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Coarse grained approach for volume conserving models

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HIGHLIGHTS

- We introduced a coarse-grained approach via theory of generalized functions.
- We determined the coarse-grained coefficients for volume conserving surface (VCS) models.
- The employed method makes use of small changes in a test space.
- We applied the approach to symmetric and asymmetric VCS models.
- The approach connects the coefficients to the SPDF for each model.

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ABSTRACT

Volume conserving surface (VCS) models without deposition and evaporation, as well as ideal molecular-beam epitaxy models, are prototypes to study the symmetries of conserved dynamics. In this work we study two similar VCS models with conserved noise, which differ from each other by the axial symmetry of their dynamic hopping rules. We use a coarse-grained approach to analyze the models and show how to determine the coefficients of their corresponding continuous stochastic differential equation (SDE) within the same universality class. The employed method makes use of small translations in a test space which contains the stationary probability density function (SPDF). In case of the symmetric model we calculate all the coarse-grained coefficients of the related conserved Kardar–Parisi–Zhang (KPZ) equation. With respect to the symmetric model, the asymmetric model adds new terms which have to be analyzed, first of all the diffusion term, whose coarse-grained coefficient can be determined by the same method. In contrast to other methods, the used formalism allows to calculate all coefficients of the SDE theoretically and within limits numerically. Above all, the used approach connects the coefficients of the SDE with the SPDF and hence gives them a precise physical meaning.

1. Introduction

The roughening properties of nonequilibrium surface systems with well-defined power-law behavior can be classified into universality classes by a unique set of exponents, which determine their dynamical scaling [1]. Discrete models and continuous equations within the same universality class share the same scaling exponents, which can be shown by numerical and analytical methods. In order to determine these exponents, many discrete models and continuous stochastic differential equations (SDE) have been studied using simulations, symmetry analyses, dynamical renormalization group theory, or numerical integration [2].

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Discrete models and continuous SDE within the same universality class share not only the same scaling exponents, but also the same linearities and (or) nonlinearities [3]. In this context, models belonging the Kardar–Parisi–Zhang (KPZ) [4] or to the conserved KPZ universality class are of special importance, since for these models it is possible to determine the nonlinearities via Monte Carlo simulations using the interface tilting method [5,6]. Another method, which is not limited to the calculation of the KPZ-nonlinearities, was introduced by Vvedensky et al. [7]. They start this calculation from a discrete SDE (or discrete Langevin equation) and determine the continuous counterpart of the discrete SDE using an analytical approach. The approach is based on the regularization of the Heaviside Θ-function and on the coarse grain approximation using a lattice constant which tends to zero [8–11]. The standard procedure to regularize a function is to replace each Heaviside Θ-function by a smooth function θ_ε, which is continuously differentiable to any order and depends on a regularization parameter ε which has to be chosen in a way that $\theta_\epsilon \to \Theta$ when $\varepsilon \to 0$. For details, see Appendix A. The regularization function θ_ε has to be analytic throughout its domain, but especially at zero, in order to enable a Taylor series expansion. The Taylor coefficients depend on both, the regularization prescription (*i.e.* the regularization function chosen) and the regularization parameter ε. As pointed out by Katzav and Schwartz [12] this expansion is problematic since in the limit $\varepsilon \to 0$ the Heaviside Θ-function is not analytic around zero. Consequently the ε parameter cannot be removed in the process of coarse-graining. Another weak point of the method is the difficulty of reaching conclusive results in models of higher dimensions than one. Finally, although the mathematical derivation is direct, it can generate discrepancies in interpretation of coarse coefficients of the continuous differential equation.

Recently, we introduced a different coarse-grained approach based on generalized function or distribution theory [13]. We showed, that using our approach, it is possible to calculate not only nonlinear, but also, all coefficients of the stochastic differential equation for a given discrete model of the KPZ universality class. In this work we use our formalism to show, how to determine the coarse-grained coefficients of two volume conserving surface models.

