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Equivalence of operator-splitting schemes for the integration of the Langevin equation

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Abstract. We investigate the equivalence of different operator-splitting schemes for the integration of the Langevin equation. We consider a specific problem, the so called directed percolation process, which can be extended to a wider class of problems. We first give a compact mathematical description of the operator-splitting method and introduce two typical splitting schemes that will be useful in numerical studies. We show that the two schemes are essentially equivalent through the map that turns out to be an automorphism. An associated equivalent class of operator-splitting integrations is also defined by generalizing the specified equivalence.

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Several kinds of models for lattice-based dynamic processes have been studied for decades in efforts to understand the characteristics of non-equilibrium systems, especially focusing on the critical phenomena. To mention a few, directed percolation (DP) [1]–[6], contact processes [7, 8], and catalytic reactions [9] are examples. In these studies, it was found that, in spite of the diversity in microscopic details, various models exhibit critical phenomena that are essentially identical to those for the absorbing phase transition in the DP model and the DP universality class was inferred for them [10, 11].

In order to explain the DP universality class from a unified point of view, a so called DP Langevin equation was proposed [3, 4] as

$$\partial_t \rho = a\rho - b\rho^2 + D\nabla^2\rho + \sigma\sqrt{\rho}\xi, \tag{1}$$

where $\rho = \rho(\mathbf{r}, t)$ is a non-negative field variable for concentration and ξ is a white noise with zero mean satisfying $\langle \xi(\mathbf{r}, t)\xi(\mathbf{r}', t')\rangle = 2\delta(\mathbf{r} - \mathbf{r}')\delta(t - t')$. The coefficient a is the tuning parameter for the phase transition, and b, D, σ are positive constants.

The field theoretical approach to equation (1), named the *Reggeon field theory* [12], unveils the critical behaviour of the DP universality class for spatial dimensions comparable to or higher than the critical one $d_c = 4$. The mean field theory applies in high dimensions ($d > d_c = 4$) and the perturbative results are well established near to and below d_c through the standard $\epsilon = d_c - d$ expansion. In lower dimensions, the series expansion methods for lattice-based DP models provide the most precise estimates for the critical scaling exponents [13], which have also been confirmed by extensive numerical simulations [10].

Attention has also been paid to the direct numerical integration of equation (1), especially in the quantitative study of the lower dimensional cases [14]. This seems to be a simple numerical integration of the partial differential equation at a glance. However, as long as the absorbing transition is involved, one encounters an annoying block which is by no means easily tractable. The conventional Euler integration technique using a discrete time interval Δt may result in a negative value of ρ due to the uncontrolled random noise term, and then any further sensible integration of the equation is impossible. In particular, this nuisance may appear very easily for small ρ where the noise term ($\sim\sqrt{\rho}$) is dominant over the deterministic term ($\sim\rho$). As the absorbing critical behaviour occurs in the $\rho \to 0$ limit, a proper treatment for guaranteeing a small but positive value of ρ is not only of technical interest, but also a critical issue in the numerical study of the absorbing phase transition. Some numerical schemes have been put forward for overcoming such numerical fragility [14], but without much success.

Recently, Dornic *et al* [15] utilized the operator-splitting method for integrating the Langevin equations (a similar idea appeared earlier in [16]) describing various kinds of absorbing critical phenomena [17]. In this method, the evolution in time is divided into two parts, each of which is exactly solvable. The successive integration of the two parts during Δt is regarded as one-step time evolution of equation (1), getting exact as $\Delta t \to 0$. This method has a couple of outstanding advantages over the preceding ones [14]. As the noise term is treated exactly, the non-negativity of ρ is always guaranteed. Therefore one can use a relatively large value for Δt to stay in the critical region where ρ is small, which can also save computing time considerably. An astonishing observation is that the critical behaviour seems to be fairly insensitive to the magnitude of Δt. In fact, even if $\Delta t = 0.25$ in their paper, the critical point is shifted only by 1% from the extrapolated

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value in the limit of $\Delta t \to 0$. They have reported many successful applications of this method for various kinds of absorbing critical phenomena.

