EPJ Web of Conferences **226**, 02005 (2020) https://doi.org/10.1051/epjconf/202022602005
Mathematical Modeling and Computational Physics 2019

Two-Species Reaction-Diffusion System: the Effect of Long-Range Spreading

Šarlota Birnšteinová[1,⋆], *Michal* Hnatič[1,2,3], and *Tomáš* Lučivjanský[1]

[1] *Pavol Jozef Šafárik University, Šrobárova 2, 041 54 Košice, Slovakia*
[2] *Institute of Experimental Physics, Slovak Academy of Sciences, Watsonova 47, 040 01 Košice, Slovakia*
[3] *Joint Institute for Nuclear Research, 141980 Dubna, Russia*

Abstract. We study fluctuation effects in the two-species reaction-diffusion system $A + B \to \emptyset$ and $A + A \to (\emptyset, A)$. In contrast to the usually assumed ordinary short-range diffusion spreading of the reactants we consider anomalous diffusion due to microscopic long-range hops. In order to describe the latter, we employ the Lévy stochastic ensemble. The probability distribution for the Lévy flights decays in d dimensions with the distance r according to a power-law $r^{-d-\sigma}$. For anomalous diffusion (including Lévy flights) the critical dimension $d_c = \sigma$ depends on the control parameter σ, $0 < \sigma \leq 2$. The model is studied in terms of the field theoretic approach based on the Feynman diagrammatic technique and perturbative renormalization group method. We demonstrate the ideas behind the B particle density calculation.

1 Introduction

Genuine reaction-diffusion models describe a multitude of phenomena in various disciplines, from population dynamics in ecology, competition of bacterial colonies in microbiology, dynamics of magnetic monopoles in the early universe in cosmology, to the stock market in economy, opinion exchange in sociology, etc [1].

We consider a system consisting of two particle species A and B, with the corresponding diffusion constants D_{nA} and D_{nB}. The reacting particles are assumed to undergo two kinds of reaction processes

$$A + A \to \begin{cases} \emptyset, & \text{with probability } p, \\ A, & \text{with probability } 1 - p, \end{cases} \qquad A + B \to A. \tag{1}$$

The problem where both particle species are mobile due to diffusion was studied in [2–4]. Neglecting the initial conditions, the mean-field equations for the process (1) take the simple form

$$\frac{\partial a}{\partial t} = D_{nA} \boldsymbol{\nabla}^2 a - \lambda a^2, \quad \frac{\partial b}{\partial t} = D_{nB} \boldsymbol{\nabla}^2 b - \lambda' ab, \tag{2}$$

where a and b denote the densities of corresponding reacting particles A and B, parameters λ and λ' are the reaction rates.

⋆e-mail: sarlota.birnsteinova@student.upjs.sk

For a space dimension d larger than the upper critical dimension d_c ($d_c = 2$ for the ordinary diffusion) the result for particle density A decreases with time as $a \sim 1/(\lambda t)$ [3–5]. The density of B particles decays with time as $b \sim t^{-\theta}$, where exponent θ depends on the ratio $\delta = D_{nB}/D_{nA}$ and the probability p [2, 3, 6]. For dimensions $d \leq 2$ the fluctuations become relevant and θ can not be determined from the rate equations (2).

To model a long-range spreading, we consider a generalized diffusion process, in which hopping distances are governed by the Lévy distribution [7]. The Fourier transforms of such distributions are $P(k) = \mathrm{e}^{-D_A k^\sigma}$, $P(k) = \mathrm{e}^{-D_B k^\sigma}$ for the Lévy index $0 < \sigma \leq 2$, where the anomalous diffusion constants D_A and D_B scale the distributions [8]. The exponent σ is a free parameter that controls the characteristic shape of the distribution. It should be emphasized that σ does not introduce any new length scale, rather it changes the scaling properties of the underlying (anomalous) diffusion process [9]. The anomalous diffusion modeled by the Lévy flights is effectively captured by the following substitutions:

$$D_{nA}\boldsymbol{\nabla}^2 \to D_{nA}\boldsymbol{\nabla}^2 + D_A\boldsymbol{\nabla}^\sigma, \quad D_{nB}\boldsymbol{\nabla}^2 \to D_{nB}\boldsymbol{\nabla}^2 + D_B\boldsymbol{\nabla}^\sigma. \tag{3}$$

