On the Segregation Phenomenon in Complex Langevin Simulation

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Abstract

In the numerical simulation of certain field theoretical models, the complex Langevin simulation has been believed to fail due to the violation of ergodicity. We give a detailed analysis of this problem based on a toy model with one degree of freedom \( S = -\beta \cos \theta \). We find that the failure is not due to the defect of complex Langevin simulation itself, but rather to the way how one treats the singularity appearing in the drift force. An effective algorithm is proposed by which one can simulate the \( 1/\beta \) behaviour of the expectation value \( < \cos \theta > \) in the small \( \beta \) limit.

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1 Introduction

The complex Langevin simulation is a challenging idea for quantum systems with complex actions [1, 2], where the conventional Monte Carlo methods are not efficient. It has been applied to a variety of physical systems such as QCD at finite temperature and chemical potential [3, 4, 5, 6], gauge theories with external charges or fermions [7, 8, 9, 10]. Big successes could be obtained in case the complex Langevin simulation works. In some cases, however, it fails to give correct results.

One typical reason for the failure of the complex Langevin simulation are instabilities, where blow-up solutions are observed due to the non-positive definite Fokker-Planck Hamiltonian [11, 7]. To tackle this problem, the role of a kernel is investigated and some progress has been made [12, 13, 14]. In principle, if a suitable kernel is introduced, blow-up solutions could be avoided and correct results may be obtained. Recently some more discussions about the convergence of the complex Langevin equation [15, 16] and its spurious solutions [17] have been presented.

In this paper another type of failure is concerned. In the practical simulation of certain models, no blow-up solutions are observed but the results are not correct. One important example is the non-Abelian gauge theory coupled to external charges [8, 18]. The violation of ergodicity due to the so-called segregation theorem has been blamed for this failure [18]. This defect may not be remedied by the introduction of a kernel (at least up to now no suitable one has been found) [17]. It has been pointed out that the singular points corresponding to the zeroes in the probability distribution may play an important role in this problem [19].

The purpose of this paper is to present a detailed analysis of the latter problem above. In the next section a brief review in the context of a simplified model with one-degree of freedom is given. Our new observation to the failure and some theoretical supports are discussed in section 3 and 4. In sections 5 and 6 the possible algorithms for simulating the δ-type singular drift forces are presented. Finally the conclusions follow.

2 Brief review of the problem
2.1 The idea and its failure

Let us consider the following simple integral,

\[
\langle \cos \theta \rangle = \int_0^{2\pi} d\theta \cos^2 \theta \exp \{\beta \cos \theta\} = \frac{I_0(\beta)}{I_1(\beta)} - \frac{1}{\beta}.
\] (1)

The analytical result shows that the quantity is singular \(\sim 1/\beta\) in the limit \(\beta \to 0\). In this limit the denominator becomes very small, therefore, to simulate the quantity to high precision by calculating numerator and denominator separately becomes very difficult. In order to overcome this difficulty, an idea is to apply the Langevin method. For this purpose one first rewrites the integral as

\[
\langle \cos \theta \rangle = \int_0^{2\pi} d\theta \cos \theta P_{\text{eff}}(\theta) = \frac{\int_0^{2\pi} d\theta \cos \theta \exp \{-S_{\text{eff}}\}}{\int_0^{2\pi} d\theta \exp \{-S_{\text{eff}}\}},
\] (2)

where

\[
P_{\text{eff}} \propto e^{-S_{\text{eff}}}, \quad S_{\text{eff}} = -\beta \cos \theta - \ln(\cos \theta).
\] (3)

This action is complex for \(\cos \theta < 0\). As the distribution \(P_{\text{eff}} \propto e^{-S_{\text{eff}}}\) is not positive definite, usual Monte Carlo method cannot be applied. On the other hand the Langevin equation

\[
\dot{\theta} = -\beta \sin \theta - \tan \theta + \eta
\] (4)

can in principle be solved and may be used for the simulation of (2). Unfortunately, this Langevin equation turns out to fail completely to generate the desired configurations for \(\beta \approx 2.5\), and therefore cannot give the correct \(1/\beta\) behaviour. This can be seen in Fig. 1.

