates, as reported in Refs. [152, 155]. We remark that the stronger effects of varying predation rates λ in the LV system can be largely traced to the sensitivity $\sim 1/\lambda$ of the stationary species densities already on the mean-field approximation level [173].

4.5 Summary and Conclusions

In this chapter, we have investigated the dynamics of the RPS and ML models up to one-loop order in the fluctuation corrections by means of a perturbative field-theoretical analysis. We utilized the Doi–Peliti formalism to obtain the dynamical probability functional for the stochastic Markovian dynamics, and also extracted the equivalent generalized Langevin equations. In the Gaussian theory, as expected, the RPS model displays only purely oscillatory modes in addition to the strictly diffusive conserved total particle density. In the ML model, a Hopf bifurcation point appears at $2\kappa - \sigma = 0$ that separates the parameter space into stable and unstable regions; in the latter regime, spiral structures are spontaneously generated.

The one-loop fluctuation corrections in the RPS model, which are of first order in the effective nonlinear coupling $\lambda/D \ll 1$, generate dissipation. We have found that in the physically accessible dimensions $d = 1, 2, 3$, the damping coefficient is always positive. This indicates the stability of the spatially uniform stationary state in the RPS model, at least in the perturbative regime. Thus, our analysis sheds light on the absence of spatio-temporal structures in the RPS model. In addition, the one-loop correction to the oscillation frequency is IR divergent due to the dissipation-free nature of the mean-field modes, very similar to the LV model. However, outside the range of validity of the perturbation expansion, the damping terms become sizeable; hence we argue that this IR divergence becomes naturally regularized. This explains why no significant fluctuation corrections to the oscillation frequency have as yet been numerically observed in computer simulations, which have invariably been situated far away from the perturbative regime.

In the ML model, as both the dissipation and oscillation frequencies are already finite at mean-field level, the one-loop fluctuation corrections should not qualitatively modify the mean-field conclusions. Since both propagating modes are massive due to the finite damping coefficients, the ML system does not display any IR singularities. Hence the ML model is insensitive to fluctuations at least perturbatively, and in the region where the homogeneous steady state is stable. Moreover, we have argued that uniformly distributed quenched random disorder in the reaction rates only weakly influences fluctuation corrections in either system, which is in agreement with earlier Monte Carlo simulation data.

Finally, we provided two decisive criteria that determine the possibility of spatio-temporal structures in the LV, RPS, and ML models. The first argument considers a single lattice site point of view, while the second is based on studying the global stability of the spatially homogeneous stationary state of the system. From a single lattice site perspective, a necessary (but not sufficient) condition for the emergence of spatially extended coherent oscillatory behavior is that the oscillation frequency is constant over space and time in each run. Different oscillation frequencies on distinct sites would not allow the formation of stable coherent patterns. From a global point of view, only if the spatially uniform quasi-steady state is unstable against finite-wavelength fluctuations can non-trivial spatio-temporal struc-

tures be generated, as is evident in the ML model. Both these criteria explain the absence of spatio-temporal patterns in the RPS system, as a consequence of the relevant conservation law for the total particle number, in contrast with the otherwise apparently similar LV and ML models. We remark that adding some external noise to the RPS model that explicitly invalidates total particle number conservation might induce the formation of spiral patterns at sufficiently large length and long time scales.

4.6 Appendix

4.6.1 Doi–Peliti Formalism and the Asymmetric RPS Model

In this appendix, we provide a brief overview of the construction of the time evolution operator and the resulting field-theoretic action via the Doi–Peliti mapping of stochastic reactions to a non-Hermitean many-body quantum action [181, 182, 183, 184] (for recent reviews and additional details, see Refs. [50, 178, 185, 186]). We then proceed to construct coupled Langevin equations describing the dynamics of the system similar to previous work in the context of the LV system [50, 170, 177], plankton-based predator-prey models [187], and Turing patterns [188]. An interesting corner limit is analyzed via the generalized Langevin equations; we will show that the strongly asymmetric RPS system reduces to an effective LV model. Finally, we construct the diagonalized action for the RPS model and briefly compare the general situation with the symmetric version discussed in the bulk of this chapter. This appendix is written in a self-consistent way and we hope it will be of use to readers who would like to delve into the Doi–Peliti formalism.

Stochastic Time Evolution Operator

The RPS rules (4.1) mandate that particle numbers are discrete, hence the occupation numbers of lattice sites can be written as positive integers $n_{i\alpha}$, where the index i accounts for different particle species, while α enumerates the sites on a d -dimensional hyper-cubic lattice. The master equation for the local, on-site RPS reactions then reads:

$$\begin{aligned} \frac{\partial P(n_{i\alpha}; t)}{\partial t} = & \sum_{i=1,2,3} \lambda'_i [(n_{i\alpha} - 1)(n_{i+1\alpha} + 1)P(n_{i\alpha} - 1, n_{i+1\alpha} + 1; t) \\ & - n_{i\alpha} n_{i+1\alpha} P(n_{i\alpha}, n_{i+1\alpha}; t)] , \end{aligned} \quad (4.60)$$

where the index i wraps around (i.e., $i = 4$ is to be identified with $i = 1$). Note that for brevity we have not included hopping to adjacent lattice sites here. As an initial state, we assume a uniform distribution of particles with an average initial number of particles N_i per lattice site of species i . This corresponds to a Poisson distribution for the occupation number of each species i at all lattice sites α , $P(n_{i\alpha}; t) = \prod_{i=1,2,3} N_i^{n_{i\alpha}} e^{-N_i} / (n_{i\alpha}!)$. The

discrete nature of the possible states of the RPS systems suggests the introduction of a product Fock space state vector

$$|\Phi(t)\rangle = \sum_{\{n_{i\alpha}\}} P(n_{i\alpha}; t) \prod_{i=1,2,3} \prod_{\alpha=1}^{L^d} |n_{i\alpha}\rangle , \quad (4.61)$$

where the $|n_{i\alpha}\rangle$ represent the occupation states of species i on lattice site i . In analogy with the quantum-mechanical harmonic oscillator, the single-site states (and thereby the full state vector) can be acted upon by bosonic ladder operators obeying the commutation relations $[a_{i\alpha}, a_{j\beta}] = 0$ and $[a_{i\alpha}, a_{j\beta}^\dagger] = \delta_{\alpha\beta}\delta_{ij}$. The occupation number eigenstates are constructed via $a_{i\alpha}|n_{i\alpha}\rangle = n_{i\alpha}|n_{i\alpha}-1\rangle$, $a_{i\alpha}^\dagger|n_{i\alpha}\rangle = |n_{i\alpha}+1\rangle$, and the empty state $|0\rangle$ is defined by $a_{i\alpha}|0\rangle = 0$.

The time evolution of the state vector (4.61) follows directly from the master equation (4.60) and can be written in the form

$$\frac{\partial}{\partial t}|\Phi(t)\rangle = -H|\Phi(t)\rangle \iff |\Phi(t)\rangle = e^{-Ht}|\Phi(0)\rangle , \quad (4.62)$$

where H denotes the (time-independent) Liouville operator which can be split into a diffusion and a reaction term, $H = H_{\text{diff}} + H_{\text{reac}}$, where the on-site reaction contribution is a sum of local terms $H_{\text{reac}} = \sum_{i=1}^{L^d} H_\alpha$, and specifically for the RPS model

$$H_\alpha = \sum_{i=1,2,3} \lambda'_i (a_{i+1\alpha}^\dagger - a_{i\alpha}^\dagger) a_{i\alpha}^\dagger a_{i\alpha} a_{i+1\alpha} . \quad (4.63)$$

Similarly, since on-lattice diffusion is implemented by particles performing simple jumps between nearest-neighbor lattice sites, the diffusion part of H reads

$$H_{\text{diff}} = \sum_{i=1,2,3} \frac{D_i}{c^2} \sum_{\langle\alpha\beta\rangle} (a_{i\alpha}^\dagger - a_{i\beta}^\dagger)(a_{i\alpha} - a_{i\beta}) , \quad (4.64)$$

where $\langle\alpha\beta\rangle$ indicates a sum over all possible nearest-neighbor lattice site pairs in the system.

Coherent-State Path Integral and Equivalent Langevin Partial Differential Equations

Following the steps of Refs. [50, 177, 178], we write averages for observables $O = O(\{n_{i\alpha}\})$ as a multi-dimensional integral over coherent states

$$\langle O(t) \rangle \propto \int \prod_{i=1,2,3} \prod_{\alpha=1}^{L^d} d\psi_{i\alpha}^* d\psi_{i\alpha} O(\{\psi_{i\alpha}\}) e^{-\mathcal{A}(\psi_{i\alpha}^*, \psi_{i\alpha}; t)} , \quad (4.65)$$

where the $\psi_{i\alpha}$ and $\psi_{i\alpha}^*$ are complex eigenvalues describing the coherent right and left eigenstates of the ladder operators $a_{i\alpha}$ and $a_{i\alpha}^\dagger$, respectively. The coherent-state “action” is given by

$$\begin{aligned} \mathcal{A}(\psi_{i\alpha}^*, \psi_{i\alpha}; t') = & \sum_{i=1,2,3} \sum_{\alpha=1}^{L^d} \left[\int_0^{t'} dt \psi_{i\alpha}^*(t) \frac{\partial \psi_{i\alpha}(t)}{\partial t} dt - \psi_{i\alpha}(t') - N_i \psi_{i\alpha}^*(0) \right] \\ & + \int_0^{t'} dt H(a_{i\alpha}^\dagger \rightarrow \psi_{i\alpha}^*(t), a_{i\alpha} \rightarrow \psi_{i\alpha}(t)) , \end{aligned} \quad (4.66)$$

where we have to replace the ladder operators by their eigenvalues in the Liouville operator H .

In the spatial continuum limit (lattice constant $c \rightarrow 0$) we may replace the sum over lattice sites with a d -dimensional volume integral $\sum_{\alpha=1}^{L^d} \rightarrow c^{-d} \int d^d x$, and the discretely spaced coherent-state values with continuous fields $\psi_{i\alpha}(t) \rightarrow c^d a_i(\vec{x}, t)$ and $\psi_{i\alpha}^*(t) \rightarrow 1 + \tilde{a}_i(\vec{x}, t)$. Hence, the “bulk” part of action (not considering the terms from the initial conditions at $t = 0$ and the projection states at $t = t'$) of the RPS system is given by

$$\begin{aligned} \mathcal{A} = \int dt d^d x \left[\sum_{i=1,2,3} \tilde{a}_i \left(\partial_t - D_\alpha \nabla^2 \right) a_i + \lambda_1 a_1 a_2 (\tilde{a}_1 + 1)(\tilde{a}_2 - \tilde{a}_1) \right. \\ \left. + \lambda_2 a_2 a_3 (\tilde{a}_2 + 1)(\tilde{a}_3 - \tilde{a}_2) + \lambda_3 a_3 a_1 (\tilde{a}_3 + 1)(\tilde{a}_1 - \tilde{a}_3) \right] . \end{aligned} \quad (4.67)$$

In the continuum limit we can thus write averages in the following coherent-state path integral form

$$\langle O(t) \rangle \propto \int \prod_{i=1,2,3} \mathcal{D}[\tilde{a}_i] \mathcal{D}[a_i] O(\{a_i\}) e^{-\mathcal{A}(\tilde{a}_i, a_i; t)} . \quad (4.68)$$

Our aim here is to derive stochastic partial differential (Langevin) equations for the species concentrations that accurately capture the intrinsic reaction noise. To this end, we note that the Janssen–de Dominicis response functional [11, 12, 50, 189]

$$\mathcal{A} = \int dt d^d x \sum_i \tilde{a}_i \left(\partial_t a_i - D_i \nabla^2 a_i - F_i[\{a_i\}] - \sum_j L_{ij}[\{a_i\}] \tilde{a}_j \right) \quad (4.69)$$

is equivalent to the set of SPDEs

$$\partial_t a_i = D_i \nabla^2 a_i(\vec{x}, t) + F_i[\{a_i(\vec{x}, t)\}] + \zeta_i(\vec{x}, t) , \quad (4.70)$$

with the associated noise (cross-)correlations

$$\langle \zeta_i(\vec{x}, t) \zeta_j(\vec{x}', t') \rangle = 2L_{ij}[\{a_i(\vec{x}, t)\}] \delta(t - t') \delta(\vec{x} - \vec{x}') . \quad (4.71)$$

This correspondence allows the immediate derivation of a coupled Langevin equation formulation of any system that exhibits an action functional of the form (4.69). Hence, via a direct comparison with the action of the RPS system (4.66), we can extract the deterministic part of the SPDEs describing the RPS system

$$F_1 = (\lambda_1 a_2 - \lambda_3 a_3) a_1, \quad F_2 = (\lambda_2 a_3 - \lambda_1 a_1) a_2, \quad F_3 = (\lambda_3 a_1 - \lambda_2 a_2) a_3, \quad (4.72)$$

which equal the right-hand side of the mean-field equations, as they should. Furthermore, the effective noise correlations are given by the matrix L_{ij} :

$$\begin{aligned} L_{11} &= \lambda_1 a_1 a_2, & L_{12} &= -\frac{\lambda_1}{2} a_1 a_2, & L_{13} &= -\frac{\lambda_3}{2} a_1 a_3, \\ L_{22} &= \lambda_2 a_2 a_3, & L_{23} &= -\frac{\lambda_2}{2} a_2 a_3, & L_{33} &= \lambda_3 a_1 a_3. \end{aligned} \quad (4.73)$$

Hence, the SPDEs (4.70) can be constructed from the mean-field equations by including a term that accounts for diffusion and multiplicative noise terms obeying the given (cross-)correlations. Note that the noise auto-correlations L_{ii} are always determined by the concentration of the predator species A_i and its respective prey A_{i+1} , and the scale is set by the associated predation rate λ_i . Thus, the noise directly associated with a given species is solely determined by its role as predator.