The analysis of the canonical dimensions shows that for the case $\sigma < 2$ the ordinary diffusion terms $\propto \boldsymbol{\nabla}^2$ are infrared irrelevant with respect to the anomalous diffusion terms $\propto \boldsymbol{\nabla}^\sigma$. Both ordinary diffusion terms and anomalous diffusion terms have to be included for $\sigma \to 2$ [10, 11]. However, we are not interested in this case, and in the rest of the paper we assume that $\sigma \ll 2$ and discard the ordinary diffusion terms. Considering the Lévy flights also enables us to continuously vary the upper critical dimension with the Lévy index [12], since introducing the Lévy flights causes the critical dimension to be of the form $d_c = \sigma$.

In order to calculate the large-time behavior of the B particle density below the critical dimension, it is advantageous to employ the field theoretic approach followed by the perturbative renormalization group formalism. Here, we do not focus on the renormalization procedure itself, which can be found elsewhere for the ordinary diffusion case [2, 4] or for a simpler reaction-diffusion process $A + A \to \emptyset$ with anomalous diffusion [13]. Rather, we concentrate on explaining how the density of B particles can be calculated.

2 Field theoretic model

The field theory corresponding to the two-species reaction-diffusion model (2) with the Lévy flights can be derived from the master equation using the standard formalism of Doi [14, 15] and Peliti [16]. The ensuing field theoretic action [5, 17, 18] takes the form

$$\begin{aligned}\mathcal{S} = \int_0^\infty \mathrm{d}t \int_{-\infty}^\infty \mathrm{d}^d x \Big[&\psi_A^\dagger(\partial_t - \nabla^\sigma)\psi_A + \psi_B^\dagger(\partial_t - \delta\nabla^\sigma)\psi_B + \lambda_0\psi_A^\dagger\psi_A^2 + \lambda_0\psi_A^{\dagger 2}\psi_A^2 + \lambda_0' Q\psi_B^\dagger\psi_A\psi_B \\ &+ \lambda_0'\psi_A^\dagger\psi_B^\dagger\psi_A\psi_B\Big] - \int_{-\infty}^\infty \mathrm{d}^d x\,(\psi_A^\dagger a_0 + \psi_B^\dagger b_0).\end{aligned} \tag{4}$$

A simpler form of the action is obtained provided the new parameters $\delta = D_B/D_A$ and $Q = 1/(2-p)$ are introduced, the time t, λ and λ' are rescaled to absorb the anomalous diffusion constant D_A and fields as follows: $\psi_A \to Q\psi_A$, $\psi_A^\dagger \to \psi_A^\dagger/Q$.

The action (4) of the studied model has a convenient form for the standard Feynman diagrammatic technique [17, 18], the elements of which are depicted in Fig. 1. This technique allows us to construct an expression for the B-particle density, which is of interest here, in the form of a perturbation expansion. The order of the perturbation theory is set by the number of loops. The calculation of one-loop diagrams corrects the mean-field approximation, which is not valid below the upper critical dimension. To take into account all possible contributions of the initial conditions, we first need to find the mean-field expressions for the particle densities and propagators [17].

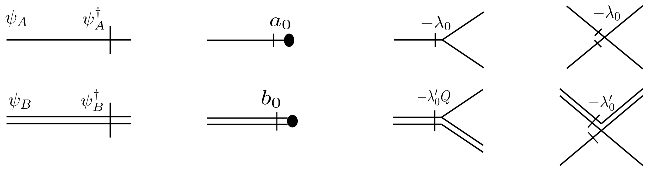


Figure 1. Propagators, initial conditions and vertices of the theory described by the action (4).