2.2 Conventional interpretation of the failure and the segregation phenomenon

In order to give the \(1/\beta\) singularity, the solution of the Langevin equation \(\theta = \theta_r + i\theta_i\) should get a big imaginary part. This is clear because \(\Re \cos \theta = \cos \theta_r \cosh \theta_i\) and \(\cos \theta_r \leq 1\). Contrary to this expectation, an important observation given in [20, 18] is that the configurations obtained through the updations by use of the Langevin equation (4) are almost real.
This phenomenon is always observed independently of which initial configuration one takes, and was called “the collapse of the complex distribution to the real distribution”.

This is surely the direct reason why the Langevin simulation fails to give the $1/\beta$-singularity at $\beta \to 0$ as is shown in Fig. 1.

In addition, in [18] the segregation theorem has been applied to explain the wrong result obtained by the Langevin simulation. Due to the collapse of the complex distribution to a real one we can restrict the discussion to the stochastic process on the real axis. Let us assume that there exists a domain $D$ on the real axis with a boundary on which the probability distribution vanishes. In this case, the segregation theorem states that the probability that a real diffusion process starting inside $D$ exits the domain or stays permanently near the boundary of the domain, is zero. In case of our model (3), the zeros of $P_{eff}$ divide the total configuration space $D \equiv [0, 2\pi]$ (note that we will adopt periodic boundary conditions) into two subdomains: $D_1 \equiv [0, \frac{\pi}{2}) \oplus (\frac{3\pi}{2}, 2\pi]$ and $D_2 \equiv (\frac{\pi}{2}, \frac{3\pi}{2})$. If the segregation theorem is applied, the Langevin simulation should give one of the following results,

$$< \cos \theta >_i \equiv \frac{\int_{D_i} \cos \theta e^{-S_{eff}}}{\int_{D_i} e^{-S_{eff}}}, \quad i = 1 \text{ or } 2. \quad (5)$$

depending on the starting point of the simulation.

Note that the the above integrals have the same form as (3), while the integration regions are restricted to the subdomain $D_1$ or $D_2$. These results have also been plotted in Fig. 1 by dotted and dot-dashed lines. In this figure one may see the clear discrepancy between the result of the Langevin simulation and the above prediction from the segregation phenomenon. The situation was quite different in [18]. In that paper the simulated result and the prediction given by the segregation assumption (especially $< \cos \theta >_1$) agree quite well, by which the authors concluded that the failure of their simulation is connected to the segregation phenomenon or, in other words, the violation of the ergodicity.

3 A new observation
3.1 It is not the segregation but!

Before discussing the difference between the result of the Langevin simulation obtained here and that of [18], let us first describe the algorithm used in more detail.

In numerically solving the Langevin equation, it sometimes happens that the configuration comes near to the singular points where the drift force becomes very big. To get an accurate numerical solution in such a case, one should adjust the fictitious time step. Here we have followed the way used in [18]. Let us write the discretized Langevin equation as $\Delta \theta = D(\theta) \Delta t + \sqrt{2 \Delta t} \xi$ ($< \xi^2 > = 1$). The criterion to get an accurate numerical solution is represented by $|D(\theta)\Delta t| \ll |\sqrt{2\Delta t}\xi|$, which gives $\Delta t \ll \frac{2}{D^2(\theta)}$ (we have used $\xi^2 \sim 1$). In discretizing the Langevin equation, we normally use a certain prefixed fictitious time step $\Delta t = \Delta t_p$. In case that the configuration comes near to the singular points and therefore the relation $\Delta t_p < \frac{2}{D^2(\theta)}$ is not satisfied we replace $\Delta t_p$ by $\Delta t = \frac{2}{D^2(\theta)}$. Repeating the updatings by the use of this adjusted time step until $\sum \Delta t = \Delta t_p$, we include the last configuration in the set of ensemble elements.

Let us come back to the discussion about the difference of our Langevin result in Fig. 1 and that in [18]. As was mentioned above the algorithm used here to update the configuration is almost the same as that used in [18]. The big difference in the result, however, arises from the number of iterations taken in solving the Langevin equation. In order to show this we plot in Fig. 2 the result of $<\cos \theta>$ versus the number of iterations.

When one calculates the average from less than 500 iterations, the result coincides with $<\cos \theta>_{i}$, ($i = 1$ or $i = 2$) in (3), given by the segregation assumption. Which value ($<\cos \theta>_1$ or $<\cos \theta>_2$) will result from the simulation depends in which region, $D_1$ or $D_2$, the starting point of the iteration was chosen. Calculates the same quantity from a much bigger ensemble, the result converges to a different value that does not depend on the choice of the initial configuration. See Fig. 1, which is clearly showing that the segregation is observed only within those configurations in which the number of updatings is too small.

