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Stability of complex Langevin dynamics in effective models

Gert Aarts,[a] **Frank A. James,**[b] **Jan M. Pawlowski,**[c] **Erhard Seiler,**[d] **Dénes Sexty**[c] **and Ion-Olimpiu Stamatescu**[c,e]

[a] *Department of Physics, College of Science, Swansea University, Swansea, United Kingdom*
[b] *Institute for Theoretical Physics, Universität Regensburg, Regensburg, Germany*
[c] *Institut für Theoretische Physik, Universität Heidelberg, Heidelberg, Germany*
[d] *Max-Planck-Institut für Physik (Werner-Heisenberg-Institut), München, Germany*
[e] *FEST, Heidelberg, Germany*

E-mail: g.aarts@swan.ac.uk, Frank.James@physik.uni-regensburg.de, J.Pawlowski@thphys.uni-heidelberg.de, ehs@mppmu.mpg.de, d.sexty@thphys.uni-heidelberg.de, i.o.stamatescu@thphys.uni-heidelberg.de

Abstract: The sign problem at nonzero chemical potential prohibits the use of importance sampling in lattice simulations. Since complex Langevin dynamics does not rely on importance sampling, it provides a potential solution. Recently it was shown that complex Langevin dynamics fails in the disordered phase in the case of the three-dimensional XY model, while it appears to work in the entire phase diagram in the case of the three-dimensional SU(3) spin model. Here we analyse this difference and argue that it is due to the presence of the nontrivial Haar measure in the SU(3) case, which has a stabilizing effect on the complexified dynamics. The freedom to modify and stabilize the complex Langevin process is discussed in some detail.

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1 Introduction

Because the fermion determinant in QCD at nonzero baryon chemical potential is complex, standard lattice QCD algorithms based on importance sampling cannot be used. As a result, a nonperturbative study of the QCD phase structure in the temperature — chemical potential plane is still missing [1]. Complex Langevin dynamics [2–5] may provide a solution, since it is not based on importance sampling, but instead on a stochastic exploration of an enlarged (complexified) field space. However, the method is not guaranteed to work: the numerical solution of a complex Langevin process may converge to a wrong answer. This problem was observed immediately [6, 7] after complex Langevin dynamics

was proposed in the early 1980s and is still present in current complex Langevin simulations [8–10]. However, recently it has also been shown convincingly that in some cases complex Langevin simulations converge to the seemingly correct answer, even when the sign problem is severe, i.e. in the thermodynamic limit of one-, three- and four-dimensional field theories at nonzero chemical potential [11–14]. Given the importance of understanding strongly-coupled theories such as QCD at nonzero chemical potential numerically, this issue clearly needs to be addressed.

The outstanding questions are therefore (1) to quantify whether the results from complex Langevin simulations have converged correctly; (2) to understand why the (in)correct convergence occurs; (3) to find a cure in the case of incorrect convergence. Recently we have clarified question (1) in some detail by putting the mathematical foundation of complex Langevin dynamics on firmer footing and deriving a set of criteria for correctness that need to be satisfied [15, 16]. These consistency conditions can be calculated during the complex Langevin simulation.

In this paper we focus on question (2), yielding insight that can be used to address the third question. This is done in the context of two three-dimensional spin models recently studied: the abelian XY model and the nonabelian SU(3) spin model, both at nonzero chemical potential. The XY model was studied in ref. [10]. Here it was shown that correct convergence is obtained deep in the ordered phase, but incorrect convergence was found in the disordered phase and the transition region. This conclusion was based on a study of the expected analyticity of observables around $\mu^2 = 0$, of properties of distributions in the complexified field space, and from a comparison with an alternative world-line formulation, which is sign-problem free [17]. The SU(3) spin model was studied in ref. [14], extending the classic papers [18, 19]. Using similar criteria as in the XY model (analyticity and Taylor series expansion around $\mu^2 = 0$, localized distributions in the complexified field space) as well as a test of the criteria for correctness mentioned above, we concluded that complex Langevin dynamics yields the correct results in the entire phase diagram. This conclusion was subsequently supported by a study using a dual formulation, which is again sign-problem free [20, 21].

In the present paper we address this observed difference in performance of the complex Langevin method between the XY and the SU(3) spin model. Surprisingly, we find that the nonabelian nature of the SU(3) spin model is crucial. In particular we demonstrate that in the disordered phase of the XY model the real manifold is unstable against complex fluctuations while in the SU(3) spin model it is stable. Stability of the real manifold is important for understanding the expected analyticity of observables around $\mu^2 = 0$.