Strongly Asymmetric RPS Model: Mapping to the LV System

In order to investigate the asymmetric “corner” limit of the RPS system, we re-define the interaction rates as $\lambda_1 = \lambda/x$, $\lambda_2 = \lambda$ and $\lambda_3 = \kappa\lambda$. The dimensionless variable x varies in the interval $(0, 1]$ and describes the asymmetry of the rates, while the equally dimensionless parameter κ is of order unity and describes the difference between the predation rates of species A_2 and A_3 . We are interested in the limit $x \rightarrow 0$ in which the predation reactions between species A_1 and A_2 dominate. The concentrations at the coexistence fixed point become

$$(\Omega_1, \Omega_2, \Omega_3) = \rho(x, \kappa x, 1 - [1 + \kappa]x) + \mathcal{O}(x^2). \quad (4.74)$$

Hence, the densities of species A_1 and A_2 become small as $x \rightarrow 0$, while species A_3 makes up most of the overall species abundance. This is the “corner” limit in which RPS can be approximated by a two-species Lotka–Volterra system, with the third, most abundant species serving as a mean-field like reservoir to feed the first species, and to provide the effective spontaneous death reaction for the second species, as explained above [190]. Species A_1 thus effectively turns into prey, while A_2 becomes the sole predator species. The noise correlation matrix L in this corner case reads

$$\begin{aligned} L_{11} &= \frac{\lambda}{x} a_1 a_2, & L_{12} &= -\frac{\lambda}{2x} a_1 a_2, & L_{13} &\approx -\frac{\kappa\lambda}{2} a_1 \rho, \\ L_{22} &\approx \lambda a_2 \rho, & L_{23} &\approx -\frac{\lambda}{2} a_2 \rho, & L_{33} &= \kappa\lambda a_1 \rho. \end{aligned}$$

The noise strength of species A_1 , as well as the noise cross-correlations between species A_1 and A_2 , are inversely proportional to the large rate scaling factor x , indicating that fluctuations of species A_1 and A_2 (the LV predator and prey, respectively) become strong in the limit $x \rightarrow 0$. Indeed, writing the resulting effective SPDEs in the limit of large λ_1 and assuming a homogeneous and stationary distribution of species A_3 yields

$$\partial_t a_1 \approx D_1 \nabla^2 a_1 + \lambda_1 a_1 a_2 - \rho \left(1 - \frac{\lambda_2 + \lambda_3}{\lambda_1} \right) \lambda_3 a_1 + \zeta_1 , \quad (4.75)$$

$$\partial_t a_2 \approx D_2 \nabla^2 a_2 + \rho \left(1 - \frac{\lambda_2 + \lambda_3}{\lambda_1} \right) \lambda_2 a_2 - \lambda_1 a_1 a_2 + \zeta_2 , \quad (4.76)$$

with the noise correlations

$$\langle \zeta_1(\vec{x}, t) \zeta_1(\vec{x}', t') \rangle = 2\lambda_1 a_1 a_2 \delta(\vec{x} - \vec{x}') \delta(t - t') , \quad (4.77)$$

$$\langle \zeta_1(\vec{x}, t) \zeta_2(\vec{x}', t') \rangle = -\lambda_1 a_1 a_2 \delta(\vec{x} - \vec{x}') \delta(t - t') , \quad (4.78)$$

$$\langle \zeta_2(\vec{x}, t) \zeta_2(\vec{x}', t') \rangle = 2\lambda_2 \rho \left(1 - \frac{\lambda_2 + \lambda_3}{\lambda_1} \right) a_2 \delta(\vec{x} - \vec{x}') \delta(t - t') . \quad (4.79)$$

This set of Langevin equations precisely matches those derived directly for the LV model [177].

Fluctuation Corrections

In order to gain more insight into the role of fluctuations in the RPS system, we study the non-linear vertices arising from the Doi–Peliti action (4.66). To this end, we first need to diagonalize the action by transforming to appropriate field combinations. We then list the resulting vertices that capture fluctuation corrections beyond the Gaussian mean-field approximation.

To start, we transform the fields to describe the fluctuations around the fixed-point species concentrations. To this end we employ the linear transformation

$$a_i(\vec{x}, t) = \Omega_i + c_i(\vec{x}, t) , \quad \tilde{a}_i(\vec{x}, t) = \tilde{c}_i(\vec{x}, t) , \quad (4.80)$$

here ignoring higher-order shifts of the steady-state coexistence concentrations induced by stochastic fluctuations (i.e., the counter-terms or additive renormalizations in Ref. [177]). The action for these new fluctuating fields becomes

$$\mathcal{A} = \int dt \, d^d x \left[\sum_{i=1,2,3} \tilde{c}_i (\partial_t - D_i \nabla^2) c_i + \bar{\mathcal{A}} \right] , \quad (4.81)$$

with the reduced part

$$\begin{aligned} \bar{\mathcal{A}} = \frac{-1}{\bar{\lambda}^2} & \left[\lambda_1 (\tilde{c}_1 + 1) (\tilde{c}_1 - \tilde{c}_2) (\bar{\lambda} c_1 + \lambda'_2 \rho) (\bar{\lambda} c_2 + \lambda_3 \rho) \right. \\ & + \lambda'_2 (\tilde{c}_2 + 1) (\tilde{c}_2 - \tilde{c}_3) (\bar{\lambda} c_2 + \lambda_3 \rho) (\bar{\lambda} c_3 + \lambda_1 \rho) \\ & \left. + \lambda_3 (\tilde{c}_3 + 1) (\tilde{c}_3 - \tilde{c}_1) (\bar{\lambda} c_3 + \lambda_1 \rho) (\bar{\lambda} c_1 + \lambda_2 \rho) \right] , \end{aligned} \quad (4.82)$$

Two-point (noise) sources $\rightrightarrows$	
$\tilde{\phi}_\pm^2$	$+\frac{\rho\lambda_2}{(\lambda_1+\lambda_3)^2}\left(\rho\frac{\lambda_1^2(\lambda_2-\lambda_3)-\lambda_3^2(\lambda_1-\lambda_2)}{\lambda_1+\lambda_2+\lambda_3}\pm i\omega_0[\lambda_1-\lambda_3]\right)$
$\tilde{\phi}_+\tilde{\phi}_-$	$-\frac{2\rho^2\lambda_2}{\lambda_1+\lambda_3}\frac{\lambda_1\lambda_2+\lambda_1\lambda_3+\lambda_2\lambda_3}{\lambda_1+\lambda_2+\lambda_3}$
Merging three-point vertices $\leftarrow\leftarrow$	
$\tilde{\phi}_\pm\phi_\pm\psi$	$\pm 2i\frac{\omega_0}{\rho\lambda_2}\frac{(\lambda_1+\lambda_2+\lambda_3)^2}{\lambda_1+\lambda_3}$
$\tilde{\phi}_\pm\phi_\pm^2$	$+\left(\frac{\lambda_1+\lambda_2+\lambda_3}{\lambda_1+\lambda_3}\right)^2([\lambda_1-\lambda_3]\pm i\frac{\omega_0}{\rho\lambda_2}[\lambda_1-2\lambda_2+\lambda_3])$
$\tilde{\phi}_\pm\phi_\mp^2$	$-\left(\frac{\lambda_1+\lambda_2+\lambda_3}{\lambda_1+\lambda_3}\right)^2([\lambda_1-\lambda_3]\pm i\frac{\omega_0}{\rho\lambda_2}[\lambda_1+2\lambda_2+\lambda_3])$
Splitting three-point vertices $\rightrightarrows\leftarrow$	
$\psi\tilde{\phi}_\pm^2$	$\frac{2}{(\lambda_1+\lambda_3)^2}(\rho[\lambda_1^2(\lambda_2-\lambda_3)+\lambda_3^2(\lambda_2-\lambda_1)]\pm i\omega_0[\lambda_1-\lambda_3][\lambda_1+\lambda_2+\lambda_3])$
$\psi\tilde{\phi}_+\tilde{\phi}_-$	$-\frac{4\rho}{\lambda_1+\lambda_3}(\lambda_1\lambda_2+\lambda_1\lambda_3+\lambda_2\lambda_3)$
$\phi_\pm\tilde{\psi}\tilde{\phi}_\pm$	$\pm 2i\omega_0\frac{\lambda_1+\lambda_2+\lambda_3}{\lambda_1+\lambda_3}$
$\phi_\pm\tilde{\phi}_\pm^2$	$\frac{\rho}{(\lambda_1+\lambda_3)^2}(\lambda_1\lambda_2[\lambda_1-\lambda_2]-\lambda_1\lambda_3[\lambda_1+\lambda_3]+2\lambda_2\lambda_3^2\pm\frac{\lambda_2\rho}{i\omega_0}[\lambda_2(\lambda_1^2-\lambda_3^2)+\lambda_1\lambda_3(\lambda_2+\lambda_3-2\lambda_1)])$
$\phi_\pm\tilde{\phi}_\mp^2$	$-\frac{\rho}{(\lambda_1+\lambda_3)^3}(\lambda_1^2\lambda_2[\lambda_1+3\lambda_2-\lambda_3]+\lambda_1\lambda_3[\lambda_1\lambda_2]^2+2(\lambda_1^2+\lambda_2^2)\lambda_3^2+\lambda_1\lambda_3^3\pm\frac{\lambda_2\rho}{i\omega_0}[-\lambda_1^3\lambda_2+\lambda_1\lambda_3^3+\lambda_2\lambda_3^3+\lambda_1^2\lambda_3(2\lambda_2+\lambda_3)])$
$\phi_\pm\tilde{\phi}_+\tilde{\phi}_-$	$\frac{2\rho}{(\lambda_1+\lambda_3)^2}(2\lambda_1\lambda_2^2+[\lambda_2^2-\lambda_1^2]\lambda_3-[\lambda_1+\lambda_2]\lambda_3^2\mp\frac{\lambda_2\rho}{i\omega_0}[\lambda_1^2(\lambda_2+\lambda_3)-\lambda_2\lambda_3^2-\lambda_1\lambda_2\lambda_3])$

Table 4.1: Coefficients of the vertices in the action after the transformation to fluctuating fields.

and $\bar{\lambda} = \lambda_1 + \lambda_2 + \lambda_3$. The harmonic part of this action can be cast in a bilinear matrix form $\bar{s}_h = \sum_{ij} \tilde{c}_j A_{ij} c_i$ with the mass matrix

$$A = \frac{\rho}{\bar{\lambda}} \begin{pmatrix} 0 & -\lambda_1\lambda_2 & \lambda_2\lambda_3 \\ \lambda_1\lambda_3 & 0 & -\lambda_2\lambda_3 \\ -\lambda_1\lambda_3 & \lambda_1\lambda_2 & 0 \end{pmatrix} = -A_s, \quad (4.83)$$

where A_s is the stability matrix of the system at mean-field level. We note that it reduces to the stability matrix (4.4) in the symmetric limit $\lambda_1 = \lambda_2 = \lambda_3 = \lambda$.

Our goal is to find a transformation that diagonalizes the mass matrix A , and thus the harmonic part of the action (4.66), if we set all diffusivities equal, $D_i = D$. The matrix A is asymmetric, hence we make use of its orthogonal left and right eigenvectors $\vec{u}_i A = e_i \vec{u}_i$ and $A \vec{v}_i = e_i \vec{v}_i$, respectively. The resulting eigenvector matrices $Q = (\vec{u}_1, \vec{u}_2, \vec{u}_3)$ and $P = (\vec{v}_1, \vec{v}_2, \vec{v}_3)$ read

$$Q = \begin{pmatrix} 1 & 1 & 1 \\ 1 & -\frac{\lambda_2(\lambda_1+\lambda_2)}{\lambda_2\lambda_3+i\Lambda} & -\frac{\lambda_2(\lambda_1+\lambda_2)}{\lambda_2\lambda_3-i\Lambda} \\ 1 & -\frac{\lambda_2(\lambda_2+\lambda_3)}{\lambda_1\lambda_2-i\Lambda} & -\frac{\lambda_2(\lambda_2+\lambda_3)}{\lambda_1\lambda_2+i\Lambda} \end{pmatrix}, \quad (4.84)$$

where $\Lambda = \sqrt{\lambda_1 \lambda_2 \lambda_3 (\lambda_1 + \lambda_2 + \lambda_3)}$, and

$$P = \begin{pmatrix} 1 & 1 & 1 \\ \frac{\lambda_3}{\lambda_2} & -\frac{\lambda_3(\lambda_1+\lambda_2)}{\lambda_2\lambda_3-i\Lambda} & -\frac{\lambda_3(\lambda_1+\lambda_2)}{\lambda_2\lambda_3+i\Lambda} \\ \frac{\lambda_1}{\lambda_2} & -\frac{\lambda_1(\lambda_2+\lambda_3)}{\lambda_1\lambda_2+i\Lambda} & -\frac{\lambda_1(\lambda_2+\lambda_3)}{\lambda_1\lambda_2-i\Lambda} \end{pmatrix}. \quad (4.85)$$

The right and left eigenvector matrices then transform the mass matrix to the diagonal form $Q^T A P (Q^T P)^{-1} = \text{diag}(e_i)$. Defining new fields $\tilde{\phi}_i$ and ϕ_i according to the transformation $\tilde{c}_i = \sum_j Q_{ji}^T \phi_j$ and $c_i = \sum_j P_{ij} \phi_j$, we arrive at³

$$\begin{aligned} \tilde{c}_1 &= \tilde{\psi} + \tilde{\phi}_+ + \tilde{\phi}_-, \\ \tilde{c}_{2/3} &= \tilde{\psi} - \frac{\lambda_2}{\lambda_1 + \lambda_3} (\tilde{\phi}_+ + \tilde{\phi}_-) \pm \frac{i\Lambda/\lambda_{3/1}}{\lambda_1 + \lambda_3} (\tilde{\phi}_+ - \tilde{\phi}_-), \end{aligned} \quad (4.86)$$

$$\begin{aligned} c_1 &= \psi + \phi_+ + \phi_-, \\ c_{2/3} &= \frac{\lambda_{3/1}}{\lambda_2} \psi - \frac{\lambda_{3/1}}{\lambda_1 + \lambda_3} (\phi_+ + \phi_-) \mp \frac{i\Lambda/\lambda_2}{\lambda_1 + \lambda_3} (\phi_+ - \phi_-). \end{aligned} \quad (4.87)$$

It is already obvious from this structure that the fields $\tilde{\psi}$ and ψ describe the fluctuation of the total population, while the other fields are oscillatory in nature. Employing these transformations, one arrives at the diagonalized harmonic action

$$\begin{aligned} \mathcal{A}_0 &= \int dt \int d^d x (\lambda_1 + \lambda_2 + \lambda_3) \left[\frac{1}{\lambda_2} \tilde{\psi} (\partial_t - D\nabla^2) \psi \right. \\ &\quad \left. + \frac{1}{\lambda_1 + \lambda_3} \tilde{\phi}_+ (\partial_t - D\nabla^2 + i\omega_0) \phi_+ + \frac{1}{\lambda_1 + \lambda_3} \tilde{\phi}_- (\partial_t - D\nabla^2 - i\omega_0) \phi_- \right]. \end{aligned} \quad (4.88)$$

The field $\psi = \lambda_2(c_1 + c_2 + c_3)/(\lambda_1 + \lambda_2 + \lambda_3)$ is massless, encodes no reactions, and is purely diffusive, as it represents the total local concentration of all three species. The corresponding harmonic propagator is given in Fourier space by

$$\langle \tilde{\psi}(\vec{q}, \omega) \psi(\vec{q}', \omega') \rangle = \frac{\lambda_2}{\lambda_1 + \lambda_2 + \lambda_3} \frac{(2\pi)^{d+1} \delta(\vec{q} + \vec{q}') \delta(\omega + \omega')}{-i\omega + Dq^2}, \quad (4.89)$$

while the oscillating field propagators display poles at finite eigenfrequencies $\mp\omega_0$, similar to the LV case [177]. The action transformed to the new fields becomes quite cumbersome to write out in full, hence we merely provide the coefficients of the possible field combinations in the vertices in Table 4.1. Note that we omit the coefficients of any four-point vertices as these do not contribute to one-loop order corrections.

³Note that we have employed a different diagonalization convention in this appendix as compared to the main text. This difference is reflected in the constant factors in the propagators.