There are two well-defined groups of models and equations as distinguished by their noise, which is either non-conservative or conservative. Growth models and equations which describe deposition or evaporation process are included in the first group. In contrast, volume conserving surface (VCS) models without deposition or evaporation are included in second group. The models studied in this work are VCS models and consequently have conservative noise. Volume conserving processes are defined as physical processes which occur on the surface of a solid and preserve the total volume enclosed by the surface. These processes describe the movement of a particle from a site of the surface to another, and exclude particle deposition or evaporation. The conserved noise is assumed to be Gaussian distributed and uncorrelated. It has an expectation value of zero and the correlation is

$$\langle \eta(\vec{x}, t)\, \eta(\vec{x}', t')\rangle = -2\, Q\, \nabla^2 \delta(\vec{x} - \vec{x}')\, \delta(t - t'), \tag{1}$$

with $\vec{x} \in \mathbb{R}^d$ and where the conserved noise intensity Q is proportional to the temperature of the system.

The conserved KPZ (cKPZ) equation ($h = h(\vec{x}, t)$, $\nu < 0$, and $\lambda < 0$)

$$\frac{\partial h}{\partial t} = \nabla^2 \left[\nu\, \nabla^2 h + \frac{\lambda}{2} \left(\nabla h\right)^2 \right] + \eta(\vec{x}, t), \tag{2}$$

proposed by Sun et al. [14] describes the first continuous VCS process with conserved noise. The expression in the brackets of Eq. (2) we call KPZ kernel of the equation. In the first molecular-beam epitaxy (MBE) models, Eq. (2) reappears with an additive constant F that takes the deposition flux into account. This extended equation is called Villain–Lai–Das Sarma (VLD) equation, named by the authors of the article it was first time mentioned [15,3]. In contrast to the noise term of the cKPZ equation, the noise term of the VLD equation describes non-conservative noise. It has an expectation value of zero and the correlation $\langle \eta(\vec{x}, t)\, \eta(\vec{x}', t')\rangle = -2\, D\, \delta(\vec{x} - \vec{x}')\, \delta(t - t')$, where the noise intensity D is proportional to the flux F. Although the cKPZ and VLD equations have the same KPZ kernel, the equations show distinct macroscopic properties, which have been identified and studied in various scientific works [16]. Since both equations have the same kernel, these distinct properties can be attributed the different nature of their noise.

A VCS model can be described by the continuity differential equation or conservation law

$$\frac{\partial h}{\partial t} + \nabla \cdot \mathbf{j} = \eta, \tag{3}$$

where $\mathbf{j} = \mathbf{j}(\vec{x}, t)$ is the surface diffusion current and $\eta = \eta(\vec{x}, t)$ is the conserved noise. The form of the current $\mathbf{j}$ is determined by the symmetries of the system. The current cannot depend explicitly on h, since this would break the invariance under constant height translations. It is expected that under nonequilibrium conditions the total current $\mathbf{j}$ has two terms, *i.e.* $\mathbf{j} = -\nabla \mu_{\text{ne}} + \mathbf{j}_{\text{ne}}$. Here μ_{ne} is the nonequilibrium chemical potential and $\mathbf{j}_{\text{ne}}$ is the nonequilibrium current. From symmetry consideration it is expected that μ_{ne} is a function of $\nabla^2 h$ and ∇h.

The first model studied in this work has both of these terms. Its dynamic rules are axial symmetric, which means, that a randomly chosen particle hops independently from the actual surface configuration with the same probability to left as it hops to the right. Its KPZ kernel (see the Eq. (2)) is proportional to μ_{ne}. Furthermore it is expected that $\mathbf{j}_{\text{ne}}$ is an odd function of ∇h.

The second model studied in this work has both types of current contribution, $\nabla \mu_{\text{ne}}$ and $\mathbf{j}_{\text{ne}}$. Its dynamic rules are not axial symmetric, which means, that it depends on the surface configuration whether a randomly chosen particle hops to