The paper is organized as follows. In section 2 we remind the reader of the SU(3) and XY models and reduce them to effective one-link models with complex couplings. In section 3 the effective one-link models are discussed in detail and the difference between the abelian and nonabelian models is stressed. In section 4 we use the insight to illustrate how coordinate transformations may stabilize the dynamics. Conclusions and an outlook are given in ref. 5. Appendix A contains a detailed discussion of possible modifications of the complex Langevin approach.

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2 SU(3) and U(1) spin models

2.1 SU(3) spin model

We consider the three-dimensional SU(3) spin model at nonzero chemical potential, with the action

$$S = S_B + S_F, \tag{2.1}$$

where

$$S_B = -\beta \sum_x \sum_{\nu=1}^{3} \left(\mathrm{Tr}\, U_x \mathrm{Tr}\, U^\dagger_{x+\hat{\nu}} + \mathrm{Tr}\, U^\dagger_x \mathrm{Tr}\, U_{x+\hat{\nu}} \right), \tag{2.2}$$

$$S_F = -h \sum_x \left(e^{\mu} \mathrm{Tr}\, U_x + e^{-\mu} \mathrm{Tr}\, U^\dagger_x \right). \tag{2.3}$$

The matrices U_x are elements of SU(3). The action is complex and satisfies the usual symmetry, $S^*(\mu) = S(-\mu^*)$. The 'fermion' contribution follows from the full QCD determinant by preserving only propagation in the temporal direction at leading order in the hopping expansion (i.e. heavy quarks). The model is part of a whole family of effective Polyakov loop models with heavy quarks [22, 23]. A detailed complex Langevin study can be found in ref. [14].

We want to construct a one-link model that captures the essential dynamics. We therefore focus on a site x and consider the interaction of U_x with its nearest neighbours. Treating all six neighbours equally and denoting their contribution as $u \in \mathbb{C}$, we write the effective one-link model as[1]

$$S_U = -\beta_1 \mathrm{Tr}\, U - \beta_2 \mathrm{Tr}\, U^{-1}, \tag{2.4}$$

where the effect of the neighbours is captured, to a certain extent, by a simplified parametrization

$$\beta_1 = 6\beta u + h e^{\mu}, \qquad \beta_2 = 6\beta u^* + h e^{-\mu}, \tag{2.5}$$

with $\beta_1^*(\mu) = \beta_2(-\mu^*)$.

Typical values of $\beta_{1,2}$ are determined by β, h and μ, and by the contribution from the nearest neighbours, represented by u, in the original three-dimensional theory. We first note that the critical β value in the SU(3) spin model at vanishing μ is $\beta_c \sim 0.133$ [14, 21].[2] We therefore consider β values around this value, as in refs. [14, 21]. Writing $u = |u| e^{i\gamma}$, the correlation between its phase and amplitude can be determined using simulations in the full, three-dimensional theory. The result is shown in figure 1, from a study on a 12^3 lattice for 15 combinations of β and μ at fixed $h = 0.02$. Note that during a Langevin simulation, u takes values in the familiar triangular shape with corners at $3e^{2\pi i q/3}$ $(q = 0, 1, 2)$. This explains the three spikes at $\gamma/\pi = 0, \pm 2/3$. At larger β and/or μ, u lies predominantly in the trivial direction $(q = 0)$ and γ is closer to zero. Note also that at nonzero μ,

[1] As always, U^{-1} is written instead of $U^\dagger$ to allow for the correct extension to SL(3,$\mathbb{C}$).

[2] Its relation with the four-dimensional coupling can be ultimately be understood from a combined strong-coupling/hopping parameter expansion [22].

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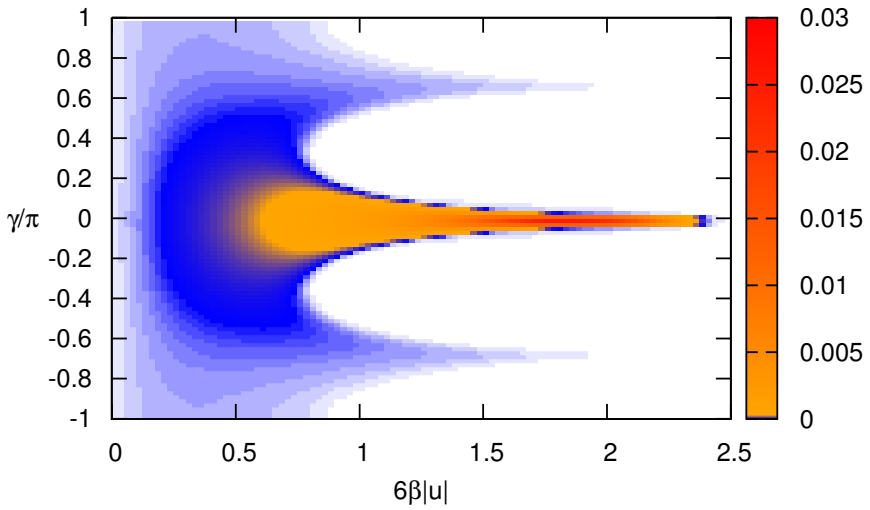