4.6.2 Detailed Calculations for the ML Model

Here we provide intermediate steps for the one-loop calculation of the ML model. The renormalized frequencies are

$$\begin{aligned} \gamma_r \pm i\nu_r = & \gamma_0 \pm i\nu_0 + (\sigma + \kappa) \left[M_1^{(\pm)} \int_k \frac{1}{k^2 + \frac{\gamma_0}{D}} + M_2^{(\pm)} \int_k \frac{1}{k^2 + \frac{\gamma_0 \mp i\nu_0}{D}} \right. \\ & \left. + M_3^{(\pm)} \int_k \frac{1}{k^2 + \frac{\mu + \gamma_0 \pm i\nu_0}{2D}} + M_4^{(\pm)} \int_k \frac{1}{(k^2 + \frac{\gamma_0 \mp i\nu_0}{D})^2} + M_5^{(\pm)} \int_k \frac{1}{(k^2 + \frac{\mu + \gamma_0 \pm i\nu_0}{2D})^2} \right], \end{aligned} \quad (4.90)$$

with the coefficients $M_i^{(\pm)} = \text{Re}M_i \pm i\text{Im}M_i$, where

$$\begin{aligned} \text{Re}M_1 = & \frac{\gamma_0}{\sqrt{3}D\mu^2\nu_0[(\gamma_0 - \mu)^2 + \nu_0^2]^2} \left[\gamma_0^2\mu(\gamma_0 - \mu)^4 - \nu_0^4(4\gamma_0^3 - 19\gamma_0^2\mu + 2\gamma_0\mu^2 + 8\mu^3) \right. \\ & \left. - \nu_0^2(\gamma_0 - \mu)^2(2\gamma_0^3 - 5\gamma_0^2\mu + 2\gamma_0\mu^2 + 3\mu^3) - \nu_0^6(2\gamma_0 + 5\mu) \right], \\ \text{Im}M_1 = & \frac{1}{\sqrt{3}D\mu^2[(\gamma_0 - \mu)^2 + \nu_0^2]^2} \left[-\gamma_0^2\mu(\gamma_0 - \mu)^4 - \nu_0^4(4\gamma_0^3 - 17\gamma_0^2\mu + 2\gamma_0\mu^2 + 2\mu^3) \right. \\ & \left. - \nu_0^2(2\gamma_0^5 - \gamma_0^4\mu + 6\gamma_0^3\mu^2 - 8\gamma_0^2\mu^3 + \mu^5) - \nu_0^6(2\gamma_0 + \mu) \right], \\ \text{Re}M_2 = & -\frac{\gamma_0^2(\sqrt{3}\gamma_0 + \nu_0)}{3D\mu\nu_0}, \quad \text{Im}M_2 = \frac{\gamma_0(\sqrt{3}\gamma_0 + \nu_0)}{3D\mu}, \\ \text{Re}M_3 = & -\frac{\gamma_0}{3D\mu[(\gamma_0 - \mu)^2 + \nu_0^2]^2} \left[2\sqrt{3}\nu_0^3(6\gamma_0^2 - \gamma_0\mu - 3\mu^2) + \nu_0^4(\gamma_0 + \mu) \right. \\ & \left. + 2\nu_0^2(\gamma_0 - \mu)^2(\gamma_0 + \mu) - 2\sqrt{3}\mu\nu_0(\gamma_0 - \mu)^2(\gamma_0 + \mu) + (\gamma_0 - \mu)^4(\gamma_0 + \mu) - 4\sqrt{3}\nu_0^5 \right], \\ \text{Im}M_3 = & \frac{\gamma_0\nu_0}{3D\mu[(\gamma_0 - \mu)^2 + \nu_0^2]^2} \left[2\sqrt{3}\nu_0(2\gamma_0^3 + \gamma_0^2\mu - 4\gamma_0\mu^2 + \mu^3) + 2\sqrt{3}\nu_0^3(\mu - 6\gamma_0) \right. \\ & \left. - 2\nu_0^2(\gamma_0 - \mu)^2 - (\gamma_0 - \mu)^4 - \nu_0^4 \right], \\ \text{Re}M_4 = & -\frac{(\gamma_0 + \sqrt{3}\nu_0)(\gamma_0^2 + \nu_0^2)}{6D^2\mu}, \quad \text{Im}M_4 = \frac{\gamma_0(\gamma_0^2 + \nu_0^2)}{\sqrt{3}D^2\mu}, \\ \text{Re}M_5 = & -\frac{\gamma_0}{6D^2\mu[(\gamma_0 - \mu)^2 + \nu_0^2]} \left[\gamma_0^4 - \gamma_0^3(\mu - 2\sqrt{3}\nu_0) - \gamma_0^2\mu^2 \right. \\ & \left. + \gamma_0(\mu - 2\sqrt{3}\nu_0)(\mu^2 + 3\nu_0^2) - \nu_0^2(\mu^2 + \nu_0^2) \right], \\ \text{Im}M_5 = & -\frac{\gamma_0\nu_0}{6D^2\mu[(\gamma_0 - \mu)^2 + \nu_0^2]} \left[2\gamma_0^3 - 3\gamma_0^2(\mu - 2\sqrt{3}\nu_0) + 2\gamma_0\nu_0^2 \right. \\ & \left. + (\mu - 2\sqrt{3}\nu_0)(\mu^2 + \nu_0^2) \right]. \end{aligned} \quad (4.91)$$

The renormalized diffusivity is

$$\begin{aligned}
D_r^\pm = & D - (\kappa + \sigma) \left[\frac{(\gamma_0 - \sqrt{3}\nu_0)}{3dD\mu} (\gamma_0 \mp i\nu_0) \int_k \frac{k^2}{\left(k^2 + \frac{\gamma_0 \mp i\nu_0}{D}\right)^3} \right. \\
& - \frac{\gamma_0}{3dD\mu} (\gamma_0 + \mu \pm i\nu_0) \int_k \frac{k^2}{\left(k^2 + \frac{\mu + \gamma_0 \pm i\nu_0}{2D}\right)^3} \\
& \mp i \frac{2\sqrt{3}\gamma_0}{3dD^2\mu} (\gamma_0^2 + \nu_0^2) (\gamma_0 \mp i\nu_0) \int_k \frac{1}{\left(k^2 + \frac{\gamma_0 \mp i\nu_0}{D}\right)^3} \\
& + \frac{2\sqrt{3}\gamma_0}{3dD\mu\nu_0} (\gamma_0^2 + \nu_0^2) \int_k \frac{1}{\left(k^2 + \frac{\gamma_0 \mp i\nu_0}{D}\right)^2} \pm i \frac{2\sqrt{3}\gamma_0}{3d\mu\nu_0^2} (\gamma_0^2 + \nu_0^2) \int_k \frac{1}{k^2 + \frac{\gamma_0 \mp i\nu_0}{D}} \\
& - \frac{\sqrt{3}\gamma_0\nu_0(\gamma_0 + \mu \pm i\nu_0)^2}{3dD^2\mu(-\gamma_0 + \mu \pm i\nu_0)} \int_k \frac{1}{\left(k^2 + \frac{\mu + \gamma_0 \pm i\nu_0}{2D}\right)^3} \\
& - \frac{4\sqrt{3}\gamma_0^2\nu_0(\gamma_0 + \mu \pm i\nu_0)}{3dD\mu(-\gamma_0 + \mu \pm i\nu_0)^2} \int_k \frac{1}{\left(k^2 + \frac{\mu + \gamma_0 \pm i\nu_0}{2D}\right)^2} \\
& - \frac{8\sqrt{3}\gamma_0^2\nu_0(\gamma_0 + \mu \pm i\nu_0)}{3d\mu(-\gamma_0 + \mu \pm i\nu_0)^3} \int_k \frac{1}{k^2 + \frac{\mu + \gamma_0 \pm i\nu_0}{2D}} \\
& \left. + \frac{2\gamma}{\sqrt{3}d\mu\nu_0^2} \left[\frac{4\gamma\nu_0^3(\gamma + \mu + i\nu_0)}{(-\gamma + \mu + i\nu_0)^3} - i(\gamma^2 + \nu_0^2) \right] \int_k \frac{1}{k^2 + \frac{\gamma_0}{D}} \right], \tag{4.92}
\end{aligned}$$

and can be further simplified to

$$\begin{aligned}
D_r^\pm = & D + \frac{\kappa + \sigma}{d} \left[P_3^{(\pm)} \int_k \frac{1}{\left(k^2 + \frac{\gamma_0 \mp i\nu_0}{D}\right)^3} + P_2^{(\pm)} \int_k \frac{1}{\left(k^2 + \frac{\gamma_0 \mp i\nu_0}{D}\right)^2} + P_1^{(\pm)} \int_k \frac{1}{k^2 + \frac{\gamma_0 \mp i\nu_0}{D}} \right. \\
& + Q_3^{(\pm)} \int_k \frac{1}{\left(k^2 + \frac{\mu + \gamma_0 \pm i\nu_0}{2D}\right)^3} + Q_2^{(\pm)} \int_k \frac{1}{\left(k^2 + \frac{\mu + \gamma_0 \pm i\nu_0}{2D}\right)^2} + Q_1^{(\pm)} \int_k \frac{1}{k^2 + \frac{\mu + \gamma_0 \pm i\nu_0}{2D}} \\
& \left. - \left(P_1^{(\pm)} + Q_1^{(\pm)} \right) \int_k \frac{1}{k^2 + \frac{\gamma_0}{D}} \right], \tag{4.93}
\end{aligned}$$

where $P_i^{(\pm)} = \text{Re}P_i \pm i\text{Im}P_i$ and $Q_i^{(\pm)} = \text{Re}Q_i \pm i\text{Im}Q_i$, with

$$\begin{aligned}
\text{Re}P_1 = & 0, \quad \text{Im}P_1 = \frac{2\gamma_0(\gamma_0^2 + \nu_0^2)}{\sqrt{3}\mu\nu_0^2}, \\
\text{Re}P_2 = & \frac{\gamma_0(2\sqrt{3}\gamma_0^2 - \gamma_0\nu_0 + 3\sqrt{3}\nu_0^2)}{3d\mu\nu_0}, \quad \text{Im}P_2 = \frac{\nu_0(\gamma_0 - \sqrt{3}\nu_0)}{3D\mu}, \\
\text{Re}P_3 = & \frac{(\gamma_0^3 - 3\sqrt{3}\gamma_0^2\nu_0 - \gamma_0\nu_0^2 - \sqrt{3}\nu_0^3)}{3D^2\mu}, \quad \text{Im}P_3 = -\frac{2\gamma_0^2(\sqrt{3}\gamma_0 + \nu_0)}{3D^2\mu}, \\
\text{Re}Q_1 = & \frac{8\gamma_0^2\nu_0[6\gamma_0\nu_0^2(\mu - \gamma_0) + (\gamma_0 - \mu)^3(\gamma_0 + \mu) + \nu_0^4]}{\sqrt{3}\mu[(\gamma_0 - \mu)^2 + \nu_0^2]^3},
\end{aligned}$$

$$\begin{aligned}
\text{Im}Q_1 &= \frac{16\gamma_0^2\nu_0^2(2\gamma_0^3 - 3\gamma_0^2\mu - 2\gamma_0\nu_0^2 + \mu^3 + \mu\nu_0^2)}{\sqrt{3}\mu[(\gamma_0 - \mu)^2 + \nu_0^2]^3}, \\
\text{Re}Q_2 &= -\frac{\gamma_0}{3D\mu[(\gamma_0 - \mu)^2 + \nu_0^2]^2} \left[\gamma_0^5 + \gamma_0^4(4\sqrt{3}\nu_0 - 3\mu) \right. \\
&\quad \left. + 2\gamma_0^3(\mu^2 - 2\sqrt{3}\mu\nu_0 + \nu_0^2) + 2\gamma_0^2(\mu^3 - 2\sqrt{3}\mu^2\nu_0 - \mu\nu_0^2 - 6\sqrt{3}\nu_0^3) \right. \\
&\quad \left. - \gamma_0(\mu^2 - 4\sqrt{3}\mu\nu_0 - \nu_0^2)(\mu^2 + \nu_0^2) + \mu(\mu^2 + \nu_0^2)^2 \right], \\
\text{Im}Q_2 &= \frac{\gamma_0\nu_0[-2\nu_0^2(\gamma_0 - \mu)^2 - 4\sqrt{3}\gamma_0\nu_0(3\gamma_0 + \mu)(\gamma_0 - \mu) - (\gamma_0 - \mu)^4 + 4\sqrt{3}\gamma_0\nu_0^3 - \nu_0^4]}{3D\mu[(\gamma_0 - \mu)^2 + \nu_0^2]^2}, \\
\text{Re}Q_3 &= \frac{\gamma_0}{6D^2\mu[(\gamma_0 - \mu)^2 + \nu_0^2]} \left[\gamma_0^4 + 2\sqrt{3}\gamma_0^3\nu_0 - 2\gamma_0^2\mu(\mu - \sqrt{3}\nu_0) \right. \\
&\quad \left. - 2\gamma_0\nu_0(\sqrt{3}\mu^2 - 2\mu\nu_0 + 3\sqrt{3}\nu_0^2) + (\mu^2 - 2\sqrt{3}\mu\nu_0 - \nu_0^2)(\mu^2 + \nu_0^2) \right], \\
\text{Im}Q_3 &= \frac{\gamma_0\nu_0[\nu_0^2(\gamma_0 + \mu) + \sqrt{3}\nu_0(3\gamma_0 - \mu)(\gamma_0 + \mu) + (\gamma_0 - \mu)^2(\gamma_0 + \mu) - \sqrt{3}\nu_0^3]}{3D^2\mu[(\gamma_0 - \mu)^2 + \nu_0^2]}. \quad (4.94)
\end{aligned}$$

4.6.3 Renormalized Variables in the ML Model at Physically Accessible Dimensions

Finally, we list the expressions of the renormalized variables at physically accessible dimensions $d = 1, 2$, and 3 .