This can much more directly be seen in Fig. 3, where the probability distribution within an ensemble of, respectively, 300, 1000 and 30000 configurations are shown. In Fig. 3a, the configurations are distributed in only one of the regions $D_1$ and $D_2$. On the other hand, in Fig. 3b and in Fig. 3c the
Figure 1:

$< \cos \theta >$ simulated by the complex Langevin equation compared with the theoretical curve (solid line) given by (1). The dashed line and the dot-dashed line corresponds, respectively, to the theoretical prediction $< \cos \theta >_1$ and $< \cos \theta >_2$ explained in subsection 2.2. The dotted line corresponds to $< \cos \theta >_{abs}$ explained in section 3.

Figure 2:

$< \cos \theta >$ simulated by the complex Langevin equation versus the number of iterations. Dotted line, dashed line and dot-dashed line corresponds respectively to $< \cos \theta >_{abs}$, $< \cos \theta >_1$ and $< \cos \theta >_2$.  

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distribution of the configuration covers the whole region of \( \mathcal{D} \).

Within the above two results, another important point needs to be stressed. It is the fact that the simulated results in Fig. 2 coincide exactly with

\[
< \cos \theta >_{\text{abs}} = \int_0^{2\pi} d\theta \cos \theta P_{\text{abs}}(\theta) = \frac{\int_0^{2\pi} d\theta \cos \theta \exp\{-S_{\text{abs}}\}}{\int_0^{2\pi} d\theta \exp\{-S_{\text{abs}}\}},
\]

(1)

where

\[
P_{\text{abs}} \propto e^{-S_{\text{abs}}}, \quad S_{\text{abs}} = -\beta \cos \theta - \ln |\cos \theta|.
\]

(2)

Also note that in Fig. 3c the probability distribution coincides exactly with \( P_{\text{abs}} \), given by the line represented by circles.

The reason why this happens will be discussed in section 4.

### 3.2 What is missing then? – the \( \delta \)-function

The difference between what we should get, see Eqs.(2,3), and what we have got, see Eqs.(1,2), may be found in the following simple formula

\[
S_{\text{eff}} = S_{\text{abs}} \pm i\pi \Theta(\cos \theta).
\]

(3)

where \( \Theta \) is the real step-function

\[
\Theta(x) = \begin{cases} 
1 & x > 0, \\
0 & x < 0.
\end{cases}
\]

(4)

From this action one gets the drift force

\[
-\frac{\delta S_{\text{eff}}}{\delta \theta} = -\frac{\delta S_{\text{abs}}}{\delta \theta} \mp i\pi \sin \theta \delta(\cos \theta),
\]

(5)

and the corresponding Langevin equation

\[
\dot{\theta} = -\beta \sin \theta - P(\tan \theta) \mp i\pi \sin \theta \delta(\cos \theta) + \eta,
\]

(6)

which is different from the normal one in Eq.(4).

As was stated in the first paragraph of section 2.2, one will never get the \( 1/\beta \)-behaviour in case the complex distribution collapses to the real one, independently of whether the segregation phenomenon is observed or not.
Figure 3:

Probability distribution within an ensemble of configurations. The figure (a),(b) and (c), respectively, is that of ensembles obtained by 300, 1000 and 30000 iterations using the Langevin equation (4). A line plotted by circles represents the distribution $P_{abs} \propto e^{-S_{abs}}$, while the solid line shows the theoretical prediction from the segregation assumption in $D_1$. The double-circle is the starting point of the iterative solution.
An important term missing in (4) is an imaginary part in the drift to allow for a complex distribution.

In this context, the additional drift force \( i\pi \delta(-\cos \theta) \) in (3) is expected to work well because it kicks the configuration into the deep imaginary region. This pushes the distribution collapsed on the real axis to that in the whole complex plane and may help to give the \( 1/\beta \) singularity.

4 Theoretical support of the idea

In the previous section we have discussed how one may simulate correctly a system whose drift force is singular. Before starting to solve the new Langevin equation obtained there, we give some theoretical support for the idea of a \( \delta \)-function-like drift. Furthermore, an important question to be answered is “whether our observation contradicts to the segregation theorem or not?”