Figure 1. Correlation between the phase γ and the modulus $6\beta|u|$, where $u = |u|e^{i\gamma} = \mathrm{Tr}\, U$ in the three-dimensional SU(3) spin model, for 15 combinations of $\beta = 0.125, 0.13, 0.135$, and $\mu = 0.5, 1, 2, 3, 4$, at $h = 0.02$ on a 12^3 lattice.

the dynamics takes place slightly outside SU(3) [14] and $|u|$ is not strictly bounded by 3. Typical values of h and μ are determined by the relation with four-dimensional theory [24]: for Wilson quarks, $h = (2\kappa)^{N_\tau}$ with $\kappa \sim 0.12$ and $N_\tau = 4, 6, 8$, etc. Relevant values of h are therefore small. Upon identification with the four-dimensional theory, μ as used here in fact corresponds to μ/T (with $1/T = a_\tau N_\tau$).

We finally express the complex couplings as

$$\beta_1 = \beta_{\mathrm{eff}} e^{i\gamma} + h e^{\mu}, \qquad \beta_2 = \beta_{\mathrm{eff}} e^{-i\gamma} + h e^{-\mu}, \tag{2.6}$$

where $\beta_{\mathrm{eff}} = 6\beta|u| \lesssim 2.5$.

2.2 XY model

The action for the three-dimensional XY model at nonzero chemical potential reads

$$\begin{aligned} S &= -\frac{\beta}{2} \sum_x \sum_{\nu=1}^{3} \left(e^{\mu\delta_{\nu,3}} U_x U^\dagger_{x+\hat{\nu}} + e^{-\mu\delta_{\nu,3}} U^\dagger_x U_{x+\hat{\nu}} \right) \\ &= -\beta \sum_x \sum_\nu \cos\left(\phi_x - \phi_{x+\hat{\nu}} - i\mu\delta_{\nu,3}\right), \end{aligned} \tag{2.7}$$

where $U_x = e^{i\phi_x}$ are in this case U(1) phase variables. A complex Langevin study of this model can be found in ref. [10].

We first note that deep in the ordered phase, where $\phi_x - \phi_{x+\hat{\nu}} \ll 1$, the action reduces to

$$S \sim \frac{1}{2} \sum_{x,\nu} \beta_\nu \left(\phi_x - \phi_{x+\hat{\nu}}\right)^2, \tag{2.8}$$

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with $\beta_{1,2} = \beta$, $\beta_3 = \beta \cosh \mu$. Here we dropped an overall constant and employed the periodicity of the lattice. Since this action is real, the sign problem is absent in this limit. Indeed, in the corresponding part of the phase diagram (large β and/or μ), no problems were encountered in ref. [10].

As in the SU(3) case, we consider an effective one-link model of the form

$$S_U = -\beta_1 U - \beta_2 U^{-1}, \qquad U = e^{i\phi}, \tag{2.9}$$

with complex couplings $\beta_{1,2}$. If we follow the approach from the SU(3) model and replace the six nearest neighbours by a common contribution $u \in \mathbb{C}$, we find that

$$\beta_1 = \beta u^* \left(2 + \cosh \mu\right), \qquad \beta_2 = \beta u \left(2 + \cosh \mu\right), \tag{2.10}$$

so that $\beta_1^* = \beta_2$ and the action S_U is in fact real. Hence we are forced to represent the nearest neighbours by independent complex phases and we consider the general effective U(1) one-link model,

$$S_U = -\beta_1 U - \beta_2 U^{-1} = -\beta_1' \cos \phi - \beta_2' \sin \phi, \tag{2.11}$$

where we take $\beta_{1,2}, \beta_{1,2}' \in \mathbb{C}$ without further restrictions.

