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One-dimensional lattices topologically equivalent to two-dimensional lattices within the context of the lattice gas model, III. The hexagonal lattice

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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 within the context of the lattice gas model. A procedure allowing to construct one-dimensional lattices that are topologically equivalent to two-dimensional lattices is described in detail in the case of a hexagonal lattice which has the particular feature that need four types of dynamical variables. This example shows additional features to the general procedure and some extensions are also suggested in order to provide a wider insight in the present approach.

1. Introduction

The present paper is the third of a series of companion papers [1], where it was studied the diffusion of monomers in a rectangular and triangular two-dimensional lattices and the corresponding one-dimensional lattices that is topologically equivalent within the context of the lattice gas model. Here, a two-dimensional hexagonal lattice will be considered and the corresponding one-dimensional lattice that is topologically equivalent will be studied within the context of the diffusion of monomers and the partial differential equations could be obtained with the same procedure as the one used in paper I of Ref. [1], *mutatis mutandis*.

This paper will be worked within the framework of the so called Discrete Stochastic Evolution Equations (DSEE). In addition some papers dealing with examples of evolution equations were written considering only one-dimensional lattices that evolves according to the stochastic lattice gas model [2]. Some examples, showing the versatility of the DSEE approach,

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can be found in Refs. [2–7]. In Ref. [8], a topological theorem was proved that states that every lattice is topologically equivalent to a one-dimensional one, allowing to construct the corresponding one-dimensional lattice.

Only a hexagonal lattice will be studied, but other interesting lattices could be included within this context without a considerable effort. 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 Refs. [9–15].

The paper is organized as follows. In Section 2 the abbreviated basic definitions necessary for the *mise en scène* of the model and notations are introduced and the detailed version can be found in paper I of Ref. [1]. In Section 3, an example, with the special feature that need four types of dynamical variables for to be described, that shows not only the way and steps needed to construct the one-dimensional lattice that is topologically equivalent to a two-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 de diffusion of particles in a two-dimensional hexagonal lattice is studied in detail. In Section 3.2 the procedures needed to construct a one-dimensional lattice that is topologically equivalent to the two-dimensional hexagonal 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 wrap the lattices on a hexagonal torus and on a skewed torus, according to whether the lattice is 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 Ref. [1]. Here, it will be said that the stochastic updating that will be considered is of the form,

$$q_s^{(r)}(\overrightarrow{x}, t+a_0) = q_s^{(r)}(\overrightarrow{x}, t) + \sum_{\{s,k\}} w_{s,k}^{(r)}\, q_s^{(r)}(\overrightarrow{x_k}, t) + \sum_{\{s,s',k,k'\}} w_{\{s,s',k,k'\}}^{(r)}\, q_s^{(r)}(\overrightarrow{x_k}, t) q_{s'}^{(r)}(\overrightarrow{x_{k'}}, t) + \cdots + B_s^{(r)}(\overrightarrow{x_k}, t), \quad \forall\, s, s' \in \{1, \ldots, S\}, t \geq 0, \overrightarrow{x_k}, \overrightarrow{x_{k'}} \in \Lambda \tag{1}$$

within the context of the lattice gas model, which is a particular case of

$$q_s^{(r)}(\overrightarrow{x}, t+a_0) = q_s^{(r)}(\overrightarrow{x}, t) + G_s^{(r)}(X_{l_{01}}, \ldots, X_{l_{0k}}, X_j, X_\xi, t, \ldots, t - l_k a_0), \quad \forall\, s \in \{1, \ldots, S\}, t \geq 0, \overrightarrow{x} \in \Lambda, \tag{2}$$

as explained in Ref. [1].

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 two-dimensional hexagonal 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

$$q_s(\overrightarrow{x}, t+a_0) = q_s(\overrightarrow{x}, t) + G_s, \quad \forall\, s \in \{1, \ldots, S\}, t \geq 0, \overrightarrow{x} \in \Lambda, \tag{3}$$

where $q_s(\overrightarrow{x}, t+a_0) = \overline{q_s^{(r)}(\overrightarrow{x}, t+a_0)}$, $G_s = \overline{G_s^{(r)}}$, 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 $q_s(\overrightarrow{x}, t+a_0) - q_s(\overrightarrow{x}, t) \approx a_0 \partial q_s(\overrightarrow{x}, t)/\partial t$, obtaining the following partial differential equation

$$\frac{\partial q_s(\overrightarrow{x}, t)}{\partial t} = \frac{1}{a_0} G_s, \quad \forall\, s \in \{1, \ldots, S\}, t \geq 0, \overrightarrow{x} \in V_d, \tag{4}$$

where now the set of points Λ 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 simple 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) and (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.

The present example is a little bet complex than the two previous lattices studied in the two companion papers [1], in the sense that the index s takes four values, R, Y, B, and G, corresponding to the red, yellow, blue and green colors, respectively, shown in Fig. 1(a). Note that it was used letters instead of number in order to provide a best description of the corresponding type of sites. 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 two-dimensional one and both two lattices, the two-dimensional hexagonal and the corresponding one-dimensional one, are described by almost the same continuum evolution equation.