To make the discussion clearer we consider an alternative model which is simpler but has a similar structure as the \( \cos \theta \)-model in (2) and (3).

4.1 A simpler model (modified Rayleigh-model)

Let us consider the following integral,

\[
<x> \equiv \frac{\int_{-\infty}^{+\infty} dx x^2 \exp\left(-\alpha^2 (x - \beta)^2\right)}{\int_{-\infty}^{+\infty} dx x \exp\left(-\alpha^2 (x - \beta)^2\right)} = \beta + \frac{1}{\alpha \beta}, \tag{1}
\]

One can rewrite it as

\[
<x> = \int_{-\infty}^{+\infty} dx x P_{eff}(x) = \frac{\int_{-\infty}^{+\infty} dx x \exp\{-S_{eff}\}}{\int_{-\infty}^{+\infty} dx \exp\{-S_{eff}\}}, \tag{2}
\]

where

\[
S_{eff} = \frac{\alpha}{2} (x - \beta)^2 - \ln x. \tag{3}
\]

As is seen in (4), the quantity \( <x> \) is also singular in the limit of \( \beta \to 0 \). This singularity arises from the fact that the denominator in (4) vanishes in this limit although the numerator remains finite. The situation is very similar to that of the \( \cos \theta \)-model. Therefore, this model will be a good candidate
to check all of the points discussed in the previous sections. Exactly in the same way as in case of the \( \cos \theta \)-model, the naive Langevin equation

\[
\dot{x} = -\alpha (x - \beta) + \frac{1}{x} + \eta(t). \tag{4}
\]

fails to reproduce the \( 1/\beta \) singularity given in (1). Based on this simple model, therefore, we will first study the segregation theorem in more detail in the next subsection.

### 4.2 The segregation phenomenon

Let us start from the Fokker-Plank equation equivalent to the above Langevin equation,

\[
\dot{P}(x; t) = \frac{1}{2} \frac{\partial^2}{\partial x^2}[B(x, t)P(x, t)] - \frac{\partial}{\partial x}[A(x, t)P(x, t)],
\]

\[
B(x, t) = 2, \quad A(x, t) = A(x) \equiv -\alpha(x - \beta) + \frac{1}{x} \tag{5}
\]

This is a second-order parabolic differential equation. In order to specify its solution one needs an initial condition, e.g., \( P(x; t_0) = \delta(x - x_0) \), and boundary conditions. In case the drift force \( A(x, t) \) is singular (or the diffusion coefficient \( B(x, t) \) vanishes) at some point \( x = x_b \), a certain boundary condition should be imposed at this point which is called a \textit{prescribed boundary condition}. What kind of boundary condition one should take at \( x = x_b \) is determined by the form of the drift and the diffusion coefficient. An extensive analysis of this problem has been given by Feller [21]. See also [22] for a review.

For our Langevin equation (4) the prescribed boundary condition will be given at the singular point of the drift, \( x = x_b = 0 \). \([x_b, x_0] \). Following the classification of Feller [21], the singular point \( x = x_b = 0 \) should be treated as an \textit{entrance boundary}. In this case the solution of the Langevin equation (4) should be such that if the configuration starting from, e.g., \( x = x_0 > x_b \) comes near to that boundary it should be pushed back to the

\[\text{Note that this Langevin equation is closely related to the well known Rayleigh process, } \dot{x} = -\alpha x + \frac{\mu}{x} + \eta(t).\]
original direction $x > x_b$. Therefore, the configuration starting from $x > x_b$
can never leave that region\(^3\). This is the so called segregation phenomenon.

4.3 The reason for the failure of the naive Langevin equation and the role of the $\delta$-function-like drift

Similar to what we saw in Fig. 2 and Fig. 3, however, this is not the case when one naively does a numerical simulation for solving the Langevin equation (4) by discretizing the time $t$. The configuration turned out to pass through the barrier at $x = x_b$ easily and the segregation theorem looks to be violated. The main reason why this happens may come from the fact that by discretizing the time we cannot treat the singularity in the drift rigorously. The adjusted time step has been introduced in order to take into account the effect of the singular region as rigorous as possible. But this seems still not enough. The system which are simulated by the discretized version of the Langevin equation (4) can not exactly be the process given by (4) but that with some regularized drift $A(x)_R$. In Figure 4, $A(x)_R$ is taken to be constant $\pm 1/r_0$ for $|x| < r_0$. The form of $A(x)_R$ in $|x| < r_0$ is, by no means, unique. However, one can easily check that the following discussion does not depend on the way how one regularizes $A(x)$ in this region.