$d = 1$:

For the ψ_o mode, the renormalized parameters read

$$\begin{aligned}
\mu_r &= \mu \left[1 - \frac{5(\sigma + \kappa)}{24D} \sqrt{\frac{D}{\mu}} - \frac{\sigma + \kappa}{D} \sqrt{\frac{D}{\gamma_0}} \left(\frac{1}{12} + \frac{\gamma_0}{3\mu} + \frac{\sqrt{3}\nu_0}{16\mu} + \frac{\sqrt{3}\nu_0}{16\gamma_0} + \frac{\sqrt{3}\nu_0\gamma_0}{6\mu^2} \right) \right], \\
D_r^0 &= D - \frac{\sigma + \kappa}{48} \sqrt{\frac{D}{\mu}} - \frac{\sigma + \kappa}{24} \sqrt{\frac{D}{\gamma_0}} \left(\frac{\gamma_0}{\mu} - \frac{\sqrt{3}\nu_0}{2\mu} + \frac{\sqrt{3}\nu_0}{2\gamma_0} \right). \quad (4.95)
\end{aligned}$$

For the $\psi_{\pm}$ modes, when $\gamma_0 \geq 0$, the renormalized parameters are

$$\begin{aligned}
\gamma_r &= \gamma_0 + (\sigma + \kappa) \sqrt{\frac{D}{\nu_0}} \left[\frac{1}{2} \text{Re}M_1 \sqrt{\frac{\nu_0}{\gamma_0}} + \frac{1}{2} \left(1 + \frac{\gamma_0^2}{\nu_0^2} \right)^{-1/4} \left(\text{Re}M_2 \cos \frac{\theta}{2} - \text{Im}M_2 \sin \frac{\theta}{2} \right) \right. \\
&\quad \left. + \frac{\sqrt{2}}{2} \left(1 + \frac{(\gamma_0 + \mu)^2}{\nu_0^2} \right)^{-1/4} \left(\text{Re}M_3 \cos \frac{\eta}{2} + \text{Im}M_3 \sin \frac{\eta}{2} \right) \right]
\end{aligned}$$

$$\begin{aligned}
& + \frac{D}{4\nu_0} \left(1 + \frac{\gamma_0^2}{\nu_0^2}\right)^{-3/4} \left(\text{Re}M_4 \cos \frac{3\theta}{2} - \text{Im}M_4 \sin \frac{3\theta}{2} \right) \\
& + \frac{\sqrt{2}D}{2\nu_0} \left(1 + \frac{(\mu + \gamma_0)^2}{\nu_0^2}\right)^{-3/4} \left(\text{Re}M_5 \cos \frac{3\eta}{2} + \text{Im}M_5 \sin \frac{3\eta}{2} \right) \Big] , \\
\nu_r = & \nu_0 + (\sigma + \kappa) \sqrt{\frac{D}{\nu_0}} \left[\frac{1}{2} \text{Im}M_1 \sqrt{\frac{\nu_0}{\gamma_0}} + \frac{1}{2} \left(1 + \frac{\gamma_0^2}{\nu_0^2}\right)^{-1/4} \left(\text{Re}M_2 \sin \frac{\theta}{2} + \text{Im}M_2 \cos \frac{\theta}{2} \right) \right. \\
& + \frac{\sqrt{2}}{2} \left(1 + \frac{(\gamma_0 + \mu)^2}{\nu_0^2}\right)^{-1/4} \left(-\text{Re}M_3 \sin \frac{\eta}{2} + \text{Im}M_3 \cos \frac{\eta}{2} \right) \\
& + \frac{D}{4\nu_0} \left(1 + \frac{\gamma_0^2}{\nu_0^2}\right)^{-3/4} \left(\text{Re}M_4 \sin \frac{3\theta}{2} + \text{Im}M_4 \cos \frac{3\theta}{2} \right) \\
& \left. + \frac{\sqrt{2}D}{2\nu_0} \left(1 + \frac{(\mu + \gamma_0)^2}{\nu_0^2}\right)^{-3/4} \left(-\text{Re}M_5 \sin \frac{3\eta}{2} + \text{Im}M_5 \cos \frac{3\eta}{2} \right) \right] ; \tag{4.96}
\end{aligned}$$

yet if $\gamma_0 < 0$, the first term in both parameters changes:

$$\begin{aligned}
\gamma_r = & \gamma_0 + (\sigma + \kappa) \sqrt{\frac{D}{\nu_0}} \left[-\frac{1}{2} \text{Im}M_1 \sqrt{\frac{\nu_0}{|\gamma_0|}} + \frac{1}{2} \left(1 + \frac{\gamma_0^2}{\nu_0^2}\right)^{-1/4} \left(\text{Re}M_2 \cos \frac{\theta}{2} - \text{Im}M_2 \sin \frac{\theta}{2} \right) \right. \\
& + \frac{\sqrt{2}}{2} \left(1 + \frac{(\gamma_0 + \mu)^2}{\nu_0^2}\right)^{-1/4} \left(\text{Re}M_3 \cos \frac{\eta}{2} + \text{Im}M_3 \sin \frac{\eta}{2} \right) \\
& + \frac{D}{4\nu_0} \left(1 + \frac{\gamma_0^2}{\nu_0^2}\right)^{-3/4} \left(\text{Re}M_4 \cos \frac{3\theta}{2} - \text{Im}M_4 \sin \frac{3\theta}{2} \right) \\
& \left. + \frac{\sqrt{2}D}{2\nu_0} \left(1 + \frac{(\mu + \gamma_0)^2}{\nu_0^2}\right)^{-3/4} \left(\text{Re}M_5 \cos \frac{3\eta}{2} + \text{Im}M_5 \sin \frac{3\eta}{2} \right) \right] , \\
\nu_r = & \nu_0 + (\sigma + \kappa) \sqrt{\frac{D}{\nu_0}} \left[\frac{1}{2} \text{Re}M_1 \sqrt{\frac{\nu_0}{|\gamma_0|}} + \frac{1}{2} \left(1 + \frac{\gamma_0^2}{\nu_0^2}\right)^{-1/4} \left(\text{Re}M_2 \sin \frac{\theta}{2} + \text{Im}M_2 \cos \frac{\theta}{2} \right) \right. \\
& + \frac{\sqrt{2}}{2} \left(1 + \frac{(\gamma_0 + \mu)^2}{\nu_0^2}\right)^{-1/4} \left(-\text{Re}M_3 \sin \frac{\eta}{2} + \text{Im}M_3 \cos \frac{\eta}{2} \right) \\
& + \frac{D}{4\nu_0} \left(1 + \frac{\gamma_0^2}{\nu_0^2}\right)^{-3/4} \left(\text{Re}M_4 \sin \frac{3\theta}{2} + \text{Im}M_4 \cos \frac{3\theta}{2} \right) \\
& \left. + \frac{\sqrt{2}D}{2\nu_0} \left(1 + \frac{(\mu + \gamma_0)^2}{\nu_0^2}\right)^{-3/4} \left(-\text{Re}M_5 \sin \frac{3\eta}{2} + \text{Im}M_5 \cos \frac{3\eta}{2} \right) \right] . \tag{4.97}
\end{aligned}$$

The renormalized diffusivity is not affected by the sign of γ_0 ,

$$\begin{aligned}
\text{Re}D_r = & D + (\kappa + \sigma) \sqrt{\frac{D}{\nu_0}} \left[-\frac{1}{2} \left(1 + \frac{\gamma_0^2}{\nu_0^2}\right)^{-1/4} \text{Im}P_1 \sin \frac{\theta}{2} - \frac{1}{2} \text{Re}Q_1 \sqrt{\frac{\nu_0}{\gamma_0}} \right. \\
& \left. + \frac{D}{4\nu_0} \left(1 + \frac{\gamma_0^2}{\nu_0^2}\right)^{-3/4} \left(\text{Re}P_2 \cos \frac{3\theta}{2} - \text{Im}P_2 \sin \frac{3\theta}{2} \right) \right]
\end{aligned}$$

$$\begin{aligned}
& + \frac{3D^2}{16\nu_0^2} \left(1 + \frac{\gamma_0^2}{\nu_0^2}\right)^{-5/4} \left(\text{Re}P_3 \cos \frac{5\theta}{2} - \text{Im}P_3 \sin \frac{5\theta}{2}\right) \\
& + \frac{\sqrt{2}}{2} \left(1 + \frac{(\mu + \gamma_0)^2}{\nu_0^2}\right)^{-1/4} \left(\text{Re}Q_1 \cos \frac{\eta}{2} + \text{Im}Q_1 \sin \frac{\eta}{2}\right) \\
& + \frac{\sqrt{2}D}{2\nu_0} \left(1 + \frac{(\mu + \gamma_0)^2}{\nu_0^2}\right)^{-3/4} \left(\text{Re}Q_2 \cos \frac{3\eta}{2} + \text{Im}Q_2 \sin \frac{3\eta}{2}\right) \\
& + \frac{3\sqrt{2}D^2}{4\nu_0^2} \left(1 + \frac{(\mu + \gamma_0)^2}{\nu_0^2}\right)^{-5/4} \left(\text{Re}Q_3 \cos \frac{5\eta}{2} + \text{Im}Q_3 \sin \frac{5\eta}{2}\right) \Big] . \quad (4.98)
\end{aligned}$$

$d = 2$:

For the ψ_o mode, the renormalized parameters read

$$\begin{aligned}
\mu_r = & \mu \left[1 - \frac{\sigma + \kappa}{6D\pi} \frac{\gamma_0}{\mu} \ln \frac{D\Lambda^2}{\gamma_0} - \frac{\sigma + \kappa}{12D\pi} \ln \frac{D\Lambda^2}{\mu} - \frac{\sigma + \kappa}{24D\pi} \right. \\
& \left. - \frac{\sigma + \kappa}{12D\pi} \left(1 + \frac{\sqrt{3}\nu_0}{2\mu} + \frac{\sqrt{3}\nu_0}{2\gamma_0} + \frac{2\sqrt{3}\nu_0\gamma_0}{\mu^2} \right) \right] , \\
D_r^o = & D - \frac{\sigma + \kappa}{48\pi} - \frac{\sigma + \kappa}{24\pi} \left(\frac{\gamma_0}{\mu} - \frac{2\sqrt{3}\nu_0}{3\mu} + \frac{\sqrt{3}\nu_0}{3\gamma_0} \right) . \quad (4.99)
\end{aligned}$$

For the $\psi_{\pm}$ modes, the renormalized parameters are

$$\begin{aligned}
\gamma_r = & \gamma_0 + \frac{\sigma + \kappa}{2\pi} \left[\frac{\text{Re}M_1}{2} \ln \frac{D\Lambda^2}{\gamma_0} + (\text{Re}M_2 + \text{Re}M_3) \ln \Lambda - \theta \text{Im}M_2 + \eta \text{Im}M_3 \right. \\
& - \frac{1}{4} \left[\text{Re}M_2 \ln \frac{\gamma_0^2 + \nu_0^2}{D^2} + \text{Re}M_3 \ln \frac{(\mu + \gamma_0)^2 + \nu_0^2}{4D^2} \right] \\
& + \frac{D}{2\nu_0} \left(1 + \frac{\gamma_0^2}{\nu_0^2} \right)^{-1/2} (\text{Re}M_4 \cos \theta - \text{Im}M_4 \sin \theta) \\
& \left. + \frac{D}{\nu_0} \left(1 + \frac{(\mu + \gamma_0)^2}{\nu_0^2} \right)^{-1/2} (\text{Re}M_5 \cos \eta + \text{Im}M_5 \sin \eta) \right] , \\
\nu_r = & \nu_0 + \frac{\sigma + \kappa}{2\pi} \left[\frac{\text{Im}M_1}{2} \ln \frac{D\Lambda^2}{\gamma_0} + (\text{Im}M_2 + \text{Im}M_3) \ln \Lambda + \theta \text{Re}M_2 - \eta \text{Re}M_3 \right. \\
& - \frac{1}{4} \left[\text{Im}M_2 \ln \frac{\gamma_0^2 + \nu_0^2}{D^2} + \text{Im}M_3 \ln \frac{(\mu + \gamma_0)^2 + \nu_0^2}{4D^2} \right] \\
& \left. + \frac{D}{2\nu_0} \left(1 + \frac{\gamma_0^2}{\nu_0^2} \right)^{-1/2} (\text{Re}M_4 \sin \theta + \text{Im}M_4 \cos \theta) \right]
\end{aligned}$$

$$+ \frac{D}{\nu_0} \left(1 + \frac{(\mu + \gamma_0)^2}{\nu_0^2} \right)^{-1/2} (-\text{Re}M_5 \sin \eta + \text{Im}M_5 \cos \eta) \Big] , \quad (4.100)$$

and the renormalized diffusivity is

$$\begin{aligned} \text{Re}D_r = D + \frac{\kappa + \sigma}{2\pi} \Big[& -\frac{\text{Re}Q_1}{8} \ln \frac{\nu_0^2 + (\mu + \gamma_0)^2}{4\gamma_0^2} + \frac{1}{4} (\eta \text{Im}Q_1 - \theta \text{Im}P_1) \\ & + \frac{D}{4\nu_0} \left(1 + \frac{\gamma_0^2}{\nu_0^2} \right)^{-1/2} (\text{Re}P_2 \cos \theta - \text{Im}P_2 \sin \theta) \\ & + \frac{D^2}{8\nu_0^2} \left(1 + \frac{\gamma_0^2}{\nu_0^2} \right)^{-1} (\text{Re}P_3 \cos 2\theta - \text{Im}P_3 \sin 2\theta) \\ & + \frac{D}{2\nu_0} \left(1 + \frac{(\mu + \gamma_0)^2}{\nu_0^2} \right)^{-1/2} (\text{Re}Q_2 \cos \eta + \text{Im}Q_2 \sin \eta) \\ & + \frac{D^2}{2\nu_0^2} \left(1 + \frac{(\mu + \gamma_0)^2}{\nu_0^2} \right)^{-1} (\text{Re}Q_3 \cos 2\eta + \text{Im}Q_3 \sin 2\eta) \Big] . \end{aligned} \quad (4.101)$$

$d = 3$:

For the ψ_o mode, the renormalized parameters read

$$\begin{aligned} \mu_r = \mu \Big[& 1 + \frac{\sigma + \kappa}{16D\pi} \sqrt{\frac{\mu}{D}} + \frac{\sigma + \kappa}{6D\pi} \sqrt{\frac{\gamma_0}{D}} \left(-\frac{1}{4} + \frac{\gamma_0}{\mu} - \frac{\sqrt{3}\nu_0}{16\mu} - \frac{\sqrt{3}\nu_0}{16\gamma_0} - \frac{\sqrt{3}\nu_0\gamma_0}{2\mu^2} \right) \Big] , \\ D_r^o = D - \frac{\sigma + \kappa}{96\pi} \sqrt{\frac{\mu}{D}} - \frac{\sigma + \kappa}{48\pi} \sqrt{\frac{\gamma_0}{D}} \Big(& \frac{\sqrt{3}\nu_0}{6\gamma_0} + \frac{\gamma_0}{\mu} - \frac{5\sqrt{3}\nu_0}{6\mu} \Big) . \end{aligned} \quad (4.102)$$

