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# Monte Carlo simulations of bosonic reaction-diffusion systems and comparison to Langevin equation description

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**Abstract.** Using the Monte Carlo simulation method for bosonic reaction-diffusion systems introduced recently [S.-C. Park, Phys. Rev. E **72**, 036111 (2005)], one dimensional bosonic models are studied and compared to the corresponding Langevin equations derived from the coherent state path integral formalism. For the single species annihilation model, the exact asymptotic form of the correlation functions is conjectured and the full equivalence of the (discrete variable) master equation and the (continuous variable) Langevin equation is confirmed numerically. We also investigate the cyclically coupled model of bosons which is related to the pair contact process with diffusion (PCPD). From the path integral formalism, Langevin equations which are expected to describe the critical behavior of the PCPD are derived and compared to the Monte Carlo simulations of the discrete model.

**PACS.** 64.60.Ht Dynamic critical phenomena – 05.10.Ln Monte Carlo methods – 89.75.Da Systems obeying scaling laws

## 1 Introduction

The reaction-diffusion (RD) systems have played a paradigmatic role in studying certain physical, chemical, and biological systems [1]. In the study of the RD systems on a lattice via Monte Carlo (MC) simulations, particles are usually assigned hard core exclusion property. On the other hand, the renormalization group (RG) calculations which have been successfully applied to several RD systems are often performed with boson systems [2–4]. Hence, the comparison of the numerical studies with the RG calculations can sometimes become a nontrivial issue.

There are two ways to bridge this gap between numerical and analytical studies. One is to make a path integral formula for hard core particles which is suitable for the RG calculations. This path has indeed been sought and some formalisms are suggested [5–7]. The other is to find a numerical method that would simulate boson systems. In this context, numerical integration studies of equivalent Langevin equations to the boson systems have been performed, too [8–11]. However, it is not always possible to find an equivalent Langevin equation [12] and hence the applicability of this approach is somewhat restricted. Therefore, another numerical method is called for.

Recently, a general algorithm to simulate the bosonic RD systems was proposed [13]. Section 2 is devoted to a heuristic explanation of this algorithm to simulate general bosonic RD systems. In Section 3, the numerical method is applied to two bosonic RD systems. First, the single species annihilation model is studied with the emphasis on the pair correlation functions. We conjecture an exact asymptotic behavior of these quantities. We then present the numerical comparison of the discrete model to Langevin equation of continuous variables. Then, the cyclically coupled model of bosons is introduced and Langevin equations for this model with/without bias are derived from the well-trodden path integral formalism and compared to MC simulations. Section 4 summarizes the work.

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## 2 Algorithm

This section explains the method proposed in reference [13] that is suitable for MC simulations of bosonic RD systems. After describing how single species boson systems can be simulated, a brief remark regarding the generalization to multiple species will be followed.

The reaction dynamics of diffusing bosons is represented as

$$nA \xrightarrow{\lambda_{nm}} (n+m)A, \tag{1}$$

where $n \geq 0$, $m \geq -n$ ($m \neq 0$), and $\lambda_{nm}$ is the transition rate. Each particle diffuses with rate $D$ on a $d$ dimensional hypercubic lattice. The periodic boundary conditions are always assumed, but other boundary conditions do not limit the validity of the algorithm below. Configurations are specified by the occupation number $\rho_{\mathbf{x}}$ ($\geq 0$) at each lattice point $\mathbf{x}$. A configuration is denoted as $\{\rho\}$ which means $\{\rho_{\mathbf{x}} | \mathbf{x} \in \mathbf{L}^d\}$, where $\mathbf{L}^d$ stands for the set of lattice points and the cardinality of $\mathbf{L}^d$ is $L^d$.

The master equation which describes stochastic processes modeled by equation (1) takes the form [12,14]

$$\frac{\partial P}{\partial t} = D \sum_{\langle \mathbf{x},\mathbf{y} \rangle} \left( (\rho_{\mathbf{x}} + 1)\hat{E}_{\mathbf{x},\mathbf{y}} - \rho_{\mathbf{x}} \right) P + \sum_{n,m} \lambda_{nm} \sum_{\mathbf{x}} \left( f(\rho_{\mathbf{x}} - m, n)\hat{C}_{\mathbf{x},m} - f(\rho_{\mathbf{x}}, n) \right) P, \quad (2)$$