For the stochastic process with the above regularized drift $A(x)_R$, no prescribed boundary condition exists by definition. The solution, therefore, can pass through the point $x = 0$ without any problem. In addition to this, an interesting point is that for this regularized process the stationary solution for $P(x)$ (at $|x| > r_0$) is given by $P_{\text{abs}} \propto |x| \exp(-\frac{\alpha}{2}(x - \beta)^2)$ and not by $x \exp(-\frac{\alpha}{2}(x - \beta)^2)$. To show this, let us try to solve the stationary solution $P(x)$ in the case of the regularized drift,

$$\left(\frac{\partial}{\partial x} + A(x)_R\right) P(x) = 0$$

The solution can be represented as (for simplicity we take $\beta = 0$ in the following)

$$r_0 < x : P(x) = c_1 e^{-\frac{x^2}{2} + \ln x},$$

\(^3\) When the configuration starts exactly from that point $x = x_b$ it should enter either the region $x > x_b$ or $x > x_b$, which is the origin of the name entrance boundary.
\[ 0 < x < r_0 : \quad P(x) = c_2 e^{-\frac{\alpha}{2}x^2 + \frac{1}{r_0}x}, \]
\[ -r_0 < x < 0 : \quad P(x) = c_3 e^{-\frac{\alpha}{2}x^2 - \frac{1}{r_0}x}, \]
\[ x < -r_0 : \quad P(x) = c_4 e^{-\frac{\alpha}{2}x^2 + \ln x}, \]
\[ x < -r_0 : \quad P(x) = c_4 e^{-\frac{\alpha}{2}x^2 + \ln x}, \]

with \( c_1, c_2, c_3 \) and \( c_4 \) being constants. The continuity conditions of \( P(x) \) at \( x = \pm r_0 \) and \( x = 0 \) give an interesting relation between \( c_1 \) and \( c_4 \), namely
\[ c_4 = c_1 e^{\ln(-1)} = -c_1. \]

This proves that, outside of the singular region, the Fokker-Planck distribution has the form of
\[ P(x) \propto |x| \exp\left\{\left(-\frac{\alpha}{2}\right)x^2\right\}. \]

From those discussions, it may be clear why our numerical simulation gave the results corresponding to \( P_{abs}(\theta) \) given in (1) and in (2) in the previous section.

Our proposal for the way out of this problem mentioned in the last subsection is to include an extra \( \delta \)-function type drift in the Langevin equation due to the relation \( \ln x = \ln |x| \pm i\pi \Theta(-x) \). The drift coming from \( \ln |x| \), i.e., \( -\delta(\ln |x|)/\delta x = P(1/x) \), is corresponding in some sense to the regularized drift \( A(x)_R \) discussed above. Then the total drift should be \[ \tilde{A}(x) = A(x)_R + i\pi \delta(x) \] It is interesting to repeat the same discussion as above using the new drift \( \tilde{A}(x) \). For this drift \( \tilde{A}(x) \), the solution of \( \tilde{J} \equiv (\partial_x + \tilde{A}(x)) P(x) = 0 \) can not, in general, be continuous at \( x = 0 \). This is seen by integrating both sides of this equation in a small region \([-\epsilon, +\epsilon]\), and taking the limit \( \epsilon \to 0 \). On the other hand applying the same discussion to the stationary F-P equation, \( \tilde{P} = \partial_x \tilde{J} = \partial_x (\partial_x + \tilde{A}(x)) P = 0 \), one finds that \( \partial_x P(x) \) can still be continuous at \( x = 0 \). From this continuity condition of \( \partial_x P(x) \) one gets \( c_4 = c_1 \) rather than that in (8). This means that \( P(x) \propto x \exp(-\alpha x^2/2) \) rather than \( P(x) = P_{abs}(x) \propto |x| \exp(-\alpha x^2/2) \).

This shows that if we succeed to estimate the effect of the \( \delta \)-function type drift in the Langevin equation, we will get the correct result.