For the $\psi_{\pm}$ modes, if $\gamma_0 \geq 0$, the renormalized parameters are

$$\begin{aligned} \gamma_r = \gamma_0 + \frac{\sigma + \kappa}{4\pi} \sqrt{\frac{\nu_0}{D}} \Big[& -\text{Re}M_1 \sqrt{\frac{\gamma_0}{\nu_0}} - \left(1 + \frac{\gamma_0^2}{\nu_0^2} \right)^{1/4} \left(\text{Re}M_2 \cos \frac{\theta}{2} + \text{Im}M_2 \sin \frac{\theta}{2} \right) \\ & - \frac{\sqrt{2}}{2} \left(1 + \frac{(\mu + \gamma_0)^2}{\nu_0^2} \right)^{1/4} \left(\text{Re}M_3 \cos \frac{\eta}{2} - \text{Im}M_3 \sin \frac{\eta}{2} \right) \\ & + \frac{D}{2\nu_0} \left(1 + \frac{\gamma_0^2}{\nu_0^2} \right)^{-1/4} \left(\text{Re}M_4 \cos \frac{\theta}{2} - \text{Im}M_4 \sin \frac{\theta}{2} \right) \\ & + \frac{\sqrt{2}D}{2\nu_0} \left(1 + \frac{(\mu + \gamma_0)^2}{\nu_0^2} \right)^{-1/4} \left(\text{Re}M_5 \cos \frac{\eta}{2} + \text{Im}M_5 \sin \frac{\eta}{2} \right) \Big] , \\ \nu_r = \nu_0 + \frac{\sigma + \kappa}{4\pi} \sqrt{\frac{\nu_0}{D}} \Big[& -\text{Im}M_1 \sqrt{\frac{\gamma_0}{\nu_0}} - \left(1 + \frac{\gamma_0^2}{\nu_0^2} \right)^{1/4} \left(-\text{Re}M_2 \sin \frac{\theta}{2} + \text{Im}M_2 \cos \frac{\theta}{2} \right) \\ & - \frac{\sqrt{2}}{2} \left(1 + \frac{(\mu + \gamma_0)^2}{\nu_0^2} \right)^{1/4} \left(\text{Re}M_3 \sin \frac{\eta}{2} + \text{Im}M_3 \cos \frac{\eta}{2} \right) \end{aligned}$$

$$\begin{aligned}
& + \frac{D}{2\nu_0} \left(1 + \frac{\gamma_0^2}{\nu_0^2}\right)^{-1/4} \left(\operatorname{Re} M_4 \sin \frac{\theta}{2} + \operatorname{Im} M_4 \cos \frac{\theta}{2} \right) \\
& + \frac{\sqrt{2}D}{2\nu_0} \left(1 + \frac{(\mu + \gamma_0)^2}{\nu_0^2}\right)^{-1/4} \left(-\operatorname{Re} M_5 \sin \frac{\eta}{2} + \operatorname{Im} M_5 \cos \frac{\eta}{2} \right) \Big] . \tag{4.103}
\end{aligned}$$

When $\gamma_0 < 0$ and the system is rendered unstable, the renormalized parameters become

$$\begin{aligned}
\mu_r &= \left[1 + \frac{\sigma + \kappa}{16D\pi} \sqrt{\frac{\mu}{D}} + \frac{\sigma + \kappa}{6D\pi} \sqrt{\frac{\gamma_0}{D}} \left(-\frac{1}{4} + \frac{\gamma_0}{\mu} - \frac{\sqrt{3}\nu_0}{16\mu} - \frac{\sqrt{3}\nu_0}{16\gamma_0} - \frac{\sqrt{3}\nu_0\gamma_0}{2\mu^2} \right) \right] , \\
D_r^o &= D - \frac{\sigma + \kappa}{96\pi} \sqrt{\frac{\mu}{D}} - \frac{\sigma + \kappa}{48\pi} \sqrt{\frac{\gamma_0}{D}} \left(\frac{\sqrt{3}\nu_0}{6\gamma_0} + \frac{\gamma_0}{\mu} - \frac{5\sqrt{3}\nu_0}{6\mu} \right) . \tag{4.104}
\end{aligned}$$

For the $\psi_{\pm}$ modes, for $\gamma_0 \geq 0$, the renormalized parameters are

$$\begin{aligned}
\gamma_r &= \gamma_0 + \frac{\sigma + \kappa}{4\pi} \sqrt{\frac{\nu_0}{D}} \left[-\operatorname{Im} M_1 \sqrt{\frac{|\gamma_0|}{\nu_0}} - \left(1 + \frac{\gamma_0^2}{\nu_0^2}\right)^{1/4} \left(\operatorname{Re} M_2 \cos \frac{\theta}{2} + \operatorname{Im} M_2 \sin \frac{\theta}{2} \right) \right. \\
& - \frac{\sqrt{2}}{2} \left(1 + \frac{(\mu + \gamma_0)^2}{\nu_0^2}\right)^{1/4} \left(\operatorname{Re} M_3 \cos \frac{\eta}{2} - \operatorname{Im} M_3 \sin \frac{\eta}{2} \right) \\
& + \frac{D}{2\nu_0} \left(1 + \frac{\gamma_0^2}{\nu_0^2}\right)^{-1/4} \left(\operatorname{Re} M_4 \cos \frac{\theta}{2} - \operatorname{Im} M_4 \sin \frac{\theta}{2} \right) \\
& \left. + \frac{\sqrt{2}D}{2\nu_0} \left(1 + \frac{(\mu + \gamma_0)^2}{\nu_0^2}\right)^{-1/4} \left(\operatorname{Re} M_5 \cos \frac{\eta}{2} + \operatorname{Im} M_5 \sin \frac{\eta}{2} \right) \right] , \\
\nu_r &= \nu_0 + \frac{\sigma + \kappa}{4\pi} \sqrt{\frac{\nu_0}{D}} \left[\operatorname{Re} M_1 \sqrt{\frac{|\gamma_0|}{\nu_0}} - \left(1 + \frac{\gamma_0^2}{\nu_0^2}\right)^{1/4} \left(-\operatorname{Re} M_2 \sin \frac{\theta}{2} + \operatorname{Im} M_2 \cos \frac{\theta}{2} \right) \right. \\
& - \frac{\sqrt{2}}{2} \left(1 + \frac{(\mu + \gamma_0)^2}{\nu_0^2}\right)^{1/4} \left(\operatorname{Re} M_3 \sin \frac{\eta}{2} + \operatorname{Im} M_3 \cos \frac{\eta}{2} \right) \\
& + \frac{D}{2\nu_0} \left(1 + \frac{\gamma_0^2}{\nu_0^2}\right)^{-1/4} \left(\operatorname{Re} M_4 \sin \frac{\theta}{2} + \operatorname{Im} M_4 \cos \frac{\theta}{2} \right) \\
& \left. + \frac{\sqrt{2}D}{2\nu_0} \left(1 + \frac{(\mu + \gamma_0)^2}{\nu_0^2}\right)^{-1/4} \left(-\operatorname{Re} M_5 \sin \frac{\eta}{2} + \operatorname{Im} M_5 \cos \frac{\eta}{2} \right) \right] . \tag{4.105}
\end{aligned}$$

The renormalized diffusivity is not affected by the sign of γ_0 ,

$$\begin{aligned}
\operatorname{Re} D_r &= D + \frac{\kappa + \sigma}{3\pi} \sqrt{\frac{\nu_0}{D}} \left[-\frac{1}{4} \left(1 + \frac{\gamma_0^2}{\nu_0^2}\right)^{1/4} \operatorname{Im} P_1 \sin \frac{\theta}{2} + \frac{1}{4} \operatorname{Re} Q_1 \sqrt{\frac{\gamma_0}{\nu_0}} \right. \\
& \left. + \frac{D}{8\nu_0} \left(1 + \frac{\gamma_0^2}{\nu_0^2}\right)^{-1/4} \left(\operatorname{Re} P_2 \cos \frac{\theta}{2} - \operatorname{Im} P_2 \sin \frac{\theta}{2} \right) \right]
\end{aligned}$$

$$\begin{aligned}
& + \frac{D^2}{32\nu_0^2} \left(1 + \frac{\gamma_0^2}{\nu_0^2}\right)^{-3/4} \left(\operatorname{Re}P_3 \cos \frac{3\theta}{2} - \operatorname{Im}P_3 \sin \frac{3\theta}{2}\right) \\
& - \frac{\sqrt{2}}{8} \left(1 + \frac{(\mu + \gamma_0)^2}{\nu_0^2}\right)^{1/4} \left(\operatorname{Re}Q_1 \cos \frac{\eta}{2} - \operatorname{Im}Q_1 \sin \frac{\eta}{2}\right) \\
& + \frac{\sqrt{2}D}{8\nu_0} \left(1 + \frac{(\mu + \gamma_0)^2}{\nu_0^2}\right)^{-1/4} \left(\operatorname{Re}Q_2 \cos \frac{\eta}{2} + \operatorname{Im}Q_2 \sin \frac{\eta}{2}\right) \\
& + \frac{\sqrt{2}D^2}{16\nu_0^2} \left(1 + \frac{(\mu + \gamma_0)^2}{\nu_0^2}\right)^{-3/4} \left(\operatorname{Re}Q_3 \cos \frac{3\eta}{2} + \operatorname{Im}Q_3 \sin \frac{3\eta}{2}\right) \Big] . \quad (4.106)
\end{aligned}$$

Chapter 5

Active-to-Absorbing Phase Transition in Pair Contact Process with Diffusion

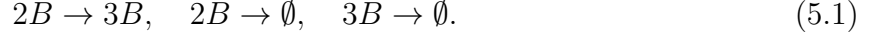
5.1 Introduction

Active-to-absorbing phase transitions are a peculiar type of phase transitions that occur between an active phase, characterized by an order parameter with a non-zero average, and an absorbing phase, where not only does the average of the order parameter go to zero, but all fluctuations also disappear. This type of transition is frequently encountered in nature, particularly in the spread of epidemics, and has garnered significant attention from researchers both theoretically and numerically (e.g., Refs. [191, 192] and the references therein). However, in contrast to phase transitions in thermal equilibrium, a comprehensive classification of universality classes of the active-to-absorbing phase transition is still lacking. Among all known universality classes, the most prominent is directed percolation (DP). DP has been observed in a wide range of systems, such as phase transition between two turbulent states in liquid crystals [193, 194], the extinction threshold for the Lotka-Volterra predator-prey system [177, 195], and the phase transition in glassy systems with blockages [196, 197], among others.

In order to classify universality classes of active-to-absorbing phase transitions in a systematic manner, one of the most effective approaches is to utilize reaction-diffusion systems with contact reactions. The study of DP [7, 8, 198] under this representation has been met with success through the use of one-particle reactions ($B \rightarrow 2B$ and $B \rightarrow \emptyset$) and two-particle soft site-restriction ($2B \rightarrow B$). The interplay between these one-particle reactions leads to a non-equilibrium phase transition between a branching-dominant active phase, characterized by a non-vanishing average particle density, and a decaying-dominant absorbing phase, where no particles survive. The implementation of soft site-restriction guarantees that this phase transition is continuous.

A natural extension of the reactions in DP is to require pair particles to react, leading to a three-particle soft site-restriction reaction, known as the pair contact process with diffusion

(PCPD) (for a review, see [199]). This reaction is defined as follows:



Numerous numerical simulations have been conducted on this system (for examples, [199, 200, 201, 202, 203, 204]). However, due to its extremely long crossover time, an unambiguous universality class has yet to be identified and the critical exponents reported are quite scattered. Three different possibilities have been proposed as follows:

- The PCPD belongs to a novel universality class. [202, 205]
- The PCPD belongs to DP. [203, 206]
- The critical regime of PCPD is non-universal and is subject to the diffusion rate. [200, 207]

To further understand the discrepancy in the numerical simulations, field-theoretic RG analysis in Doi-Peliti formalism has been applied both perturbatively [208] and non-perturbatively [209]. However, both approaches have been unsuccessful. The perturbative analysis in [208] yielded runaway RG flow trajectories and the non-perturbative RG analysis [209] resulted in finite-scale singularities.

In order to address the issues in the RG analysis, the authors in [210] proposed an effective two-species model for PCPD. This model introduces a pair particle which could potentially restore the violated Galilean symmetry and introduce another characteristic scale to address the finite-scale divergence. The authors numerically demonstrated the equivalence between the original PCPD in (5.1) and the two-species model they proposed.

This chapter aims to implement a perturbative RG analysis on the effective two-species model proposed in [210]. We show the inconsistency between the scaling behavior near the fixed point of the theory and the critical condition. We further demonstrate the equivalence between the two-species model and the original theory at the tree-level when the pair particle is massive. We conclude that the pair particle does not become massless and thus does not contribute another characteristic scale. Therefore, the effective order parameter could still be the single particle density, and the single particle field theory should be revisited.

The chapter is organized as follows: In the following section 5.2, we briefly review the field-theoretic RG analysis of DP within the reaction-diffusion system representation. We then discuss the perturbative RG analysis of the single-species PCPD in section 5.3 and review the problems with it. In section 5.4, we introduce the two-species PCPD. We first show its equivalence to the single-species PCPD and then apply a one-loop perturbative RG analysis to it. We show the inconsistency in the analysis and provide an overview of the entire problem. The appendix contains additional technical details for the one-loop perturbative analysis.

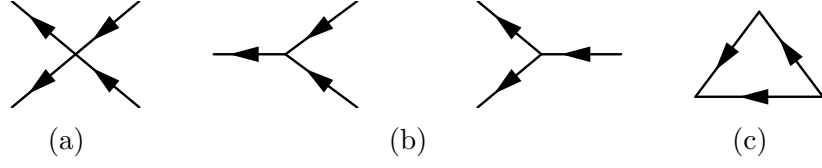


Figure 5.1: (a) Vertex corresponding to operator $\hat{\phi}^2\phi^2$, (b) vertices corresponding to operators $\hat{\phi}\phi^2$ and $\hat{\phi}^2\phi$, and (c) one-loop triangular diagram contributing through combined operators $[\hat{\phi}^2\phi][\hat{\phi}\phi^2]$.

5.2 Review of the Field-Theoretic RG Analysis of DP

In this section, we provide an overview of the field-theoretic RG analysis of the DP universality class using the reaction-diffusion system representation [198, 211, 212], also known as Reggeon field theory [213, 214, 215]. This section is primarily based on [50] and readers can refer to [216] for more in-depth information.

The DP universality class can be modeled by the following contact reactions, in combination with particle hopping:

$$B \xrightarrow{\sigma} 2B, \quad B \xrightarrow{\kappa} \emptyset, \quad 2B \xrightarrow{\lambda} B, \quad (5.2)$$

where σ , κ , and λ represent effective reaction rates. This system exhibits a continuous phase transition at $\kappa_c = \sigma$. When $\kappa < \sigma$, the average particle density is finite, and the system is in the active phase. On the other hand, when $\kappa > \sigma$, the average particle density vanishes, and the system is in an absorbing phase.

The reaction-diffusion system in Eq.(5.2) can be described by the Doi-Peliti action after the Doi shift:

$$\mathcal{A} = \int_{t,x} \hat{\phi} [\partial_t + D(r - \lambda^2)] \phi + \lambda \hat{\phi} \phi^2 - \sigma \hat{\phi}^2 \phi + \lambda \hat{\phi}^2 \phi^2, \quad (5.3)$$

where D is the diffusion constant and $r = (\kappa - \sigma)/D$. The phase transition occurs when the field ϕ becomes massless. In the perturbative analysis, the fixed point is driven by combined operators with the same number of $\hat{\phi}$ and ϕ fields. In the DP action Eq.(5.3), beyond the quadratic terms, there are two sets of operators with the same number of $\hat{\phi}$ and ϕ fields: $[\hat{\phi}^2\phi^2]$ and $[\hat{\phi}^2\phi][\hat{\phi}\phi^2]$. The coupling constant corresponding to these two operators are $u^2 = \lambda\sigma$ and λ with naive scaling dimensions $4-d$ and $2-d$, respectively. A diagrammatic representation of the vertices corresponding to these operators is shown in Fig. 5.1.