3 Mean-field approximation

The mean-field approximation corresponding to a sum of Feynman diagrams without loops and for the *A* and *B* particle densities reads

$$\langle\psi_A(t)\rangle_{mf} \equiv \text{- - - - - - - -} = \frac{a_0}{1+a_0\lambda_0 t}, \quad \langle\psi_B(t)\rangle_{mf} \equiv \text{= = = = = = = =} = \frac{b_0}{(1+a_0\lambda_0 t)^{\lambda_0' Q/\lambda_0}}, \tag{5}$$

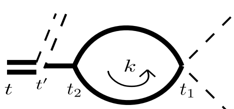
where the subscript mf stands for the mean-field approximation. Let us note that Eq. (5) corresponds to the solution of the rate equations (2). The mean-field propagators $G^{mf}_{AA} \equiv \langle\psi_A(-p,t_2)\psi_A^\dagger(p,t_1)\rangle_{mf}$ and $G^{mf}_{BB} \equiv \langle\psi_B(-p,t_2)\psi_B^\dagger(p,t_1)\rangle_{mf}$ can be written as follows:

$$\begin{aligned} G^{mf}_{AA}(p,t_2,t_1) &\equiv \overset{p}{\underset{t_2 \qquad t_1}{\overline{\qquad\qquad}}} = \mathrm{e}^{-p^\sigma(t_2-t_1)}\left(\frac{1+\lambda_0 a_0 t_1}{1+\lambda_0 a_0 t_2}\right)^2, \\ G^{mf}_{BB}(p,t_2,t_1) &\equiv \overset{p}{\underset{t_2 \qquad t_1}{\overline{\overline{\qquad\qquad}}}} = \mathrm{e}^{-\delta p^\sigma(t_2-t_1)}\left(\frac{1+\lambda_0 a_0 t_1}{1+\lambda_0 a_0 t_2}\right)^{\lambda_0' Q/\lambda_0}. \end{aligned} \tag{6}$$

Knowing the mean-field structures of the densities and propagators allows us to calculate the one-loop corrections to the *B* particle density.

4 An instance of one-loop Feynman diagram calculation

The contributions of one-loop order to the *B* particle density in the anomalous diffusion case involve three Feynman diagrams. The calculation of the simplest one, reported below, illustrates the ideas behind the general procedure.



$$= \int_0^t \mathrm{d}t_2 \int_0^{t_2} \mathrm{d}t_1 \int_{t_1}^{t_2} \mathrm{d}t'\, G^{mf}_{BB}(p,t_2,t')(-\lambda_0' Q)\langle\psi_B(t')\rangle_{mf} G^{mf}_{AA}(p,t',t_1)$$

$$\times \int \frac{\mathrm{d}^d k}{(2\pi)^d}(-\lambda_0) G^{mf2}_{AA}(k,t_2,t_1)(-\lambda_0)\langle\psi_A(t_1)\rangle^2_{mf}, \tag{7}$$

where Eqs. (5) and (6) are used. After integration over variable t' we apply the limit $a_0 \to \infty$ [2, 3] to get

$$\begin{aligned} &= -\frac{a_0^2 b_0 \lambda_0^2 \lambda_0' Q}{(1+a_0\lambda_0 t)^{\lambda_0' Q/\lambda_0}} \int_0^t \mathrm{d}t_2 \int_0^{t_2} \mathrm{d}t_1 \frac{(1+a_0\lambda_0 t_1)^2}{(1+a_0\lambda_0 t_2)^2} \int_{t_2}^t \mathrm{d}t\,(1+a_0\lambda_0 t')^{-2} \int \frac{\mathrm{d}^d k}{(2\pi)^d}, \exp\left[-2k^\sigma(t_2-t_1)\right] \\ &= -\frac{a_0 b_0 \lambda_0 \lambda_0' Q}{(a_0\lambda_0 t)^{1+\lambda_0' Q/\lambda_0}} \int_0^t \mathrm{d}t_2 \int_0^{t_2} \mathrm{d}t_1\, t_1^2 t_2^{-3} \int \frac{\mathrm{d}^d k}{(2\pi)^d} \exp\left[-2k^\sigma(t_2-t_1)\right]. \end{aligned} \tag{8}$$