5 How can one do the simulation for the \( \delta \)-function type drift?

\(^4\) Note that an addition of this \( \delta \)-function type drift will never spoil the regularity of the stochastic process at \( x = 0 \). This can easily be seen by calculating the functions \( f(x), g(x), h_1(x) \) and \( h_2(x) \) defined in (2) by using this drift. All of them turn out to be integrable in the region of \([0, x_0]\) for any finite \( x_0 \).
5.1 A model with a real $\delta$ function

In order to study how to solve the Langevin equations with the $\delta$-function type drift numerically, we first consider an even simpler model given by the real action

$$S_2 = \frac{\alpha}{2}(x - \beta)^2 - \frac{c}{2}\epsilon(x),$$  \hspace{1cm} (1)

where $c > 0$ is a real constant. Due to the existence of the $-c\epsilon(x)/2$ in the action, the distribution $P_2 \propto e^{-S_2}$ has a discontinuity at $x = 0$, see Fig. 5. The probability distribution is shifted to the direction of positive $x$, which increases the value of, e.g., $<x>$.

In the Langevin simulation, this effect will be given by the drift $-\delta/\delta x(-c/2\epsilon(x)) = c\delta(x)$ in the corresponding Langevin equation

$$\dot{x} = -\alpha(x - \beta) + c\delta(x) + \eta$$  \hspace{1cm} (2)

When the configuration crosses $x = 0$ while updating the Langevin equation, it gets a kick towards positive $x$, which works to increase the expectation value $<x>$.

5.2 A success of the numerical simulation

For the numerical solution of the Langevin equation we first have to fix how to treat the drift $c\delta(x)$. In this subsection we like to discuss two ways,

– the use of a smeared $\delta$-function, and

– an integration of the $\delta$-function around $x = 0$.

**The use of the smeared $\delta$-function:** One can replace the $\delta$-function by the smeared one,

$$\delta(x) \rightarrow \delta_\epsilon, \quad \delta_\epsilon \equiv \frac{1}{\pi x^2 + \epsilon^2},$$  \hspace{1cm} (3)

where $\epsilon$ is a small number. In Fig.6, the results for $<x>$ and $<x^2>$ simulated by the Langevin equation (2) with $\delta(x)$ being replaced by the smeared one $\delta_\epsilon(x)$ are given. One can see that, within this real model, the effect of the discontinuity in the probability distribution is nicely simulated by the effect of the $\delta$-function type drift in the Langevin equation.
Figure 4:
(a) Regularized drift force $A(x)_R$ at $x \sim 0$. (b) Solution of (3) under an assumption of continuous $P(x)$. (c) Solution of (3) under an assumption of continuous $\partial_x P(x)$.

Figure 5:
Schematic figure of the probability distribution $P_2 \propto e^{-S_2}$ with $S_2$ given in (4).
Integrating out the $\delta$-function: It is also possible to get an effective algorithm by analytically integrating out the $\delta$-function. Let us rewrite the Langevin equation (2) in a discretized form, and consider the step from $x_i$ to $x_f$ ($\Delta x \equiv x_f - x_i$),

$$\Delta x = a + c \frac{\Delta \Theta(x)}{\Delta x} \Delta t,$$

$$a \equiv \left( -\alpha(x - \beta) + \sqrt{\frac{2}{\Delta t} \xi} \right) \Delta t,$$  

(4)

where $\xi$ is a Gaussian noise with $\langle \xi^2 \rangle = 1$. When $x$ does not cross $x = 0$ within this step, $\Delta \Theta(x) = 0$ and therefore from (4) we simply get

$$\Delta x = a$$  

(5)

When $x$ crosses $x = 0$, $\Delta \Theta(x) = \pm 1$ (depending on whether $x_i > 0$ or $x_i < 0$) and the Langevin equation (4) becomes a second order algebraic equation for $\Delta x$. Solving this equation we get

$$\Delta x = \frac{a + \sqrt{a^2 + 4c\Delta t}}{2} \quad (x_i < 0, a > 0),$$

$$\Delta x = \frac{a - \sqrt{a^2 - 4c\Delta t}}{2} \quad (x_i > 0, a < 0).$$  

(6)

The simulated results for $\langle x \rangle$ by the use of this algorithm is shown in Fig. [7]. One can see that the Langevin simulation with the $\delta$-function type drift is being able to recover the exact one very nicely.