where $P = P(\{\rho\}, t)$ is the probability with which the configuration of the system is $\{\rho\}$ at time $t$, $\langle \mathbf{x}, \mathbf{y} \rangle$ means the nearest neighbor pair ($\mathbf{x}, \mathbf{y} \in \mathbf{L}^d$), $f(\rho_{\mathbf{x}}, n) = (\rho_{\mathbf{x}}!)/(\rho_{\mathbf{x}} - n)!$ is the number of ordered $n$-tuples at site $\mathbf{x}$ of the configuration $\{\rho\}$, and $\hat{E}_{\mathbf{x},\mathbf{y}}$ and $\hat{C}_{\mathbf{x},m}$ are operators affecting $P(\{\rho\}, t)$ such that

$$\hat{E}_{\mathbf{x},\mathbf{y}} P = P(\{\cdots, \rho_{\mathbf{x}} + 1, \rho_{\mathbf{y}} - 1, \cdots\}; t),$$
$$\hat{C}_{\mathbf{x},m} P = P(\{\cdots, \rho_{\mathbf{x}} - m, \cdots\}; t). \quad (3)$$

The master equation implies that the average number of transition events for the configuration $\{\rho\}$ during infinitesimal time interval $dt$ is

$$E(dt, \{\rho\}) = dt \sum_{\mathbf{x},n} \left( 2dD\delta_{n,1} + \sum_m \lambda_{nm} \right) f(\rho_{\mathbf{x}}, n) = dt \sum_{\mathbf{x},n} \left( 2dD\delta_{n,1} + \sum_m n!\lambda_{nm} \right) g(\rho_{\mathbf{x}}, n), \quad (4)$$

where $g(\rho_{\mathbf{x}}, n) = f(\rho_{\mathbf{x}}, n)/n! = \binom{\rho_{\mathbf{x}}}{n}$ is the number of (nonordered) $n$-tuples at site $\mathbf{x}$. The first line of equation (4) follows the usual convention in the field theoretical study of boson systems and the second line is introduced to save memories in actual simulations. For a later purpose, we introduce a model dependent function $h(\rho_{\mathbf{x}}, n) = \epsilon_n g(\rho_{\mathbf{x}}, n)$, where $\epsilon_n$ takes 1 (0) if $D\delta_{n,1} + \sum_m \lambda_{n,m}$ is nonzero (zero). The meaning of $\epsilon_n$ is straightforward; we have only to consider the dynamics with nonzero transition rate.

The algorithm starts by selecting one of $n$-tuples at any site, randomly. The simplest way to implement the selection is as follows: first a site $\mathbf{x}$ is picked up with probability $N_{\mathbf{x}}/M$, where $N_{\mathbf{x}} = \sum_n h(\rho_{\mathbf{x}}, n)$ is the number of accessible states (NAS) at site $\mathbf{x}$ and $M = \sum_{\mathbf{x}} N_{\mathbf{x}}$ is the total number of accessible states (TNAS). Then, $n$ is chosen with probability $h(\rho_{\mathbf{x}}, n)/N_{\mathbf{x}}$. In this procedure, the array of the number of particles at all sites, say $\boldsymbol{\rho}[\,]$ ($\boldsymbol{\rho}[\mathbf{x}] = \rho_{\mathbf{x}}$), is necessary. However, it is not efficient as there are too many floating number calculations. For a faster performance we introduce two more arrays, say $\mathsf{list}[\,]$ and $\mathsf{act}[\,][\,]$. The array $\mathsf{list}[\,]$ refers to the location of any $n$-tuple. Each element of $\mathsf{list}[\,]$ takes the form $(\mathbf{x}, \ell)$, where $\mathbf{x}$ is a site index and $\ell$ lies between 1 and the NAS at site $\mathbf{x}$. From $\ell$ and the array $\boldsymbol{\rho}[\,]$, which $n$-tuple is referred to by the array $\mathsf{list}[\,]$ is determined. If $\ell \le h(\rho_{\mathbf{x}}, 0)$, then $n = 0$ is implied. Else if $\ell \le h(\rho_{\mathbf{x}}, 0) + h(\rho_{\mathbf{x}}, 1)$, $n = 1$ is meant. Else if $\ell \le h(\rho_{\mathbf{x}}, 0) + h(\rho_{\mathbf{x}}, 1) + h(\rho_{\mathbf{x}}, 2)$, $\ell$ indicates one of pairs at site $\mathbf{x}$, and so on. In case the TNAS in the system is $M$, the size of $\mathsf{list}[\,]$ is $M$ and all elements of $\mathsf{list}[\,]$ should satisfy that $\mathsf{list}[p] \neq \mathsf{list}[q]$ if $p \neq q$ ($1 \le p, q \le M$). Hence, the random selection of an integer between 1 and $M$ is equivalent to choosing one of all $n$-tuples with an equal probability. The array $\mathsf{act}$ is the inverse of the $\mathsf{list}$. In other words, $\mathsf{list}[s] = (\mathbf{x}, \ell)$ corresponds to $\mathsf{act}[\mathbf{x}][\ell] = s$. It is clear that these two selecting mechanisms are equivalent in the statistical sense.