It is a tough task to rigorously explain why the operator-splitting method with a relatively large time interval yields a reliable result for the critical behaviour of a certain problem and find what the criterion is for this approach to be valid. Our preliminary work based on the perturbative expansion in Δt reveals that the operator-splitting scheme renormalizes the given coefficients (a, b, D, σ), and generates higher order terms and new non-Gaussian noises. Furthermore, we find that it may be possible for the renormalized and newly generated coefficients to change their signs, which could produce a diverging solution, a first-order phase transition, or a higher order multicritical point. Unfortunately the coefficients are expressed in terms of alternating infinite series, from which it seems hardly possible to derive the validity criteria for Δt for maintaining the DP critical behaviour.

In this paper, we present a compact mathematical description of the operator-splitting method. We show analytically that some seemingly different splitting schemes are mathematically equivalent in the sense that there is an exact transformation map relating different splitting schemes. We hope that our result may elucidate the structure of the Δt-dependent terms and eventually help us understand the characteristics of the upper bound for Δt in general operator-splitting schemes.

First, we summarize the operator-splitting scheme specified in [15] and then provide a compact mathematical description for it. We next consider another scheme with a different choice in splitting the dynamic process. Using the Baker–Campbell–Hausdorff (BCH) formula, we prove the equivalence of two different schemes with the analytic expression for the parameter transformation function.

In the numerical study, the embedding space is replaced with a mesh-like lattice with lattice constant Δx. Then, at site i, equation (1) becomes an ordinary differential equation for $\rho_i(t)$

$$\dot{\rho}_i = \tilde{a}\rho_i - b\rho_i^2 + \frac{D}{(\Delta x)^2}\sum_j \epsilon_{ij}\rho_j + \sigma\sqrt{\rho_i}\xi_i, \tag{2}$$

where $\dot{\rho}_i$ is the time derivative of ρ_i, $\tilde{a} \equiv a - 2dD/(\Delta x)^2$, $\epsilon_{ij} = 1$ for nearest neighbour sites i and j, and $\epsilon_{ij} = 0$ otherwise, and d is the spatial dimension. Equation (2) is a set of coupled equations where the dynamics at site i is influenced by field variables ρ_j at nearest neighbours. As an additional approximation, we assume that ρ_j is piecewise constant with an initial value $\rho_j(t)$ during the integration from t to $t + \Delta t$. During this interval, equation (2) then becomes decoupled with an effective field $c_i \equiv D/(\Delta x)^2 \sum_j \epsilon_{ij}\rho_j(t)$, which leads to

$$\dot{\rho} = c + \tilde{a}\rho - b\rho^2 + \sigma\sqrt{\rho}\xi, \tag{3}$$

where the subscript i is dropped for simplicity.

The main idea of the operator-splitting method is to separate the right hand side of equation (3) into two parts, each of which can be treated exactly. In particular, it is important to have or find the exact solution of the Fokker–Planck (FP) equation associated with the part including the noise term, guaranteeing non-negativity of ρ. Dornic *et al* [15] considered a stochastic equation without the nonlinear term $b\rho^2$ and a purely deterministic

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equation involving the nonlinear term only, given as

$$\dot{\rho} = c + \tilde{a}\rho + \sigma\sqrt{\rho}\xi, \qquad \dot{\rho} = -b\rho^2. \tag{4}$$

The FP equation associated with the first stochastic equation can be solved exactly [15, 18]. The conditional probability density $\mathcal{P}_{\mathrm{S}}(\rho, t; \rho_0)$ can be obtained analytically for an initial value ρ_0, vanishing for $\rho < 0$ at any time. The deterministic equation is trivially integrated as $\rho_{\mathrm{D}}(t; \rho_0)$, which also preserves the non-negativity of ρ.

The numerical integration during Δt is done as follows: given an initial value ρ_t at time t, ρ is updated first by sampling a value appropriate to the exact probability distribution $\mathcal{P}_{\mathrm{S}}(\rho, \Delta t; \rho_t)$, which is denoted by $\rho_{\mathrm{S}}(\Delta t; \rho_t)$. Then, resetting this updated value as an initial value at time t, we integrate the deterministic equation over Δt, which yields

$$\rho_{t+\Delta t} = \rho_{\mathrm{D}}(\Delta t; \rho_{\mathrm{S}}(\Delta t; \rho_t)). \tag{5}$$

The same procedure is performed for all sites in parallel. This constitutes a single step in discrete time dynamics with the time interval Δt. The next step follows with new initial values of $\rho_{t+\Delta t}$ and newly tuned values of c. This is the idea introduced in [15].