6 Complex $\delta$-function

In this section we come back to our original problem, the cos $\theta$-model. As discussed in section 3.2 the Langevin equation for this system is given by (2). This Langevin equation has an additional drift $i\pi \delta(\cos \theta)$ that kicks the configuration $\theta$ into the deep imaginary region. This will surely help to give a big $\langle \cos \theta \rangle$ because of the reasons explained in section 2.2. The problem, however, is how to continue this $\delta$-function into the whole complex $\theta$-plane.

In order to explain the situation more clearly, let us once more use the modified Rayleigh model given in (3). The Langevin equation for this system
Figure 6:

The result of \( \langle x \rangle \) and \( \langle x^2 \rangle \) (for \( \alpha = 0.2, \beta = 0 \)) simulated by the above Langevin algorithm versus \( c \). For each run 50000 iterations have been done with \( \Delta t = 0.04 \). Errors are estimated from 32 runs of this kind. The solid line represents the exact result.

Figure 7:

The result of \( \langle x \rangle \) and \( \langle x^2 \rangle \) (for \( \alpha = 0.2, \beta = 0 \)) simulated by the above Langevin algorithm versus \( c \). For each run 50000 iterations have been done with \( \Delta t = 0.01 \). Errors are estimated from 32 runs of this kind. The solid line represents the exact result.
is given by (4) with the additional drift $i\pi \delta(x)$. In this case, even when one starts the iteration from some point on the real axis, it becomes complex after getting a kick by the $\delta$-function. Then the question arises how to treat the $i\pi \delta(x)$ in the complex plane $z = x + iy$.

**Smeared $\delta$-function:** One possibility may be to use the smeared $\delta$-function continued into the complex plane, i.e., $\delta_\epsilon(z) = \epsilon/\pi(z^2 + \epsilon^2)$. But this does not work. The reason may be that the above smeared $\delta$ function which has been introduced in order to take into account the effect of the singularity in the drift $1/x$ has again a new singularity at $z = \pm i\epsilon$ in the complex plane. Actually we have tried to use it for simulation, it could not reproduce a correct $1/\beta$ behaviour for $< \cos \theta >$.

**Integrating out the $\delta$-function:** We also have a problem in applying this idea to the complex case, because we do not have the formula corresponding to (4) in the complex case. But neglecting this fundamental question, we may use the solution of this equation, i.e., (5) and (6), with $c = i\pi$. The result is not good enough to produce the $1/\beta$ singularity although it refines the results obtained without the $\delta$-function-type drift.

In spite of these failure, it is still very encouraging that with the idea of the $\delta$-function type kick we can find an effective algorithm by which the above $1/\beta$ behaviour in the cos $\theta$ model is successfully simulated. Let us approximate the drift $i\pi \sin \theta \delta(\cos \theta)$ in the Langevin equation (6) in the following way [19]: Consider the region $\mathcal{D}$ in the complex plane of $\theta = \theta_r + i\theta_i$ around the singular points $\theta = \pi/2$ or $3\pi/2$,

$$\theta \in \mathcal{D} \iff |\Re \cos \theta| < \hat{\delta}, \quad (1)$$

$\hat{\delta}$ being a small constant, and take

$$i\pi \sin \theta \delta(\cos \theta) \longrightarrow \begin{cases} 0, & \text{for } \theta \notin \mathcal{D} \\ i\pi, & \text{for } \theta \in \mathcal{D} \end{cases} \quad (2)$$

In Fig. 8 we show the result of $< \cos \theta >$ for the cos $\theta$ model. The data drawn by black squares are those simulated by the use of the Langevin equation (3), where the drift proportional to $\delta(\cos \theta)$ has been replaced by the kick given by equation (2) above. One can see that the simulated result coincides with the theoretical prediction quite nicely in the whole region of $\beta$.