The critical dimension of DP is suggested to be $d_c = 4$ and thus corresponds to the coupling u^2 . Near the upper critical dimension 4, the operator $[\hat{\phi}^2\phi^2]$ is irrelevant and can be ignored. Thus, the action Eq.(5.3) can be re-written as

$$\mathcal{A} = \int_{t,x} \hat{S} [\partial_t + D(r - \lambda^2)] S + u \hat{S} S^2 - u \hat{S}^2 S, \quad (5.4)$$

with the re-defined fields $\hat{S} = \sqrt{\sigma/\lambda} \hat{\phi}$ and $S = \sqrt{\lambda/\sigma} \phi$. The action in Eq.(5.4) is formally known as the Reggeon field theory and it is invariant under rapidity reversal

$$S(x, t) \longleftrightarrow -\hat{S}(x, -t). \quad (5.5)$$

To one-loop order, the structure of the loop diagrams is shown in Fig. 5.1(c) and the RG beta function reads

$$\beta_v = v_R [-\epsilon + 3v_R + \mathcal{O}(v_R^2)], \quad (5.6)$$

where v is the effective coupling defined as $v = u^2/D^2$, and $\epsilon = 4 - d$. All other scaling dimensions can be calculated from the beta function Eq.(5.6), we do not discuss the details here. For further information, we suggest consulting the review paper by Janssen and Täuber [216].

5.3 Field-Theoretic RG Analysis of the Single-Species PCPD

In the previous section, we conducted a review of the perturbative RG analysis of DP. As previously mentioned, a natural extension of DP is PCPD, which includes the reactions outlined in Eq.(5.1). In this section, we will review the RG analysis of PCPD [208] and highlight the issues the authors encountered in their paper.

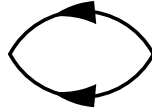


Figure 5.2: One-loop level loop structure near two dimensions in single-species PCPD.

The Doi-Peliti action of PCPD is written as

$$\mathcal{A} = \int_{t,x} \bar{b} (\partial_t - D\nabla^2) b + (2\mu - \sigma) \bar{b} b^2 + (\mu - 2\sigma) \bar{b}^2 b^2 - \sigma \bar{b}^3 b^2 + 3\nu \bar{b} b b^3 + 3\nu \bar{b}^2 b^3 + \nu \bar{b}^3 b^3, \quad (5.7)$$

where μ , σ , and ν are the reaction rates corresponding to the three reactions in (5.1). The phase transition happens when $\sigma - 2\mu = 0$. At this phase transition, there are four different combined operators with the same number of incoming and outgoing particles. These operators, along with their corresponding effective parameters, are: $[\bar{b}^2 b^2]$ with σ , $[\bar{b}^3 b^2][\bar{b}^2 b^3]$ with $\sigma\nu$, $[\bar{b}^3 b^2]^2[\bar{b} b^3]$ with $\sigma^2\nu$, and $[\bar{b}^3 b^3]$ with ν . A naive dimension analysis shows that $[\sigma] = \kappa^{2-d}$ and $[\nu] = \kappa^{1-d}$ where κ labels an arbitrary momentum scale, and the dimensions of $\sigma\nu$ and $\sigma^2\nu$ follow.

The authors of [208] studied the fixed point driven by σ near its critical dimension 2. To one-loop order, the only topology of the diagrams is by the operator $[\hat{b}^2 b^2]$ and is shown in

Fig. 5.2. The other three operator combinations become irrelevant. The RG analysis shows that there is a runaway flow in the physically-allowed region such that $\sigma \rightarrow -\infty$ and the theory is not well-defined. The fixed point is $\sigma^* = -(2-d)/3$ where σ becomes negative and thus unphysical. This further suggests the operator $[\bar{b}^2 b^2]$ governs the pair annihilation fixed point where the coupling constant of operator $[\bar{b}^2 b^2]$ is positive, instead of the PCPD fixed point.

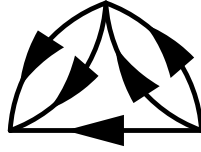


Figure 5.3: Three-loop level loop structure near $3/2$ dimensions in single-species PCPD.

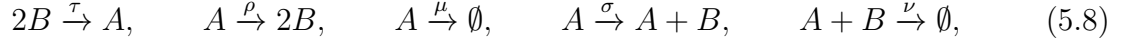
The other combined operators have not yet been explored yet. The combined operator $[\bar{b}^3 b^2][\bar{b}^2 b^3]$ has an effective coupling $\sigma\nu$ with naive scaling dimension $3 - 2d$. This operator has a critical dimension of $3/2$ and only starts to contribute at three-loop order in the perturbation expansion. The characteristic diagram at three-loop order is plotted in Fig. 5.3 and it is clear to see the correspondence between it and the triangular diagram Fig. 5.1 (c) in DP. For operator $[\bar{b}^3 b^2]^2[\bar{b} b^3]$, its effective coupling $\sigma^2\nu$ has a naive dimension of $5 - 3d$ and thus is critical near $5/3$ dimensions. It will start to contribute at even higher loop orders. The operator $[\bar{b}^3 b^3]$ governs the site-restriction reaction and it has a critical dimension 1. However, as the phase transition is driven by the competing two pair-particle reactions, it is unlikely that the fixed point is solely determined by the single reaction rate controlling the site restriction.

5.4 Coupled Pair Contact Process with Diffusion

In this section, we delve into the study of the coupled PCPD (cPCPD) [210] using the framework of dimensionally regularized perturbative RG. We begin by demonstrating that the single-species model can be obtained as an effective field theory, which analytically illustrates the equivalence between the single-species and two-species PCPD. We then examine the fixed point theory of the two-species PCPD field theory while all relevant couplings are set to zero. Our findings indicate that the scaling behavior near this fixed point is not in alignment with the critical condition, and thus does not correspond to the critical fixed point.

5.4.1 Two-species PCPD and Mean Field Analysis

The effective two-species PCPD proposed in [210] is defined by the following reactions:



where τ , ρ , μ , σ and ν are the corresponding reaction rates. The effective pair particles, denoted as A , are expected to introduce a new characteristic length scale and potentially aid in regulating the run-away flow that is present in the single-species PCPD model. The Doi-Peliti functional, which corresponds to the reactions in (5.8), is given by:

$$\mathcal{A} = \int_{t,x} \left[\bar{a} (\partial_t - D'\nabla^2 + \rho + \mu) a + \bar{b} (\partial_t - D\nabla^2) b - (2\rho + \sigma)\bar{b}a - \rho\bar{b}^2a - \sigma\bar{a}\bar{b}a - \tau\bar{a}b^2 + 2\tau\bar{b}b^2 + \tau\bar{b}^2b^2 + \nu\bar{a}ab + \nu\bar{b}ab + \nu\bar{a}\bar{b}ab \right], \quad (5.9)$$

where D and D' are the diffusion constants. The system can also be described by the following set of Langevin equations:

$$\begin{aligned} \partial_t a &= D'\nabla^2 a - (\rho + \mu)a + \tau b^2 - \nu ab + \xi, \\ \partial_t b &= D\nabla^2 b + (2\rho + \sigma)a - 2\tau b^2 - \nu ab + \eta, \end{aligned} \quad (5.10)$$

where ξ and η are noise terms with zero means and the following non-vanishing two-point correlation functions:

$$\begin{aligned} \langle \eta(x, t) \eta(x', t') \rangle &= 2(\rho a - \tau b^2) \delta(x - x') \delta(t - t'), \\ \langle \xi(x, t) \eta(x', t') \rangle &= (\sigma a - \nu ab) \delta(x - x') \delta(t - t'). \end{aligned} \quad (5.11)$$

In the mean-field limit, we can ignore the noise and spatial correlations. As t approaches infinity, there are two sets of solutions for the above equations: one is the absorbing state where the densities of A and B particles both go to 0, the other corresponds to the active phase, where:

$$a_\infty = \frac{\tau(\sigma - 2\mu)^2}{3\nu^2(3\rho + \mu + \sigma)}, \quad b_\infty = \frac{\sigma - 2\mu}{3\nu}. \quad (5.12)$$

We can see from above expression Eq.(5.12) that a continuous phase transition happens at $\sigma = 2\mu$. When $\sigma < 2\mu$, the system relaxes to the absorbing phase where all particles disappear.

5.4.2 Equivalence between PCPD and cPCPD at Tree Level

In the two-species model (5.8), while the original B particle remains massless, the pair particle A has a mass, i.e. finite decay rate. When the momentum/frequency scale is much

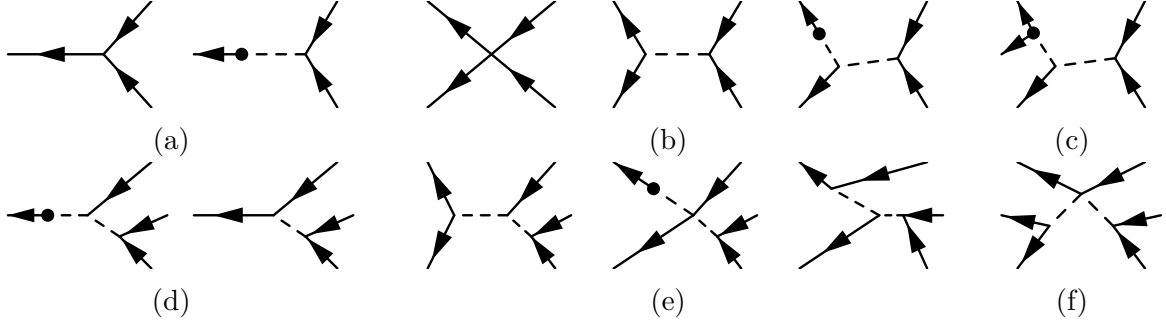


Figure 5.4: Tree-level contributions to the vertices (a) $\Gamma_{bb^2}^{\bar{b}}$, (b) $\Gamma_{b^2b^2}^{\bar{b}}$, (c) $\Gamma_{b^3b^2}^{\bar{b}}$, (d) $\Gamma_{bb^3}^{\bar{b}}$, (e) $\Gamma_{b^2b^3}^{\bar{b}}$, and (f) $\Gamma_{b^3b^3}^{\bar{b}}$. A (pair) particles are presented by dashed lines and B particles are represented by solid lines with arrows. Time flows from right to left.

lower than the mass of the A particle, we can integrate out the A particle and obtain an effective theory with only species B . We calculate the effective single-species theory to tree-level, and the tree diagrams are plotted in Fig. 5.4. By integrating out the A particles to order of $\mathcal{O}[(i\omega + p^2)/(\rho + \mu)]$, we can obtain all three pair reactions in the original PCPD. The amplitudes read:

$$\Gamma_{bb^2}^{\bar{b}} = \frac{2\mu - \sigma}{\rho + \mu}\tau, \quad \Gamma_{b^2b^2}^{\bar{b}} = \frac{\mu\tau}{\rho + \mu} - \frac{(2\rho + \sigma)\sigma\tau}{(\rho + \mu)^2}, \quad \Gamma_{b^3b^2}^{\bar{b}} = -\frac{\rho\sigma\tau}{(\rho + \mu)^2}. \quad (5.13)$$

In the limit where $\rho \gg \sigma, \mu$, the amplitudes reduce to:

$$\Gamma_{bb^2}^{\bar{b}} = \frac{2\mu - \sigma}{\rho}\tau, \quad \Gamma_{b^2b^2}^{\bar{b}} = \frac{(\mu - 2\sigma)\tau}{\rho}, \quad \Gamma_{b^3b^2}^{\bar{b}} = -\frac{\sigma\tau}{\rho}. \quad (5.14)$$

In this limit, all A particles rapidly disintegrate into pairs of B particles, effectively transforming the system into a single-species one. As a result, the ratio between the coefficients of pair reactions is consistent with that of the single-species PCPD, as specified in (5.7). The effective action then represents reactions $2B \rightarrow \emptyset$ and $2B \rightarrow 3B$ with reaction rate $\mu\tau/\rho$ and $\sigma\tau/\rho$, respectively. Additionally, the three-particle soft site restrictions are also regained through the tree-level diagrams in Fig. 5.4, and the amplitudes are given by:

$$\Gamma_{bb^3}^{\bar{b}} = \frac{3\rho + \mu + \sigma}{(\rho + \mu)^2}\nu\tau, \quad \Gamma_{b^2b^3}^{\bar{b}} = \frac{3\rho + 2\sigma}{(\rho + \mu)^2}\nu\tau, \quad \Gamma_{b^3b^3}^{\bar{b}} = \frac{\rho\tau\nu}{(\rho + \mu)^2}. \quad (5.15)$$

All three coefficients are proportional to the site restriction reaction rate ν . In the limit $\rho \gg \mu, \sigma$, the effective one-species site restriction reaction $3B \rightarrow \emptyset$ in (5.7) is regained with reaction rate $\nu\tau/\rho$ as shown

$$\Gamma_{bb^3}^{\bar{b}} = \frac{3\nu\tau}{\rho}, \quad \Gamma_{b^2b^3}^{\bar{b}} = \frac{3\nu\tau}{\rho}, \quad \Gamma_{b^3b^3}^{\bar{b}} = \frac{\tau\nu}{\rho}. \quad (5.16)$$

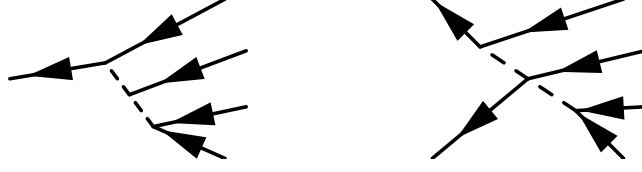


Figure 5.5: Effective four-particle reactions generated by integrating out A particles at tree-level. As in Fig. 5.4, solid lines represent B particles and dashed lines represent A particles.

Higher order reactions are also generated (for example, the four-particle reaction terms generated by diagrams shown in Fig. 5.5). However, as they are less relevant, we do not discuss them here. We have demonstrated that in the limit $\rho \rightarrow \infty$, all reactions in the single-species PCPD are exactly recovered in the tree-level effective field theory. Thus, the cPCPD is one of the possible microscopic theories that corresponds to the PCPD in the low energy limit. In the next section, we will analyze the fixed point structure of the cPCPD.