The splitting scheme can be described mathematically in terms of the probability density $\mathcal{P}(\rho, t)$. The probability density after a single step can be written as $\mathcal{P}(\rho, t+\Delta t) = \mathcal{L}(a, b, D, \sigma)\mathcal{P}(\rho, t)$, where $\mathcal{L}$ is the time evolution operator. Notice that $\mathcal{L}$ is the product of two consecutive evolution operators, having the form of $\mathrm{e}^{\Delta t L_{\mathrm{D}}}\mathrm{e}^{\Delta t L_{\mathrm{S}}}$, where $L_{\mathrm{S,D}}$ are the Fokker–Planck (FP) operators [19] associated with the stochastic and deterministic differential equations, respectively, in equation (4). In the Ito calculus, one writes

$$\mathcal{L} = \mathrm{e}^{\Delta t L_{\mathrm{D}}}\mathrm{e}^{\Delta t L_{\mathrm{S}}} = \mathrm{e}^{\Delta t \hat{P} b \rho^2}\mathrm{e}^{\Delta t(-\hat{P}(c+\tilde{a}\rho)+\hat{P}^2\sigma^2\rho)}, \tag{6}$$

where $\hat{P} \equiv \partial/\partial\rho$. We remark that equation (6) compactly contains the whole information of the operator-splitting method represented by equations (4) and (5).

The exact FP operator is given by $L = L_{\mathrm{S}} + L_{\mathrm{D}}$. Due to the non-cummutativity of two operators, $[L_{\mathrm{S}}, L_{\mathrm{D}}] \neq 0$, the exact evolution operator $\mathcal{L}_{\mathrm{exact}} = \mathrm{e}^{\Delta t L}$ differs from the operator-splitting evolution operator $\mathcal{L}$ in higher orders of Δt. The difference between $\mathcal{L}_{\mathrm{exact}}$ and $\mathcal{L}$ can be found systematically in power series of Δt using the BCH formula: for $\mathrm{e}^Z = \mathrm{e}^A\mathrm{e}^B$, Z can be expressed as [20]

$$Z = A + \int_0^1 \mathrm{d}t g\left(\mathrm{e}^{\mathrm{ad}_A}\ \mathrm{e}^{t\ \mathrm{ad}_B}\right) B, \tag{7}$$

where $g(x) \equiv 1 + \sum_{m=1}^{\infty}((-1)^{m+1}/m(m+1))(x-1)^m$ and ad_X is a linear map of which the operation is defined by $\mathrm{ad}_X Y = [X, Y]$. This leads to the rather familiar BCH formula:

$$\begin{aligned} Z = A + B + \tfrac{1}{2}[A, B] + \tfrac{1}{12}[A, [A, B]] - \tfrac{1}{12}[B, [A, B]] \\ + \cdots + k_{w_1,\ldots,w_n}[w_1, [\cdots [w_n, [A, B]]\cdots]] + \cdots, \end{aligned} \tag{8}$$

where w_i stands for either A or B, and $k_{w_1,\ldots,w_n}$ is a constant scalar. Here we do not write down the explicit expression for $k_{w_1,\ldots,w_n}$, but only note that its sign constantly changes with n.

With $A = \Delta t L_{\mathrm{D}}$ and $B = \Delta t L_{\mathrm{S}}$ as in equation (6), the commutator $[A, B]$ produces a new type of higher order noise term such as $\hat{P}^2\rho^2$ through the interplay of the nonlinear

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term $\hat{P}\rho^2$ and the noise term $\hat{P}^2\rho$. Through the nested commutators in equation (8), the operator-splitting FP operator $\ln\mathcal{L} = Z$ includes not only higher order deterministic terms like $\hat{P}\rho^n$ but also higher order noise terms like $\hat{P}^m\rho^n$. The coefficients of the pre-existing lower order terms such as $\hat{P}\rho$, $\hat{P}\rho^2$, and $\hat{P}^2\rho$ are also modified. In the renormalization group sense, the higher order terms are usually irrelevant to the DP critical behaviour, but only when the appropriate stability condition is satisfied. For example, the fixed point solution of the deterministic part in the operator-splitting FP operator should not have a structure different from that in the exact FP operator. Therefore the stability condition depends critically on the detailed Δt dependence of the coefficients. Unfortunately, the complexity of $k_{w_1,\ldots,w_n}$ prevents us from judging the stability criteria in a sensible way. Any conclusion derived from a truncated finite series in the perturbative expansion of equation (8) may not contain relevant information on the stability, especially due to the alternating nature of the series. It seems also impossible to sum the infinite series in a closed form even for the coefficients of the lower order terms. Thus it is not clear that the modified coefficients due to the operator-splitting method employed in [15] still guarantee the stability of the DP-type solutions for any value of Δt.

