One-dimensional lattices topologically equivalent to three-dimensional lattices within the context of the lattice gas model

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\textbf{HIGHLIGHTS}

• Stochastic evolution equations.
• Non-Markovian processes.
• Lattice gas model.

\textbf{ABSTRACT}

Continuum partial differential equations are obtained from a set of discrete stochastic evolution equations of both non-Markovian and Markovian processes and applied to the diffusion on a cubic lattice within the context of the lattice gas model. A procedure allowing to construct one-dimensional lattices that are topologically equivalent to a cubic three-dimensional lattice is described in detail using a successive “unfolding” process. This example shows some new features that possess the procedure and extensions are also suggested in order to provide some another uses of the present approach.

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1. Introduction

During some past decades a lot of effort was devoted to develop different approaches and techniques that allows to find the evolution equations of a set of stochastic dynamical variables that describe many models. Within the context of what could be coined Discrete Stochastic Evolution Equations (DSEE), papers dealing with different examples of evolution equations were written considering only one-dimensional lattices due to advantage of having a simpler presentation and in particular when the stochastic lattice gas model was considered [1]. Some illustrative examples that show the versatility of the DSEE approach can be found in [2–7]. In particular in [7], a topological theorem was proved which states that every lattice is topologically equivalent to a one-dimensional one. The theorem was included in [7] in order to justify the study of only one-dimensional problems. In the present paper the explicit construction of a one-dimensional lattice that is topologically equivalent to a three-dimensional cubic lattice will be considered in detail, within the context of the lattice gas model, in order to provide a procedures consisting in successive “unfoldings” that is needed in the present context. Even when the...
present approach can be used to describe non-Markovian evolution equations, in this paper, only examples whose evolution rules are Markovian will be considered for the sake of simplicity in the presentation. Moreover, only a cubic lattice will be studied, but other interesting three-dimensional lattices could be included within this context without a considerable effort, using the appropriate changes or as is usually said, mutatis mutandis. As is well known, lots of variants and approaches can be introduced in the highly versatile lattice gas model, and some of them can be found in [8–13]. Moreover, a series of papers that are closely related to the present one, can be found in [14–16].

The paper is organized as follows. In Section 2 the basic definitions necessary for the mise en scène of the model and notations are introduced for the case of non-Markovian evolution in a d-dimensional lattice and formulas and procedures are introduced. In Section 3, an example (the cubic three-dimensional lattice) that shows not only the way and steps needed to construct the one-dimensional lattice that is topologically equivalent to a three-dimensional one, but how to get rid of some “border anomalies” introducing some periodic boundary conditions according to the lattice at hand. In Section 3.1 the evolution equations that describe the diffusion of particles in a three-dimensional cubic lattice is studied in detail. In Section 3.2 the procedures needed to construct a one-dimensional lattice that is topologically equivalent to the three-dimensional one, is described step by step in order to show all possible subtleties appearing in the sequel. In Section 3.3, it is shown how to get rid of border anomalies by introducing periodic boundary conditions on the lattices according to whether the lattice is three-, two- or one-dimensional, respectively. Finally, in Section 3.3, conclusions, some generalizations, and perspectives are given.

2. The non-Markovian discrete stochastic evolution updating: basic definitions

For a detailed basic definitions see [14]. Presently only the final formulas that show the stochastic updating and the necessary steps needed for obtaining the partial differential equations will be considered. The starting stochastic updating can be given in the form,

\[ q_i^{(r)}(x, t + a_0) = q_i^{(r)}(x, t) + \sum_{\{s,k\}} w_{i,k}^{(r)}(x, k, t) + \sum_{\{s',k,k'\}} w_{i,k,k'}^{(r)}(x, k, k', t) + \cdots + B_i^{(r)}(x, t), \forall s, s' \in \{1, \ldots, S\}, t \geq 0, \overrightarrow{x}, \overrightarrow{x}' \in \Lambda \]

which can be used to obtain the following compact form

\[ q_i^{(r)}(x, t + a_0) = q_i^{(r)}(x, t) + G_i^{(r)}(X_{01}, \ldots, X_{06}, X_j, X_k, \ldots, t - l_i a_0), \forall s \in \{1, \ldots, S\}, t \geq 0, \overrightarrow{x} \in \Lambda, \]

as explained in [14].

In order to derive deterministic evolution equations, an average over realization of the corresponding stochastic equations of non-Markovian or Markovian type must be done. In the present paper the attention will be focused only on the evolution equation of the dynamical variables like the one given in Eq. (1) used to describe a three-dimensional cubic lattice like the one sown in Fig. 1. This means that the dynamical variables \( q \) will be the occupation numbers \( n \) that, as usual, takes the values one if the site is occupied and zero otherwise.

In order to obtain the corresponding deterministic evolution equations it must be averaged over realizations. The deterministic evolution equations obtained is

\[ q_i(\overrightarrow{x}, t + a_0) = q_i(\overrightarrow{x}, t) + \overline{G}_i, \forall s \in \{1, \ldots, S\}, t \geq 0, \overrightarrow{x} \in \Lambda, \]

where \( q_i(\overrightarrow{x}, t + a_0) = \overline{q_i^{(r)}(\overrightarrow{x}, t + a_0)} \), \( \overline{G}_i = \overline{G_i^{(r)}} \), etc. denote average over realizations and an overline is used to this end.

In order to obtain the partial differential equation for the evolution it is necessary to let \( q_i(\overrightarrow{x}, t + a_0) \rightarrow q_i(\overrightarrow{x}, t) \approx \overline{a_0 \partial q_i(\overrightarrow{x}, t) / \partial t} \), obtaining the following partial differential equation

\[ \overline{\partial q_i(\overrightarrow{x}, t) / \partial t} = \overline{a_0 G_i}, \forall s \in \{1, \ldots, S\}, t \geq 0, \overrightarrow{x} \in V_d, \]

where now the set of points \( \Lambda \) was replaced by \( V_d \), the hyper-volume of dimension \( d \), and will be used in the examples developed in the next sections.

3. Illustrative example

In this section a new example is worked in detail in order to show the basic procedure necessary for obtaining the evolution equations of the dynamical variables after an average over realizations on both sides of each equation as shown in Eqs. (3), (4). The example, shown below, develops particular aspects of Eq. (2) where the set of rules \( G \) are functions of the dynamical variables that at most contain products of two dynamical variables.

In the example considered below the index \( s \) takes only one value and the updating rules are only functions of the values of the dynamical variables at time \( t \). The use of a topological theorem allows to find a one-dimensional lattice topologically equivalent to a three-dimensional one (in this case a cubic lattice) and both two lattices are described by almost the same continuum evolution equation, except that the number of variables are one and three, respectively.
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