After choosing $\mathbf{x}$ and $n$, the reaction $nA \to (n+m)A$ occurs with probability $n!\lambda_{nm}\Delta t$ for all $m$, where $\Delta t$ is a configuration independent time difference. Provided $n = 1$ is selected, a particle at $\mathbf{x}$ hops to one of the nearest neighbors with probability $D\Delta t$. To make the transition probability meaningful, $\Delta t$ is made to satisfy

$$\left( 2dD\delta_{n,1} + \sum_m n!\lambda_{n,m} \right) \Delta t \le 1, \quad (5)$$

for all $n$. After this update, time increases by $\Delta t/M$. On average, this algorithm generates $E(\Delta t, \{\rho\})$ transition events during $\Delta t$.

For systems with $k$ species, all we have to do is to modify the NAS at site $\mathbf{x}$ in such a way that

$$N_{\mathbf{x}} = \sum_{i=1}^{k} \sum_n h_i(\rho_{i,\mathbf{x}}, n) + \sum_{n_1,\ldots,n_k} h_{1,\ldots,k}(\rho_{1,\mathbf{x}}, \ldots, \rho_{k,\mathbf{x}}; n_1, \ldots, n_k), \quad (6)$$

where the first (second) terms are from the dynamics in which $n$ particles of same species ($n_j$ particles of each $j$th species) are involved. For instance, for the pair annihilation of different species, so-called $A + B \to 0$ reaction, the second term of equation (6) becomes $\rho_{A,\mathbf{x}}\rho_{B,\mathbf{x}}$. Except this modification, all other steps are the same as in the single species case.

Equipped with the numerical methods, Section 3 studies some bosonic RD systems which show scaling behavior.

## 3 Applications

### 3.1 Single species annihilation model

The first example is the one dimensional single species annihilation model which corresponds to $\lambda_{nm} = 0$ unless $n = 2$ and $m = -2$. For convenience, we set $D = \frac{1}{2}$ and $\lambda_{2,-2} = \lambda$. The decaying behavior of the particle density was studied in reference [13]. This section studies the correlation function $M(r; t)$ which is defined as

$$M(r; t) = \begin{cases} \lim_{L\to\infty} \frac{1}{L} \sum_{x=1}^{L} \langle \rho_x(t)\rho_{x+r}(t) \rangle & \text{if } r \neq 0, \\ \lim_{L\to\infty} \frac{1}{L} \sum_{x=1}^{L} \langle \rho_x(t)(\rho_x(t) - 1) \rangle & \text{if } r = 0, \end{cases} \quad (7)$$