5.4.3 RG analysis of cPCPD

The critical dimension of the cPCPD is suggested to be 2 [210] and the naive dimension analysis indicates

$$[\rho] = [\mu] = [\sigma] = \kappa^2, \quad [\tau] = [\nu] = \kappa^{2-d}. \quad (5.17)$$

We found that both τ and the site-restriction reaction rate ν are marginal near two dimensions. To study the scaling behavior near the critical point in the dimensional regularized RG, it is necessary to tune relevant operators to zero and only examine the effects from the marginal operators. However, it is important to keep in mind that the critical condition $\sigma = 2\mu$ requires that the scaling dimension of σ and μ are equal near the critical fixed point. We introduce the multiplicative renormalization Z factors to absorb the ultraviolet divergences in the following way:

$$\begin{aligned} \rho_R &= Z_\rho \rho \kappa^{-2}, & \mu_R &= Z_\mu \mu \kappa^{-2}, & \sigma_R &= Z_\sigma \sigma \kappa^{-2}, & \tau_R &= Z_\tau \tau C_d \kappa^{d-2}, & \nu_R &= Z_\nu \nu C_d \kappa^{d-2} \\ a_R &= Z_a a, & \bar{a}_R &= Z_{\bar{a}} \bar{a}, & b_R &= Z_b b, & \bar{b}_R &= Z_{\bar{b}} \bar{b}, & D_R &= Z_D D, & D'_R &= Z_{D'} D', \end{aligned} \quad (5.18)$$

where $C_d = \Gamma(2 - d/2)2^{1-d}\pi^{-d/2}$ is a dimension-dependent geometric factor. We carry out a one-loop calculation and choose the normalization point at $i\omega = 2D\kappa^2$, which is located outside the infrared-singular region. Near the critical point, while taking $\rho, \sigma, \mu \rightarrow 0$, there are only two different loop structures at one-loop order, which are shown in Fig. 5.6. The renormalized vertex functions are as follows¹

¹More detailed calculations can be found in the appendix 5.6.1.

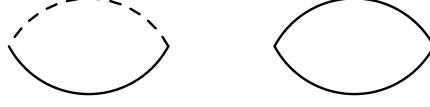


Figure 5.6: Loop structures which contribute at one-loop order near two dimensions. The dashed lines represent A particles and the solid line represents B particles. The momentum flows from right to left in our convention.

$$\begin{aligned}
 \Gamma_{\bar{a}a} &= \rho + \mu - \rho \frac{\tau}{D} \frac{C_D \kappa^{-\epsilon}}{\epsilon} + \sigma \frac{\nu}{D + D'} \left(\frac{2D\kappa^2}{D + D'} \right)^{-\epsilon/2}, \\
 \Gamma_{\bar{b}a} &= -(2\rho + \sigma) + 2\rho \frac{\tau}{D} \frac{C_D \kappa^{-\epsilon}}{\epsilon} + \sigma \frac{\nu}{D + D'} \left(\frac{2D\kappa^2}{D + D'} \right)^{-\epsilon/2}, \\
 \Gamma_{\bar{b}^2a} &= -2\rho + 2\rho \frac{\tau}{D} \frac{C_D \kappa^{-\epsilon}}{\epsilon}, \quad \Gamma_{\bar{a}\bar{b}a} = -\sigma \left[1 - \frac{\nu}{D + D'} \left(\frac{2D\kappa^2}{D + D'} \right)^{-\epsilon/2} \right], \\
 \Gamma_{\bar{a}ab} &= \nu \left[1 - \frac{\nu}{D + D'} \left(\frac{2D\kappa^2}{D + D'} \right)^{-\epsilon/2} \right], \quad \Gamma_{\bar{b}ab} = \nu \left[1 - \frac{\nu}{D + D'} \left(\frac{2D\kappa^2}{D + D'} \right)^{-\epsilon/2} \right], \\
 \Gamma_{\bar{b}b^2} &= 4\tau \left(1 - \frac{\tau}{D} \frac{C_D \kappa^{-\epsilon}}{\epsilon} \right) = \Gamma_{\bar{b}^2b^2}, \quad \Gamma_{\bar{a}b^2} = -2\tau \left(1 - \frac{\tau}{D} \frac{C_D \kappa^{-\epsilon}}{\epsilon} \right),
 \end{aligned} \tag{5.19}$$

where $\epsilon = d - 2$. From the above vertex functions, Eq.(5.19), we can extract the Z factors as follows:

$$\begin{aligned}
 Z_a &= Z_{\bar{a}} = Z_b = Z_{\bar{b}} = Z_{D'} = Z_D = 1, \quad Z_\tau = 1 - \frac{\tau}{D} \frac{C_D \kappa^{-\epsilon}}{\epsilon} = Z_\rho \\
 Z_\sigma &= 1 - \frac{\nu}{D + D'} \left(\frac{2D\kappa^2}{D + D'} \right)^{-\epsilon/2}, \quad Z_\mu = 1 + \frac{\sigma}{\mu} \frac{\nu}{D + D'} \left(\frac{2D\kappa^2}{D + D'} \right)^{-\epsilon/2} = Z_\nu.
 \end{aligned} \tag{5.20}$$

For convenience, we define the effective marginal parameters g and f as

$$g = \frac{\tau}{D}, \quad f = \frac{\nu}{D + D'}. \tag{5.21}$$

The scale-dependent anomalous dimensions and the beta functions thus follow

$$\begin{aligned}
 \beta_f &= \kappa \frac{\partial}{\partial \kappa} \bigg|_0 f_R = f_R(d - 2 + f_R), \quad \beta_g = \kappa \frac{\partial}{\partial \kappa} \bigg|_0 g_R = g_R(d - 2 + g_R), \\
 \zeta_\rho &= \kappa \frac{\partial}{\partial \kappa} \bigg|_0 \ln \frac{\rho_R}{\rho} = -2 + g_R, \quad \zeta_\sigma = \kappa \frac{\partial}{\partial \kappa} \bigg|_0 \ln \frac{\sigma_R}{\sigma} = -2 + f_R, \\
 \zeta_\mu &= \kappa \frac{\partial}{\partial \kappa} \bigg|_0 \ln \frac{\mu_R}{\mu} = -2 - \frac{\sigma_R}{\mu_R} f_R.
 \end{aligned} \tag{5.22}$$

The subscript “0” in the above equations denotes that the derivatives should be taken at fixed bare parameter values, with respect to the momentum scale κ . The nontrivial fixed

point is at $g_R = \epsilon$ and $f_R = \epsilon$. However, to maintain the critical condition $\sigma = 2\mu$, we require that the two parameters scale similarly near the fixed point, i.e. $\zeta_\sigma = \zeta_\mu$. This necessitates that either $f_R = 0$ or $\sigma_R/\mu_R = -1$. Since both σ and μ are reaction rates and are thus positive, the only possibility is $f_R = 0$, where the site restriction does not contribute. Both cases are inconsistent with the phase transition in the PCPD model and suggest that, near the critical point, at least one of the three parameters σ , ρ and μ does not go to zero. Together with the constraint $\sigma = 2\mu$, it indicates that the mass $\rho + \mu$ of the pair particles A is not zero near the active-to-absorbing phase transition. As the mass is relevant, it should go to infinity and can be integrated out as shown in the previous section. Thus, we believe that the critical behavior of the system should be fully captured by the single-species model.

5.5 Summary and Outlook

In this chapter, we delved into the active-to-absorbing phase transition in the PCPD (Pair Contact Process with Diffusion). We began by providing a brief overview of the phase transition and critical behavior in a reaction-diffusion system that belongs to the DP universality class. We then proceeded to motivate the generalization of the reactions to the PCPD model. Our analysis included a thorough examination of the structure of the field theory corresponding to the single-species PCPD, as well as a review of its fixed point structure near two dimensions. We also addressed the inconsistency in the RG flow and suggested that the fixed point found in previous research [208] is actually a pair annihilation fixed point.

Furthermore, we investigated the cPCPD model, which was introduced in a recent study [210]. We demonstrated that in the limit when the mass of the pair particle A goes to infinity, we can integrate out the pair particle at the tree-level and recover the single species PCPD exactly. We also examined the fixed-point structure of the model in the limit that all relevant parameters approach zero. Our analysis revealed that the scaling behavior near the nontrivial fixed point is not consistent with the critical condition of PCPD, and thus is not the critical point. As a result, we conclude that at least one of the relevant operators should go to infinity. Together with the critical condition, we know the mass of the pair particle goes to infinity and we can integrate the pair particle out. Therefore, we believe that the critical fixed point should be fully determined by the single species PCPD model.

There are some directions to be explored in the future:

- A phase transition is driven by a relevant operator as the system flows to one of the fixed points corresponding to a phase when it is perturbed away from the critical point. However, we have observed that the operator $\bar{b}b^2$, which appears to drive the phase transition, is not always relevant. The naive dimension of $\bar{b}b^2$ depends on the spatial dimension d , and when the spatial dimension is beyond a specific value, this operator becomes irrelevant and there should be no phase transition anymore. This specific “upper” critical dimension behaves like a reversed lower critical dimension in

the Ginzburg-Landau theory. It is meaningful to numerically check if this “upper” critical dimension exists and it would provide insights into how to rescale the fields in the RG analysis.

- In Section 5.3, we identified all possible operators that could induce a fixed point in the PCPD model. However, only one of these operators has been studied in the previous literature. To gain a deeper understanding of the model, it is important to examine the renormalization group (RG) flow near the fixed points driven by the other operators. Because of the specific structure of the Doi-Peliti field theory, the order of the ϵ expansion does not align with the order of the loop expansion for higher-order reactions. Therefore, a careful ϵ expansion, rather than loop expansion, must be performed in order to study the fixed point structures driven by these other combined operators.

5.6 Appendix

5.6.1 One-loop Results for the Vertex Functions

In this appendix, we present additional information and intermediate calculations for the explicit determination of various vertex functions. Through these calculations, we are able to obtain the renormalization Z factors. For ease of reference, we have defined the following shorthand notations:

$$\begin{aligned}
 I_1 &= \frac{1}{k^2 + \frac{q^2}{4} + \frac{i\omega}{2D}}, & I_2 &= \frac{1}{k^2 - \frac{D-D'}{D+D'}q \cdot k + \frac{q^2}{4} + \frac{i\omega+\rho+\mu}{D+D'}}, \\
 I_3 &= \frac{1}{k^2 + \frac{D}{D+D'} \left(\frac{q^2}{4} - q \cdot k \right) + \frac{i\omega/2+\rho+\mu}{D+D'}}, & I_4 &= \frac{1}{k^2 - \frac{q \cdot k}{2} + \frac{q^2}{8} + \frac{i\omega}{4D}}, \\
 I_5 &= \frac{1}{k^2 + \frac{D-D'}{D+D'}q \cdot k + \frac{q^2}{4} + \frac{i\omega+\rho+\mu}{D+D'}}, & I_6 &= \frac{1}{k^2 + \frac{q^2}{4} + \frac{i\omega/2+\rho+\mu}{D'}}.
 \end{aligned} \tag{5.23}$$

In our convention, time and hence momentum always flow from right to left in Feynman diagrams. The dashed lines represent pair particles A and the solid lines represent the single particles B .

Two-point vertices

For two-point vertices, the one-loop order diagrams are shown in Fig. 5.7 and we have the following results:

$$\begin{aligned}
 \Gamma_{\bar{b}b}(q, \omega) &= i\omega + Dq^2, \\
 \Gamma_{\bar{a}a}(q, \omega) &= i\omega + D'q^2 + \rho + \mu - \frac{\rho\tau}{D} \int_k I_1 + \frac{\sigma\nu}{D+D'} \int_k I_2 - \frac{(2\rho+\sigma)\sigma\tau}{D(D+D')} \int_k I_1 \cdot I_2, \\
 \Gamma_{\bar{b}a}(q, \omega) &= -2\rho - \sigma + \frac{2\rho\tau}{D} \int_k I_1 + \frac{\sigma\nu}{D+D'} \int_k I_2 + \frac{2(2\rho+\sigma)\sigma\tau}{D(D+D')} \int_k I_1 \cdot I_2.
 \end{aligned} \tag{5.24}$$

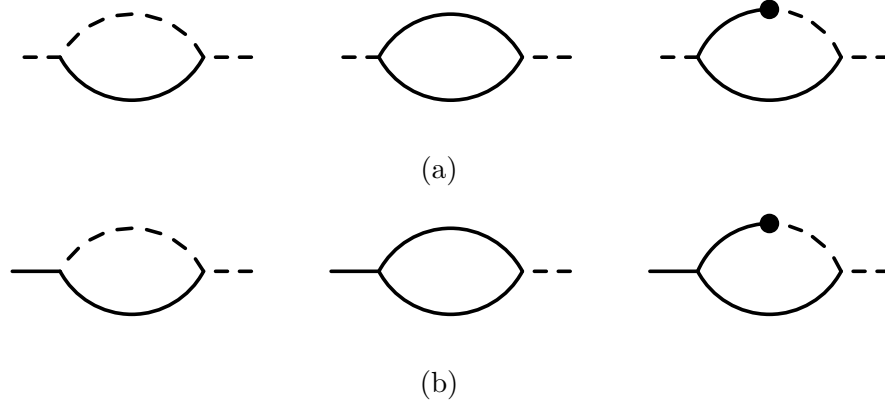


Figure 5.7: One-loop contributions to the vertex functions (a) $\Gamma_{\bar{a}a}$ and (b) $\Gamma_{\bar{b}a}$. There is no one loop contribution to the two-point vertex function $\Gamma_{\bar{b}b}$.

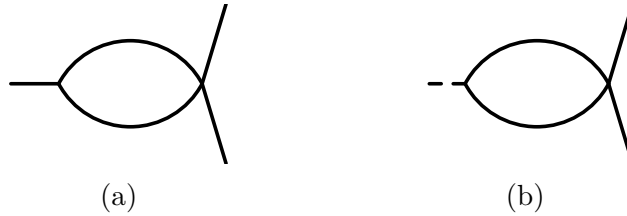


Figure 5.8: One-loop contributions to the vertex functions (a) $\Gamma_{\bar{b}b^2}$ and (b) $\Gamma_{\bar{a}b^2}$.