For momentum integration we use the expression [11]

$$2\pi^{-d/2}\Gamma(1+d/2)\int \mathrm{d}^d k\, f(|k|^\sigma) = 2\pi^{-d/\sigma}\Gamma(1+d/\sigma)\int \mathrm{d}^{2d/\sigma} k\, f(|k|^2), \tag{9}$$

which results in momentum integration taking the form

$$\int \frac{\mathrm{d}^d k}{(2\pi)^d} \exp\Big[-2k^\sigma(t_2-t_1)\Big] = \frac{2^{1-d/\sigma}\Gamma(d/\sigma)}{(4\pi)^{d/2}\Gamma(d/2)}(t_2-t_1)^{-d/\sigma}. \tag{10}$$

After time integration and also momentum integration we obtain the following expression:

$$= -\frac{b_0\lambda_0' Q}{(a_0\lambda_0 t)^{\lambda_0' Q/\lambda_0}} \frac{2^{1-d/\sigma}\Gamma[d/\sigma]}{\sigma(4\pi)^{d/2}\Gamma[d/2]} t^{\varepsilon/\sigma} \frac{2\sigma^5}{\varepsilon^2(\varepsilon+\sigma)^2(\varepsilon+2\sigma)}, \tag{11}$$

where the substitution $\varepsilon = \sigma - d$ was inserted.

5 Conclusions

A study of two-species reaction-diffusion systems in which the reactants undergo anomalous diffusion was reported. The theoretical model uses stochastic probability distribution based on Lévy flights to incorporate long-range spreading. The model is studied for the case of infra-red irrelevant ordinary diffusion employing field-theoretic perturbative renormalization group. In this short communication, preliminary calculations of the time evolution of the B particle density are given. The model calculation of a one-loop Feynman diagram opens the way to numerous future developments of the problem.

References

[1] U. C. Täuber, *Critical Dynamics: A Field Theory Approach to Equilibrium and Non-Equilibrium Scaling Behavior* (Cambridge University Press, Cambridge, 2014)
[2] B. Vollmayr-Lee, J. Hanson, R.S. McIsaac, J.D. Hellerick, J. Phys. A: Math. Theor. **51**, 034002 (2018)
[3] M. Howard, J. Phys. A: Math. Gen. **29**, 3437–3460 (1996)
[4] S. Krishnamurthy, R. Rajesh, O. Zaboronski, Phys. Rev. E **68**, 046103 (2003)
[5] B. P. Lee, J. Phys. A: Math. Gen. **27**, 2633–2652 (1994)
[6] R. Rajesh, O. Zaboronski, Phys. Rev. E **70**, 036111 (2004)
[7] J. Klafter, G. Zumofen, M.F. Shlesinger, *Lévy description of anomalous diffusion in dynamical systems* (Springer, Berlin, Heidelberg, 1995)
[8] J. P. Bouchaud, A. Georges, Phys. Rep. **195**, 127 (1990)
[9] H. Hinrichsen, M. Howard, Eur. Phys. J. B **7**, 635–643 (1999)
[10] J. Honkonent, M.Yu. Nalimov, J. Phys. A: Math. Gen. **22**, 751–763 (1989)
[11] H. K. Janssen, O. Stenull, Phys. Rev. E **78**, 061117 (2008)
[12] D. Vernon, M. Howard, Phys. Rev. E **63**, 041116 (2001)
[13] D. C. Vernon. Phys. Rev. E **68**, 041103 (2003)
[14] M. Doi, J. Phys. A **9**, 1465 (1976)
[15] M. Doi, J. Phys. A **9**, 1479 (1976)
[16] L. Peliti, J. Phys (Paris) **46**, 1469 (1985)
[17] U. C. Täuber, M. Howard, B. P. Vollmayr-Lee, J. Phys. A: Math. Gen. **38**, R79–R131 (2005)
[18] A. N. Vasil'ev, *The Field Theoretic Renormalization Group in Critical Behavior Theory and Stochastic Dynamics* (Chapman and Hall/CRC, Boca Raton, Fla 2004)