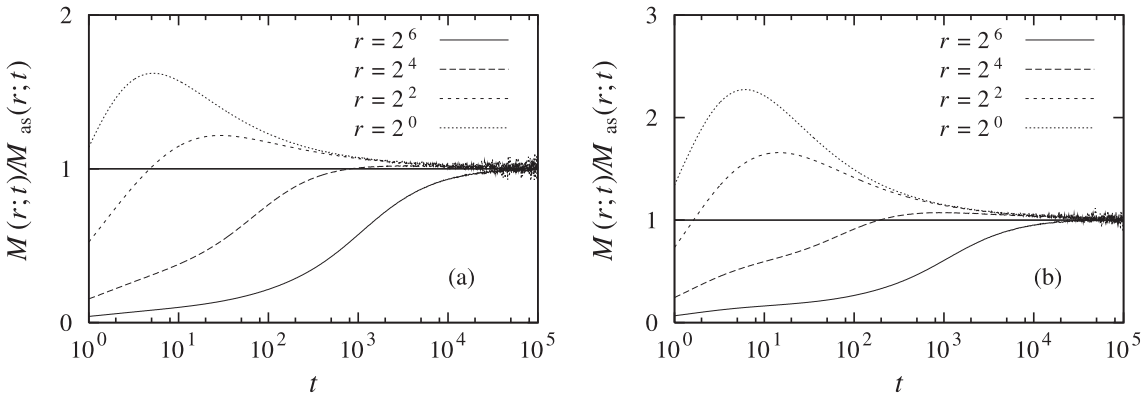


**Fig. 1.** Semi-log plots of $M(r;t)/M_{\rm as}(r;t)$ as a function of $t$ for (a) $\lambda = 1$ and (b) $\lambda = \frac{1}{2}$. All curves converge to 1 as $t$ goes to infinity.

where $\langle \ldots \rangle$ means the average over all independent realizations. Using the boson operators in references [2–4], $M(r;t)$ can be rewritten as $\frac{1}{L}\sum_x \langle a_x a_{x+r}\rangle$.

The correlation functions for the annihilation model of hard core particles with annihilation probability $p$ were studied in reference [15]. The asymptotic behavior of the correlation function is conjectured as [15]

$$M_r(t) = \frac{1}{(4\pi t)^{3/2}}\left(\pi r + c\frac{1-p}{p}\right), \qquad (8)$$

with $c = 3.4 \pm 0.2$. Note that $M_r(t)$ is not to be confused with $M(r;t)$; $M_r(t)$ and $M(r;t)$ are defined in the hard core and boson models, respectively.

In fact, the exact value of $c$ can be deduced from the differential equation

$$\frac{d\rho(t)}{dt} = -2pM_1(t), \qquad (9)$$

which relates the time derivative of the density $\rho(t)$ to the correlation function with $r = 1$. Since $\rho(t) \sim 1/\sqrt{4\pi t}$ for any finite $p$ in the asymptotic regime, it is easy to deduce that $c = \pi$ if the asymptotic behavior of the correlation function takes the form of equation (8). This value is compatible with the numerical estimation in reference [15].

By the same token, we can conjecture how the correlation function $M(r;t)$ behaves asymptotically from the equation

$$\frac{d\rho(t)}{dt} = -2\lambda M(0;t). \qquad (10)$$

If $M(r;t)$ takes the similar form to equation (8) and since $\rho(t)$ decays as $1/\sqrt{4\pi t}$ in the asymptotic regime for any nonzero value of $\lambda$ [13], one can deduce

$$M(r;t) \sim M_{\rm as}(r;t) \equiv \frac{\pi}{(4\pi t)^{3/2}}\left(r + \frac{1}{\lambda}\right) \qquad (11)$$

for all $r \geq 0$. As far as we are aware of, the correlation functions of the boson annihilation model have not been studied before. If $D \neq \frac{1}{2}$, the correlation function can be found by changing $t \mapsto 2Dt$ and $\lambda \mapsto \lambda/(2D)$. Since the boson model with infinite $\lambda$ is equivalent to the hard core particle model with $p = 1$ which is exactly soluble, equation (11) becomes exact in this limit; see equation (8).

In the following, we will check the validity of equation (11) for finite $\lambda$ and nonzero $r$ via MC simulations. Initially, particles are distributed according to the uncorrelated Poisson distribution with average density $\rho_0 = 1$. During simulations, we measured $M(r;t)$ for $r = 2^0$, $2^2$, $2^4$, and $2^6$ up to $t = 10^5$. The system size is $2^{18}$ and around $2.5 \times 10^5$ independent samples are collected for both cases of $\lambda = 1$ and $\frac{1}{2}$. Figure 1 shows that $M(r;t)$ takes the conjectured asymptotic form (11).

The MC simulations of bosonic RD systems can confirm the equivalence between the (discrete) microscopic models and (continuous) Langevin equations, if exists. From the coherent state path integral representation of the bosonic systems [2], Langevin equation can be derived in case each reaction involves at most two particles. Since the reaction of boson annihilation model requires two particles, one can write down Langevin equation which reads (Itô interpretation is employed)

$$da_x = dt(D\nabla_x^2 a_x - 2\lambda a_x^2) + i\sqrt{2\lambda}a_x dW_x, \qquad (12)$$

where $a_x$ is a complex stochastic random variable whose average is the mean number of particles at site $x$, $\nabla_x^2$ is the lattice Laplacian defined as $\nabla_x^2 f(x) = f(x+1) + f(x-1) - 2f(x)$, $i$ is the imaginary number, and $W_x$ is a Wiener process with $\langle dW_x dW_{x'}\rangle = dt\delta_{x,x'}$. Initially, $a_x$ takes the value of $\rho_0$ which is the initial density of the uncorrelated Poisson distribution used in the MC simulation.