Now we focus on classifying various operator-splitting schemes into equivalent classes, which will greatly reduce the efforts required to derive the stability criteria for Δt in general operator-splitting methods. First, we notice that the nested commutators in equations (7) and (8) can be easily summed when the commutator $[A, B]$ can be written as a linear combination of A and B only. Consider the simple case of $[A, B] = \gamma B$ with a real constant γ. As $\mathrm{ad}_B B = 0$, it is easy to show that $g(\mathrm{e}^{\mathrm{ad}_A}\mathrm{e}^{t\mathrm{ad}_B})B = (1 + \sum_{m=1}^{\infty}((-1)^{m+1}/m(m+1))(\mathrm{e}^{\gamma} - 1)^m)B$. Hence we obtain

$$Z = A + \alpha_\gamma B, \tag{9}$$

where $\alpha_\gamma = \gamma/(1-\mathrm{e}^{-\gamma})$. Therefore we find $\mathrm{e}^A\mathrm{e}^B = \mathrm{e}^{A+\alpha_\gamma B}$ or equivalently $\mathrm{e}^B\mathrm{e}^A = \mathrm{e}^{\alpha_{-\gamma}B+A}$. A general case of $[A, B] = \gamma_A A + \gamma_B B$ can be reduced to the simple case by replacing B by $\tilde{B}$ proportional to the commutator. The rather complicated result is not shown here.

Next, we observe that the components of the FP operator L satisfy the above special commutation relation such as $[\hat{P}\rho, \hat{P}] = -\hat{P}$, $[\hat{P}\rho, \hat{P}\rho^2] = \hat{P}\rho^2$, and $[\hat{P}\rho, \hat{P}^2\rho] = -\hat{P}^2\rho$. This implies that the linear term $\hat{P}\rho$ can move around rather freely between L_{S} and L_{D} without causing too much complication in the operator-splitting FP operator Z. We note that the other commutators do not satisfy the special relation and the algebra is not closed.

Consider a different splitting scheme where the linear term is included in the deterministic part. The split Langevin equations are

$$\dot{\rho} = c + \sigma\sqrt{\rho}\xi, \qquad \dot{\rho} = \tilde{a}\rho - b\rho^2. \tag{10}$$

As in the previous splitting in equation (4), both equations can be treated exactly. The corresponding evolution operator can be written as

$$\mathcal{L}'(a, b, D, \sigma) = \mathrm{e}^{\Delta t\hat{P}(b\rho^2 - \tilde{a}\rho)}\mathrm{e}^{\Delta t(-\hat{P}c + \hat{P}^2\sigma^2\rho)}. \tag{11}$$

Using the identity in equation (9), we split the first exponential map as

$$\mathcal{L}'(a, b, D, \sigma) = \mathrm{e}^{\Delta t\hat{P}(b/\alpha_{\tilde{a}\Delta t})\rho^2}\mathrm{e}^{-\Delta t\hat{P}\tilde{a}\rho}\mathrm{e}^{\Delta t(-\hat{P}c + \hat{P}^2\sigma^2\rho)}. \tag{12}$$

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The last two exponential maps can be merged together as

$$\mathcal{L}'(a,b,D,\sigma) = \mathrm{e}^{\Delta t\hat{P}(b/\alpha_{\tilde{a}\Delta t})\rho^2}\mathrm{e}^{\Delta t(-\hat{P}\tilde{a}\rho-\alpha_{\tilde{a}\Delta t}(\hat{P}c-\hat{P}^2\sigma^2\rho))}. \tag{13}$$

By comparing equations (6) and (13), one establishes the relation between the two operator-splitting schemes as

$$\mathcal{L}'(a,b,D,\sigma) = \mathcal{L}(a',b',D',\sigma'), \tag{14}$$

where

$$\begin{aligned} a' &= a + 2dD(\alpha_{\tilde{a}\Delta t}-1)/(\Delta x)^2, \qquad b' = b/\alpha_{\tilde{a}\Delta t}, \\ D' &= \alpha_{\tilde{a}\Delta t}D, \qquad \sigma' = \sqrt{\alpha_{\tilde{a}\Delta t}}\sigma. \end{aligned} \tag{15}$$

