



Clues on chemical mechanisms from renormalizability: The example of a noisy cubic autocatalytic model



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HIGHLIGHTS

- Effects of power-law noise on the renormalizability of a chemical model is studied.
- Our reaction–diffusion cubic autocatalytic model is renormalizable at one-loop.
- Effects of noise-generated higher order interactions are discussed.
- We show how ideas of effective field theory can be applied to this chemical model.

ARTICLE INFO

Article history:

Received 16 January 2017

Received in revised form 11 March 2017

Available online 4 April 2017

Keywords:

Reaction–diffusion

Chemical model

Power-law noise

Renormalization

Effective field theory

ABSTRACT

We study the effect of external power-law noise on the renormalizability of a specific reaction–diffusion system of equations describing a cubic autocatalytic chemical reaction. We show that changing the noise exponent modifies the divergence structure of loop integrals and thus the renormalizability of the model. The effects of noise-generated higher order interactions are discussed. We show how noise induces new interaction terms that can be interpreted as a manifestation of some (internal) “chemical mechanism”. We also show how ideas of effective field theory can be applied to construct a more fundamental chemical model for this system.

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1. Introduction

The nature of chemical reaction mechanisms is a scale dependent problem of great practical and theoretical importance [1], often studied using spectroscopic or other analytical (in the chemical sense) techniques. A key question in chemistry and biology is to understand the mechanisms and chemical reactions underlying the macroscopic behavior of complex systems such as cells. Answering the above question is of course a daunting task. However, given the ubiquity and relevance of these systems, it is important to try to gain insight from simpler, more tractable models.

In this paper we approach the question of inferring the small scale (ultraviolet, UV) structure of a system known at large scales (infrared, IR) in the context of stochastic reaction–diffusion equations. In other words, we fine-grain those equations in order to study the underlying mechanisms from the large scale dynamics, i.e. we are using a top-down (outside-in) approach (e.g. [2]). Although they are relatively simple, reaction–diffusion equations lead to complex patterns [3] and are thought to be an essential part of morphogenesis [4–6]. In addition to serve as models for biological pattern formation, they are also used in various contexts such as the spreading of epidemics [7], ecological invasions [8], tumor growth [9] and oscillating chemical reactions [3,10].

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For definiteness, we focus on a particular reaction–diffusion model [11,12] based on a cubic autocatalytic two-species system [13–18]. This simple model has a very interesting phenomenology. Numerical simulations of the deterministic [11] and stochastic [12] versions of the model show the formation of domains (“cells”). These domains share some characteristics with living systems like birth, growth, movement, replication and death. Understanding the inner dynamics of such a simple system might provide insight into real, more complex organisms.

The analysis of stochastic reaction–diffusion equations can be couched in the language of field theory (e.g. [19]). In the following, we outline the first steps in a new approach to study the above cubic autocatalytic reaction–diffusion (CARD) model, that could in principle be applied to other reaction–diffusion systems. A hallmark of our method is the use of a fine-graining strategy more akin to the philosophy in particle physics, in contrast to the coarse-graining methods typically used in condensed matter physics. In other words, we apply the renormalization group to the CARD model, but run it from the IR to the UV. The latter strategy is natural in the context of finding more fundamental microscopic models from the knowledge of a macroscopic one.

Another important ingredient in our approach is the use of noise to represent the combined contributions of both internal degrees of freedom and environmental effects. We argue that we may use externally tunable noise to probe reaction–diffusion equations at small scales, in the same way that varying beam energy is used to study the inner structure of particles.

The above approach has been applied to the study of small-scale structures in the CARD model [20,21]. In the present contribution, we develop the more general aspects of the approach. The rest of the paper is organized as follows. In Section 2, we present the general idea behind our fine-graining method and its potential relevance to reaction–diffusion equations and chemistry. In particular, we show how self-consistent approaches (i.e. renormalizability, effective interactions, decoupling, see for example [22–27]) could allow the analysis of the system’s inner structures. The specific details of the CARD model are introduced in Section 3. Section 4 presents the proof of renormalizability of the CARD model at one-loop and the effects of higher order interactions on the dynamics, paving the way for our discussion of effective field theory in chemistry in Section 5. We discuss our results in Section 6. Feynman rules for the CARD model and technical details about the proof of renormalizability are relegated to the [Appendices](#).

2. Methodology and goals

The goal of this section is to explain our method for studying underlying mechanisms in a broader setting. But first, let us briefly review how effective field theory is used to uncover clues about fundamental theories in particle physics.

The parameters of the Standard Model of particle physics are measured with great precision up to energies $\Lambda_{\text{SM}} \sim$ few TeV. Quantum fluctuations make the parameters of the model energy dependent, and renormalization is a tool that enables the computation of this energy dependence. The Standard Model is renormalizable, meaning that it is possible to extend its domain of validity (i.e. “run” the parameters) up to arbitrary high energies. But experiments (on neutrino oscillations, baryon asymmetry, dark matter, dark energy) show that the Standard Model is incomplete and that new physics must exist at a higher energy scale Λ_{NP} . This implies that the running of the Standard Model parameters can only be done up to energy Λ_{NP} : above this energy, a new model (with potentially new dynamical degrees of freedom) must be used.

Experimentally, it is difficult to directly detect and measure the effects of new physics if Λ_{NP} is larger than the energy of present day accelerators. Effective field theory provides another way of probing new physics at energy Λ_{NP} . The basic tenets of effective field theory [24] tell us that the values of the Standard Model parameters at low energy Λ_{SM} include corrections due to higher energy processes that are suppressed by powers of the high energy scale. In our example, if new physics appears at Λ_{NP} , then corrections to the parameters are of the form $(\Lambda_{\text{SM}}/\Lambda_{\text{NP}})^{|\text{power}|}$. Thus if $\Lambda_{\text{NP}} \gg \Lambda_{\text{SM}}$, those corrections are very small and might not be measurable. This is why Planck scale physics has no hope of being measured with current technologies. But if the ratio is not too small, it might be possible to gain insight into more fundamental theories by looking at corrections in the Standard Model parameters.

Let us now show how these concepts can be applied to chemistry. As an illustrative example, let us take the following macroscopic chemical equation:



where k is the (forward) reaction rate. This chemical equation is valid at large temporal and spatial scales (corresponding to low momentum or resolution). At shorter temporal and spatial scales, the above description might break down and must be replaced by another one. One example of microscopic description is:



Another possible microscopic description is:



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