This equation is integrated using Euler scheme with $\Delta t = 2.5 \times 10^{-5}$ and the system size of $2^{15}$. In Figure 2, numerical integration results for $\lambda = \frac{1}{2}$ are shown with comparison to MC simulations. Within statistical error, these two approaches yield the same results. Since the deviation from the mean field solution is evident, Langevin equation in the observation time properly appreciates the effect of noise. Hence, we believe that Figure 2 shows the equivalence of two approaches for the annihilation model. Needless to say, the numerical integration of Langevin equation is a much harder job than the Monte Carlo simulation.

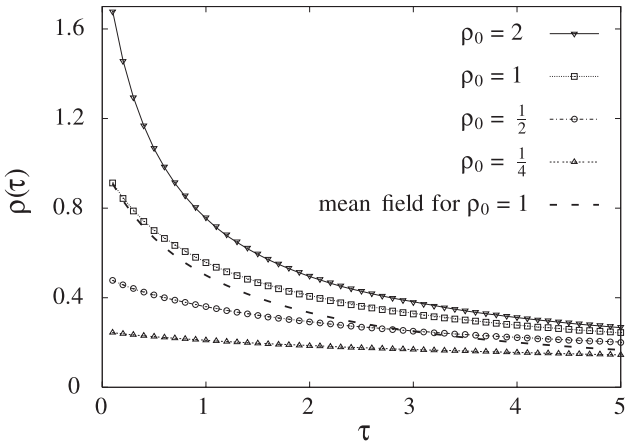


**Fig. 2.** Plots of $\rho(t)$ obtained from MC simulations (lines) and numerical integrations of Langevin equation (symbols) starting from the initial density $\rho_0$. The broken line without symbols is the mean field solution of equation (12).

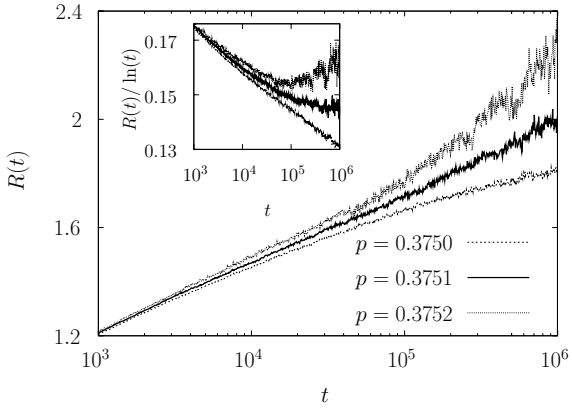


**Fig. 3.** Semi-log plot of $R(t)$ vs. $t$ for the CC with the relative bias near criticality. At criticality ($p_c = 0.3751$), clear logarithmic behavior is observed as in reference [19]. Inset: A plot of $R(t)/\ln(t)$ vs. $t$ in the semi-log scales.

### 3.2 Cyclically coupled model

The absorbing phase transition has been extensively studied as a prototype of the nonequilibrium critical phenomena [16]. The RG based on the boson systems has been applied successfully especially to the directed percolation (DP) universality class. Recently, the particle number probability distribution for boson models belonging to the DP class was studied numerically and the RG prediction was confirmed again [17].

On the other hand, the pair contact process with diffusion (PCPD) defies any numerical and analytical conclusions to date [18]. Although the driven PCPD (DPCPD) studied in reference [19] seems to conclude that the PCPD forms a different universality class from the DP, recent extensive numerical study [20] revives the scenario that the PCPD will eventually be found to belong to the DP class with a huge corrections to scaling. Still, the universality classification for the one dimensional PCPD is yet to be settled unambiguously.

To make matters worse, the recent RG study shows that the field theory starting from the single species master equation is not viable [21], which was also anticipated independently in reference [19]. As both works conclude, the field theory should account for the multispecies nature of the PCPD properly. Following this instruction, multi component Langevin equations with real random variables are introduced and studied in reference [22] to find a viable field theory for the PCPD. We will take a slightly different path and ask whether we can find a viable field theory for the PCPD, in this section.