In spite of this wonderful success of the numerical simulation, we have not yet found any smart theoretical justification of the above algorithm. Moreover the effectiveness of this algorithm can not be universal for other models.
The black square and the circle represents, respectively, the result of $\langle \cos \theta \rangle$ with and without the kick \textit{(2)}. For the parameters $\delta = 0.07, \Delta t = 0.002$ have been taken. In order to calculate the average 100000 iterations has been done for each run and the error has been estimated from 8 different kind of runs. The solid line represents the theoretical prediction. Dashed line and dotted line corresponds, respectively, to the theoretical prediction $\langle \cos \theta \rangle_1$ and $\langle \cos \theta \rangle_{abs}$ explained in subsection 2.2 and section 3.
The modified Rayleigh model discussed in section 4 is a good example. If the \( \delta \)-function type drift \( i\pi \delta(x) \) for this model is treated exactly in the same way as above, it will just give the imaginary kick \( i\pi \) to the configurations near to the singular point \( z = 0 \). The big imaginary part in \( z \), however, does not directly give a big \( \Re < z > = < x > \) contrary to the case of the \( \cos \theta \) model. We need therefore deeper understanding of the algorithm found above from more theoretical view point like that in the case of those models with real \( \delta \)-function in the previous section.

7 Conclusion

In the numerical simulation of certain field theoretical models, the complex Langevin simulation has been believed to fail due to the violation of the ergodicity. In this paper we have given a detailed analysis of this problem based on a toy model in one degree of freedom (\( \cos \theta \) model). The corresponding Langevin equations involved in the above problem have a singular drifts, e.g., \( \propto \tan \theta \). Our observation is that the failure is not due to the defect of the complex Langevin simulation itself, but rather to the way how one treats the above singular drift force. We have tried to justify this statement using also some alternative models. Under the above observation we could also give an effective algorithm by which we can simulate wonderfully the \( 1/\beta \) behaviour of the expectation value \( < \cos \theta > \) in the limit of \( \beta \to 0 \).

Unfortunately, however, the final theoretical justification of the above effective algorithm is still missing. When one succeeds in getting the rigorous theoretical background about how to treat the singular drift in the complex Langevin simulation, practical gain in the numerical simulation of lattice field theory will be extremely large.

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References

[1] G. Parisi. *Phys. Lett.* B 131 (1983) 393.

[2] J.R. Klauder. Stochastic quantization. In H. Mitter and C.B. Lang, editors, *Recent Developments in High Energy Physics*, page 251, Wien, New York, 1983. Springer.

[3] F. Karsch and H.W. Wyld. *Phys. Rev. Lett.* 55 (1985) 2242.

[4] E.M. Ilgenfritz. *Phys. Lett.* B 181 (1986) 327.

[5] N. Bilić, H. Gausterer and S. Sanielevici. *Phys. Lett.* B 198 (1987) 235.

[6] N. Bilić, H. Gausterer and S. Sanielevici. *Phys. Rev.* D 37 (1988) 3684.

[7] J. Ambjørn and S.-K. Yang. *Phys. Lett.* B 165 (1985) 140.

[8] J. Ambjørn and S.-K. Yang. *Nucl. Phys.* B 275 (1986) 18.

[9] H. Gausterer and J.R. Klauder. *Phys. Rev. Lett.* 56 (1986) 306.

[10] J.R. Klauder and S. Lee. *Phys. Rev.* D 45 (1992) 2101.

[11] J.R. Klauder and W.P. Petersen. *J. Stat. Phys.* 39 (1985) 53.

[12] H. Okamoto, K. Okano, L. Schülke and S. Tanaka. *Nucl. Phys.* B 324 (1989) 684.

[13] K. Okano, L. Schülke and B. Zheng. *Phys. Lett.* B 258 (1991) 421.

[14] B. Söderberg. *Nucl. Phys.* B 295 [FS21] (1988) 396.

[15] H. Gausterer and S. Lee. The mechanism of complex Langevin simulation. *University of Graz preprint UNIGRAZ-UTP 29-09-92 October 1992.*

[16] S. Lee. The convergence of complex langevin simulations. *preprint, University of Florida at Gainesville 1993 0.*

[17] L.L. Salcedo. *Phys. Lett.* B 305 (1993) 125.

[18] J. Flower, S.W. Otto and S. Callahan. *Phys. Rev.* D 34 (1986) 598.

[19] L. Schülke and B. Zheng. *Int. J. Mod. Phys.* C 3, 195, (1992); Proceedings of the workshop on *FERMION ALGORITHMS*, HLRZ Jülich, April 10-12, (1991).

[20] J. Ambjørn, M. Flensburg and C. Peterson. *Nucl. Phys.* B 275 [FS17] (1986) 375.
[21] W.Feller. *Ann. Math.* 55 (1952) 227.

[22] C.W. Gardiner. *Handbook of Stochastic Methods*. Springer, Berlin, 1983.
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