Three-point vertices

For the three-point vertex functions, the one-loop order diagrams are plotted in Fig. 5.8-5.10. For the reaction vertices, we have

$$\begin{aligned}
 \Gamma_{\bar{b}b^2} \left(q, \omega; \frac{q}{2}, \frac{\omega}{2}, \frac{q}{2}, \frac{\omega}{2} \right) &= 4\tau \left(1 - \frac{\tau}{D} \int_k I_1 \right), \\
 \Gamma_{\bar{a}b^2} \left(q, \omega; \frac{q}{2}, \frac{\omega}{2}, \frac{q}{2}, \frac{\omega}{2} \right) &= -2\tau \left(1 - \frac{\tau}{D} \int_k I_1 \right), \\
 \Gamma_{\bar{b}^2a} \left(\frac{q}{2}, \frac{\omega}{2}, \frac{q}{2}, \frac{\omega}{2}; q, \omega \right) &= -2\rho - \frac{2\rho\tau}{D} \int_k I_1 + \frac{2(2\rho + \sigma)\sigma\tau}{D(D + D')} \int_k I_1 \cdot I_2 + \frac{8\rho\sigma\tau}{D(D + D')} \int_k I_2 \cdot I_4, \\
 &\quad + \frac{2\sigma^2\nu}{(D + D')^2} \int_k I_2 \cdot I_3 + \frac{4(2\rho + \sigma)\sigma^2\tau}{D(D + D')^2} \int_k I_2 \cdot I_3 \cdot I_4, \\
 \Gamma_{\bar{a}b\bar{a}} \left(\frac{q}{2}, \frac{\omega}{2}, \frac{q}{2}, \frac{\omega}{2}; q, \omega \right) &= -\sigma + \frac{\sigma\nu}{D + D'} \int_k I_2 - \frac{2(\rho - \sigma)\sigma\tau}{D(D + D')} \int_k I_2 \cdot I_4, \\
 &\quad + \frac{\sigma^2\nu}{(D + D')^2} \int_k I_2 \cdot I_3 - \frac{(2\rho + \sigma)\sigma^2\tau}{D(D + D')^2} \int_k I_2 \cdot I_3 \cdot I_4.
 \end{aligned} \tag{5.25}$$

For the site restriction vertices, we have

$$\begin{aligned}
 \Gamma_{\bar{b}ab} \left(q, \omega; \frac{q}{2}, \frac{\omega}{2}, \frac{q}{2}, \frac{\omega}{2} \right) &= \nu - \frac{\nu^2}{D + D'} \int_k I_2 - \frac{2(2\rho + \sigma)\tau\nu}{D(D + D')} \int_k I_1 \cdot I_2 - \frac{8\rho\tau^2}{D^2} \int_k I_1 \cdot I_4 \\
 &\quad + \frac{2\rho\tau\nu}{D(D + D')} \int_k I_2 \cdot I_4 - \frac{2\sigma\tau\nu}{D(D + D')} \int_k I_1 \cdot I_3 - \frac{4\sigma\tau\nu}{(D + D')^2} \int_k I_3 \cdot I_5 \\
 &\quad - \frac{\sigma\nu^2}{(D + D')^2} \int_k I_2 \cdot I_3 + \frac{4(2\rho + \sigma)\rho\tau^2}{D^2(D + D')} \int_k I_1 \cdot I_2 \cdot I_4 \\
 &\quad - \frac{4(2\rho + \sigma)\sigma\tau^2}{D^2(D + D')} \int_k I_1 \cdot I_3 \cdot I_4 - \frac{4(2\rho + \sigma)\sigma\tau^2}{D^2(D + D')} \int_k I_1 \cdot I_4 \cdot I_5 \\
 &\quad - \frac{8(2\rho + \sigma)\sigma\tau^2}{D(D + D')^2} \int_k I_3 \cdot I_4 \cdot I_5 + \frac{2(2\rho + \sigma)\sigma\tau\nu}{D(D + D')^2} \int_k I_2 \cdot I_3 \cdot I_4 \\
 &\quad + \frac{(2\rho + \sigma)\sigma\tau\nu}{D'(D + D')^2} \int_k I_2 \cdot I_3 \cdot I_6 - \frac{2(2\rho + \sigma)\sigma\tau\nu}{D(D + D')^2} \int_k I_1 \cdot I_2 \cdot I_3 \\
 &\quad + \frac{(2\rho + \sigma)\sigma\tau\nu}{D'(D + D')^2} \int_k I_3 \cdot I_5 \cdot I_6 + \frac{4(2\rho + \sigma)^2\sigma\tau^2}{D^2(D + D')^2} \int_k I_1 \cdot I_2 \cdot I_3 \cdot I_4 \\
 &\quad + \frac{4(2\rho + \sigma)^2\sigma\tau^2}{D(D + D')^3} \int_k I_1 \cdot I_2 \cdot I_3 \cdot I_5 + \frac{4(2\rho + \sigma)^2\sigma\tau^2}{D^2(D + D')^2} \int_k I_2 \cdot I_3 \cdot I_5 \cdot I_6,
 \end{aligned} \tag{5.26}$$

and

$$\begin{aligned}
\Gamma_{\bar{a}ab} \left(q, \omega; \frac{q}{2}, \frac{\omega}{2}, \frac{q}{2}, \frac{\omega}{2} \right) = & \nu - \frac{\nu^2}{D+D'} \int_k I_2 + \frac{(2\rho+\sigma)\tau\nu}{D(D+D')} \int_k I_1 \cdot I_2 + \frac{4\rho\tau^2}{D^2} \int_k I_1 \cdot I_4 \\
& + \frac{2\rho\tau\nu}{D(D+D')} \int_k I_2 \cdot I_4 + \frac{\sigma\tau\nu}{D(D+D')} \int_k I_1 \cdot I_3 \\
& - \frac{4\sigma\tau\nu}{(D+D')^2} \int_k I_3 \cdot I_5 - \frac{\sigma\nu^2}{(D+D')^2} \int_k I_2 \cdot I_3 \\
& - \frac{2(2\rho+\sigma)\rho\tau^2}{D^2(D+D')} \int_k I_1 \cdot I_2 \cdot I_4 + \frac{2(2\rho+\sigma)\sigma\tau^2}{D^2(D+D')} \int_k I_1 \cdot I_3 \cdot I_4 \\
& + \frac{2(2\rho+\sigma)\sigma\tau^2}{D^2(D+D')} \int_k I_1 \cdot I_4 \cdot I_5 + \frac{4(2\rho+\sigma)\sigma\tau^2}{D(D+D')^2} \int_k I_3 \cdot I_4 \cdot I_5 \\
& + \frac{2(2\rho+\sigma)\sigma\tau\nu}{D(D+D')^2} \int_k I_2 \cdot I_3 \cdot I_4 + \frac{(2\rho+\sigma)\sigma\tau\nu}{D'(D+D')^2} \int_k I_2 \cdot I_3 \cdot I_6 \\
& + \frac{(2\rho+\sigma)\sigma\tau\nu}{D(D+D')^2} \int_k I_1 \cdot I_2 \cdot I_3 + \frac{(2\rho+\sigma)\sigma\tau\nu}{D'(D+D')^2} \int_k I_3 \cdot I_5 \cdot I_6 \\
& - \frac{2(2\rho+\sigma)^2\sigma\tau^2}{D^2(D+D')^2} \int_k I_1 \cdot I_2 \cdot I_3 \cdot I_4 - \frac{2(2\rho+\sigma)^2\sigma\tau^2}{D(D+D')^3} \int_k I_1 \cdot I_2 \cdot I_3 \cdot I_5 \\
& - \frac{2(2\rho+\sigma)^2\sigma\tau^2}{D'(D+D')^3} \int_k I_2 \cdot I_3 \cdot I_5 \cdot I_6.
\end{aligned} \tag{5.27}$$

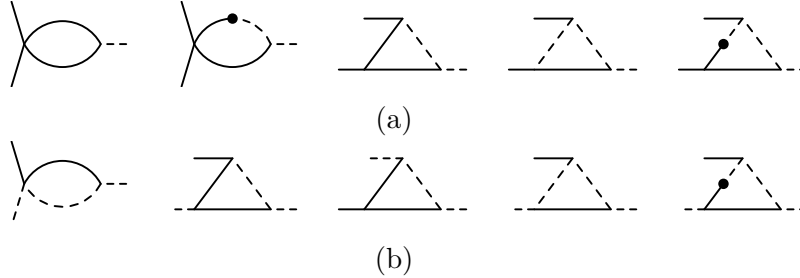


Figure 5.9: One-loop contributions to the vertex functions (a) $\Gamma_{\bar{b}^2a}$ and (b) $\Gamma_{\bar{a}b\bar{a}}$.

Four-point vertices

We only calculated the four-point vertex function $\Gamma_{\bar{b}^2b^2}$ to one-loop order. The one-loop order diagrams are shown in Fig. 5.11 and we have

$$\Gamma_{\bar{b}^2b^2} \left(\frac{q}{2}, \frac{\omega}{2}, \frac{q}{2}, \frac{\omega}{2}; \frac{q}{2}, \frac{\omega}{2}, \frac{q}{2}, \frac{\omega}{2} \right) = 4\tau \left(1 - \frac{\tau}{D} \int_k I_1 \right) \tag{5.28}$$

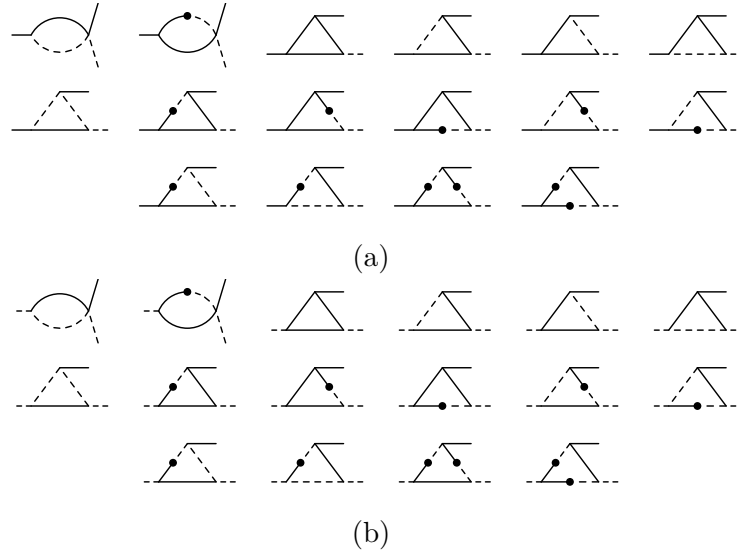


Figure 5.10: One-loop contributions to the vertex functions (a) $\Gamma_{b^2 a}$ and (b) $\Gamma_{a b a}$.

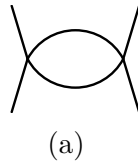


Figure 5.11: One-loop contribution to the vertex function $\Gamma_{b^2 b^2}$.

Chapter 6

Summary

In this dissertation, we investigated four distinct phenomena arising from fluctuations: the critical dynamics of antiferromagnets with conserved magnetization, a one-dimensional coined quantum walk (CQW) with spatial disorder, pattern formation and fluctuations corrections in three-species cyclic predator-prey models, and the active-to-absorbing phase transition in the pair contact process with diffusion (PCPD).

In chapter 2, we focused on studying the critical dynamics of the antiferromagnetic nonlinear sigma model with conserved total magnetization. We utilized the perturbative field-theoretic RG approach to analyze the scaling properties of the dynamical response functions of the order parameter and magnetization densities to one-loop order. As expected near thermal equilibrium, the response functions exhibit a separation of dynamics from statics. We observed an explicit symmetry breaking between the response functions of the transverse and longitudinal components of the magnetization density, indicating that the rotational symmetry cannot be recovered. Thus, approaching the critical fixed point is not feasible in this perturbative regime.

In addition, we examined the scaling behavior of the dynamical system near the ordered phase RG fixed point that characterizes the asymptotic coexistence limit by expanding around the dynamical upper critical dimension $d_c = 4$ using an $\epsilon = 4 - d$ expansion. Our investigation uncovered anomalous sub-diffusive scaling induced by Goldstone modes in the longitudinal component of the magnetization. We observed that the dynamic exponents at the coexistence ordered phase fixed point are identical to those of the SSS model, which is based on a Landau-Ginzburg-Wilson Hamiltonian. We numerically solved the RG flow equations and observed a short crossover regime towards the critical region if initiated near the critical point. By chance, we even recovered the correct dynamical critical exponent $z_c = d/2$ before reaching the coexistence limit with $z_D = z_\lambda = 2$ and $z_\Gamma = d - 2$. We predict that these relaxation properties can be experimentally observed through the dynamic scaling of neutron scattering linewidths or the temporal decay of the autocorrelation function for the longitudinal magnetization fluctuations.

In Chapter 3, the influence of quenched disorder on CQWs was analyzed. Specifically, the occupation probability of the quantum walker was studied in both the Hadamard walk and the coin-disordered version. Our findings revealed that disorder slows down the dynamics, inhibits ballistic spreading, and induces walker localization, characterized by the emergence of a new central peak. The mean squared displacement analysis also confirmed that the

dynamics becomes exceedingly slow.

Two approaches were employed to investigate the entanglement behavior between the quantum coin and the walker. The first approach assessed the entanglement entropy of individual CQW realizations, which revealed that disorder reduces the average entanglement entropy per run and induced oscillations that signify localization. The second approach quantified the entanglement negativity of the ensemble of realizations, which decreases to zero upon introducing coin disorder, indicating that entanglement is not a major factor, and further validating walker localization.

Chapter 4 focused on a perturbative field-theoretical analysis of the Rock-Paper-Scissor (RPS) and May-Leonard (ML) models up to one-loop order in fluctuation corrections. Using the Doi-Peliti formalism, we derived the dynamical probability functional and equivalent generalized Langevin equations for stochastic Markovian dynamics. In the RPS model, one-loop fluctuation corrections induce dissipation, resulting in positive damping coefficients in physically accessible dimensions. Additionally, the fluctuation corrections cause an infrared divergence in the oscillation frequency. However, outside the perturbative regime, the damping terms become significant, and the IR divergence of the oscillation frequency is naturally regularized, thereby explaining the absence of significant fluctuation corrections observed in computer simulations. As for the ML model, the one-loop fluctuation corrections do not significantly alter the mean-field conclusions, and the system remains relatively insensitive to fluctuations, at least perturbatively and in the stable region where the homogeneous steady state exists.

We also provided two criteria to determine the possibility of spatio-temporal structures in the Lotka-Volterra (LV), RPS, and ML models. The first criterion considers a single lattice site perspective, and a necessary condition for the emergence of spatially extended coherent oscillatory behavior is that the oscillation frequency remains constant over space and time in each run. The second criterion is based on studying the global stability of the spatially homogeneous stationary state of the system. Only if the spatially uniform quasi-steady state is rendered unstable against finite-wavelength fluctuations can non-trivial spatio-temporal structures be generated, as is evident in the ML model. These criteria explained the absence of spatio-temporal patterns in the RPS system, due to the relevant conservation law for the total particle number, in contrast with the LV and ML models.

In chapter 5, we focused on the active-to-absorbing phase transition in the PCPD model. First, we gave a brief overview of the phase transition and critical behavior in a reaction-diffusion system belonging to the DP universality class, before discussing the motivation behind generalizing the reactions to the PCPD model. Our analysis included a thorough examination of the field theory structure corresponding to the single-species PCPD, and a review of its fixed-point structure near two dimensions. We also addressed the inconsistency in the RG flow and suggested that the fixed point found in previous research was actually a pair annihilation fixed point.

Furthermore, we investigated the cPCPD model introduced in a recent study and showed

that in the limit where the mass of the pair particle tends to infinity, one can integrate out the pair particle field and recover the single-species PCPD. We examined the fixed-point structure of the cPCPD model in the limit where all relevant parameters approach zero and revealed that the scaling behavior near this nontrivial fixed point is not consistent with the critical condition of the PCPD, leading us to conclude that at least one of the relevant operators should go to infinity. We argued that the critical fixed point should be fully determined by the single species PCPD model, given the critical condition and the knowledge that the mass of the pair particle goes to infinity, enabling us to integrate it out.

As we conclude this dissertation, we sincerely hope that you have thoroughly enjoyed the journey with us through the exploration of four distinct systems, each exhibiting peculiar and fascinating fluctuation-induced behavior. It is our ardent wish that our studies have not only contributed to the advancement of knowledge but have also illuminated new paths for future research, as pointed out at the end of each chapter. Ultimately, we hope that our work will inspire more people to venture into the wonderland of statistical physics and uncover the many secrets that lie within.

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