Since the PCPD involves two independent "excitations" such as particles and pairs, it is natural to generalize to a two species model which captures the main physics of the PCPD. This type of two species model with hard core particles was introduced and studied in reference [23]. This section introduces a bosonic variant and studies it using both MC simulations and Langevin equations.

The model which will be called the cyclically coupled (CC) model is defined as follows: there are two species, say $A$ and $B$. Each species diffuses with rate $D_A$ and $D_B$, respectively. Each $B$ particle is annihilated ($B \to 0$) with rate $\delta$, branches another $B$ particle ($B \to 2B$) with rate $\sigma$, and mutates into two $A$ particles ($B \to 2A$) with rate $\mu$. Every pair of $B$ particles at the same site can be coagulated ($2B \to B$) with rate $\lambda$. Every pair of $A$ particles produces a $B$ particle and is removed ($2A \to B$) with rate $\tau$. The $A$ ($B$) particles have a connection, if not a exact mapping, to the isolated particles (pairs) in the PCPD.

Since the PCPD as well as the CC suffers from the strong corrections to scaling, it is nontrivial to show directly by MC simulations that the CC and the PCPD should belong to the same universality class. Fortunately, we have an alternative to check the equivalence of the CC and the PCPD in the sense of the universality. If the relative bias between two species in the CC in one dimension triggers the mean field scaling with logarithmic corrections as happens in the DPCPD [19], it is reasonable to conclude that the CC and the PCPD share the critical behavior.

The transition events of the CC with a relative bias in one dimension are almost same as those of the CC above except that $A$ particles hop only to the right with rate 1. For a numerical study, we set $D_B = 0.1$, $\mu = 0.2$, $\tau = 0.5$, $\delta = 2\lambda = 0.6 \times p$, and $\sigma = 0.6 \times (1 - p)$ with a tuning parameter $p$. Since only $A$ particles diffuse in a biased manner, the relative bias between different species can not be gauged away by the Galilean transformation. Figure 3 shows that $R(t)$ $(= A(t)/B(t))$ which is a ratio of two densities at time $t$ behaves logarithmically at criticality. Combining with the observation that $A(t) \sim t^{-0.5}$ at criticality with possible logarithmic corrections (not shown), the CC with the bias shows the same critical behavior as the DPCPD, which confirms the equivalence of the CC to the PCPD in the sense of the universality. Accordingly, Langevin equations which are equivalent to the CC are supposed to describe the critical behavior of the PCPD.

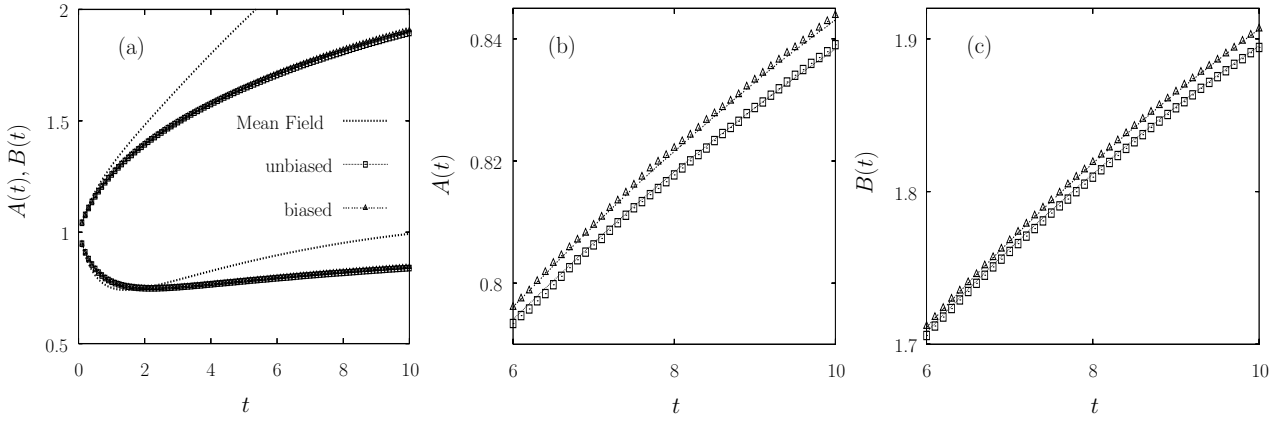


**Fig. 4.** (a) The densities of each species for both the biased and unbiased CC as a function of $t$ from the MC simulations (lines) and numerical integration (symbols) of Langevin equations (14). For comparison, mean field solutions are also shown. (b) Close-up of the interval $6 \leq t \leq 10$ for $A(t)$ in (a). (c) Close-up of the same interval as in (b), but the plots are for $B(t)$.