Since α is positive definite and does not vanish or diverge for any finite $\tilde{a}\Delta t$, the transformation between $\mathcal{L}$ and $\mathcal{L}'$ forms an *automorphism* (one-to-one and onto itself) in the parameter space of (a,b,D,σ). The transformation preserves the sign of the parameters (b,D,σ) except a (tuning parameter) where the reformulation of the discrete Laplacian is involved. Therefore, the different operator-splitting methods are related to each other only by trivial rescaling of parameters with a shift of the critical point. Any phenomenon observed in one splitting scheme is also expected in the other scheme and the stability conditions for Δt can be traced using the transformation of equation (15) if it is known for one specific operator-splitting method.

We may consider a more general splitting where the linear term is arbitrarily divided into two parts. That is, the split Langevin equations are now

$$\dot{\rho} = c + (\tilde{a}-k)\rho + \sigma\sqrt{\rho}\xi, \qquad \dot{\rho} = k\rho - b\rho^2 \tag{16}$$

where k is a real arbitrary constant. Note that we can still integrate both equations exactly. The corresponding time evolution operator is given as

$$\mathcal{L}_k(a,b,D,\sigma) = \mathrm{e}^{\Delta t\hat{P}(b\rho^2-k\rho)}\mathrm{e}^{\Delta t(-\hat{P}(c+(\tilde{a}-k)\rho)+\hat{P}^2\sigma^2\rho)}. \tag{17}$$

Similarly, we find

$$\mathcal{L}_k(a,b,D,\sigma) = \mathrm{e}^{\Delta t\hat{P}(b/\alpha_{k\Delta t})\rho^2}\mathrm{e}^{\Delta t(-\hat{P}\tilde{a}\rho+\beta_k(-\hat{P}c+\hat{P}^2\sigma^2\rho))}, \tag{18}$$

where

$$\beta_k = \alpha_{\tilde{a}\Delta t}\alpha^{-1}_{(\tilde{a}-k)\Delta t} = \frac{\tilde{a}}{\tilde{a}-k}\frac{\mathrm{e}^{\tilde{a}\Delta t}-\mathrm{e}^{k\Delta t}}{\mathrm{e}^{\tilde{a}\Delta t}-1}. \tag{19}$$

Hence one can generalize equations (14) and (15) as follows:

$$\mathcal{L}_k(a,b,D,\sigma) = \mathcal{L}(a_k,b_k,D_k,\sigma_k), \tag{20}$$

where

$$\begin{aligned} a_k &= a + 2dD(\beta_k-1)/(\Delta x)^2, \qquad b_k = b/\alpha_{k\Delta t}, \\ D_k &= \beta_k D, \qquad \sigma_k = \sqrt{\beta_k}\sigma. \end{aligned} \tag{21}$$

Due to the property of β, inherited from that of α, the transformation between $\mathcal{L}_k$ and $\mathcal{L}$ also forms an automorphism for any k. Consequently, the solution structure yielded by $\mathcal{L}_k$ is always preserved irrespective of k, and thus such operations can be represented

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by $\mathcal{L}$. This directly demonstrates that $\mathcal{L}_k$ s form an equivalent class of operator-splitting integration of the DP Langevin equation.

In summary, we present a compact mathematical description of the so-called operator-splitting method, which was proposed in [15, 16] for the numerical integration of the DP Langevin equation of equation (1). On the basis of this, we show analytically that some splitting methods are mathematically equivalent with the explicit transformation function of the model parameters. Consequently, we find that the splitting method $\mathcal{L}_k$ s form an equivalent class of integration in the sense that the solution structure and the property of transition between the solutions are always conserved for any k. In the meantime, we also address that the difference between the original dynamics and that found by the operator-splitting scheme is traceable via the perturbation theory of the mathematical description presented. However, the information from the perturbation theory seems not sufficient for deciding whether the splitting scheme still preserves the essential features of the original dynamics. Nonetheless, our work on the equivalence class will be of considerable help for examining the validity of the operator-splitting scheme in studying the universality of the DP Langevin equation.

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