Following standard path integral formalism [2], one can derive the action of the CC, which reads

$$\begin{aligned}\mathcal{L} = {} & \bar{a}_x[\partial_t a_x - D_A\nabla_x^2 a_x + v\partial_\parallel a_x - 2\mu b_x + 2\tau a_x^2] \\ & + \bar{b}_x[\partial_t b_x - D_B\nabla_x^2 b_x - r b_x + \lambda b_x^2 - \tau a_x^2] \\ & - \frac{1}{2}\bar{b}_x^2(2\sigma b_x - 2\lambda b_x^2) - \frac{1}{2}\bar{a}_x^2(2\mu b_x - 2\tau a_x^2),\end{aligned} \tag{13}$$

where the average of the field $a_x$ ($b_x$) corresponds to the density of species $A$ ($B$) at site $x$ and $r = \sigma - \mu - \delta$. Along the parallel direction denoted as $\parallel$, $A$ particles hop to the right (left) with rate $D_A + v/2$ ($D_A - v/2$). Since the number of barred fields does not exceed two in each term, one can write down the equivalent Langevin equations to the action (13), which read

$$\begin{aligned}da_x = {} & dt(D_A\nabla_x^2 a_x - v\partial_\parallel a_x + 2\mu b_x - 2\tau a_x^2) \\ & + \sqrt{2\mu b_x - 2\tau a_x^2}\, dW_x,\end{aligned} \tag{14a}$$

$$\begin{aligned}db_x = {} & dt(D_B\nabla_x^2 b_x + r b_x - \lambda b_x^2 + \tau a_x^2) \\ & + \sqrt{2\sigma b_x - 2\lambda b_x^2}\, dV_x,\end{aligned} \tag{14b}$$

where $W_x$ and $V_x$ are independent Wiener processes.

In Figure 4, we compare the MC simulations of the CC with the numerical integrations of Langevin equations (14) at $p = 0.29$. Initially, $a_x$ and $b_x$ are set to 1. The system size for the numerical integration is $2^{15}$ and around 50 samples are independently generated with $\Delta t = 2.5 \times 10^{-5}$. Up to $t = 10$, the difference between the unbiased and biased cases is minute, but, within statistical errors, the behavior of two cases can be discerned from each other. In other words, we showed that equations (14) are equivalent to the CC with/without bias. Although we compared two approaches just for one set of parameter values, the full equivalence for all parameter values is still expected.

In summary, we showed that the CC and the PCPD share the critical behavior. Then, we found Langevin equations which are equivalent to the CC. From these two observation, we can say that Langevin equations (14) with complex random variables $a$ and $b$ show the same critical behavior as the PCPD.

Although we found the representative Langevin equations for the PCPD, it is not obvious whether these equations with naive continuum limit can serve as a properly coarse-grained field theory for the PCPD. Besides, we are not sure whether equations (14) contain all relevant (or sometimes dangerously irrelevant) terms. For example, the reaction $A + B \to 0$ which is absent in our model can be generated by a chain of reactions. It is of no difficulty to write down Langevin equations with the pair annihilation of different species. However, what will happen if we include the reaction $3A \to 0$ which prohibits writing down Langevin equations like Eqs. (14)? If this reaction is also important in whichever sense (relevant or dangerously irrelevant), terms with only $a$ and $\bar{a}$ in the action take exactly the same form as those in reference [21]. Hence, it seems that the difficulty found in reference [21] still remains even in the multi component Langevin equations studied here. We only hope that this study can be a starting point of the field theoretical understanding of the PCPD in the future.

## 4 Summary

To summarize, using the algorithm proposed in reference [13] and generalized one to the multispecies models, the single species annihilation and the cyclically coupled models are studied.

For the single species annihilation model, the exact asymptotic form of the correlation functions is conjectured and numerically confirmed. In addition, the equivalence of Langevin equation derived from the coherent state path integral formalism to the discrete boson model is affirmed. From the cyclically coupled model of bosons, we derive Langevin equations for both biased and unbiased cases. By simulating discrete models and integrating the Langevin equations numerically, these continuum equations are indirectly shown to describe the critical behavior of the PCPD and the DPCPD.

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