3 Complex Langevin for effective models

3.1 U(1) one-link model

We consider complex Langevin dynamics for the one-link models constructed above. In the U(1) case, the partition function reads

$$Z_{\mathrm{U}(1)} = \int_{-\pi}^{\pi} d\phi \, e^{-S_{\mathrm{U}}(\phi)}, \tag{3.1}$$

and the corresponding complex Langevin equation is

$$\dot{\phi} = K[\phi(t)] + \eta(t), \qquad K(\phi) = -\frac{\partial S_U}{\partial \phi}, \tag{3.2}$$

with standard relations for the noise, $\langle \eta(t) \rangle = 0$, $\langle \eta(t)\eta(t') \rangle = 2\delta(t - t')$. Since the action and the drift term K are complex, ϕ will take values in the complex plane and $U = e^{i\phi}$ is no longer a phase variable.

3.2 SU(N) one-link models

In the case of the SU(3) [or more generally an SU(N)] spin model, we can express all dynamics in terms of the eigenvalues of U, subject to the constraints, i.e.,

$$U = \mathrm{diag}\left(e^{i\phi_1}, e^{i\phi_2}, \ldots, e^{i\phi_N}\right), \qquad \phi_1 + \phi_2 + \ldots + \phi_N = 0. \tag{3.3}$$

The partition function then includes integrating over the reduced Haar measure, which represents explicitly the integration over the full group manifold,

$$H(\{\phi_a\}) = \prod_{a<b} \sin^2\left(\frac{\phi_a - \phi_b}{2}\right), \tag{3.4}$$

$(a, b = 1, \ldots, N)$ and reads

$$Z_{\mathrm{SU}(N)} = \int_{-\pi}^{\pi} d\phi_1 \ldots d\phi_N \, \delta\left(\phi_1 + \phi_2 + \ldots + \phi_N\right) H(\{\phi_a\}) e^{-S_{\mathrm{U}}(\{\phi_a\})}$$
$$= \int_{-\pi}^{\pi} d\phi_1 \ldots d\phi_N \, \delta\left(\phi_1 + \phi_2 + \ldots + \phi_N\right) e^{-S_{\mathrm{eff}}(\{\phi_a\})}, \tag{3.5}$$

with

$$S_{\mathrm{eff}} = S_U + S_H = S_U - \ln H. \tag{3.6}$$

The non-abelian Haar measure, which is explicitly seen here as the reduced Haar measure, is the crucial difference between SU(N) and U(1) spin models. This is especially clear in the case of SU(2) with a simple action

$$S_U = -\frac{\beta}{2} \mathrm{Tr}\, U = -\beta \cos\phi, \qquad \beta \in \mathbb{C}. \tag{3.7}$$

As in the U(1) case, the partition function involves a single integral over $\phi \equiv \phi_1 = -\phi_2$ only and reads

$$Z_{\mathrm{SU}(2)} = \int_{-\pi}^{\pi} d\phi \, \sin^2(\phi) e^{-S_{\mathrm{U}}(\phi)}. \tag{3.8}$$

The presence of the reduced Haar measure is the important difference with eq. (3.1).

To write down the Langevin equations in the SU(N) case, we may follow several routes. Firstly, we may eliminate ϕ_N using the constraint in eq. (3.3), and write Langevin equations for the remaining $N-1$ degrees of freedom,

$$\dot{\phi}_a = K_a[\phi(t)] + \eta_a(t), \qquad K_a(\phi) = -\frac{\partial S_{\mathrm{eff}}}{\partial \phi_a}. \tag{3.9}$$

Each update requires $N-1$ stochastic kicks. This is the approach followed in refs. [14, 18].

Secondly, the constraint can also be implemented by introducing new variables z_a $(a = 1, \ldots, N)$, according to

$$\phi_a = z_a - \frac{1}{N}\left(z_1 + z_2 + \ldots + z_N\right), \tag{3.10}$$

such that the constraint $\sum_a \phi_a = 0$ is automatically satisfied. This is a singular transformation; the validity of the procedure therefore requires some justification, which is given in appendix A.4.3. It should be noted that the stochastic process, even when restricted to the first $N-1$ variables ϕ_a, is different from the one above. We then write the following dynamics for z_a,

$$\dot{z}_a = K_a[z(t)] + \eta_a, \qquad K_a(z) = -\frac{\partial S_{\mathrm{eff}}}{\partial z_a}, \tag{3.11}$$

where the ϕ_a are always considered as functions of the z_a, according to eq. (3.10). In this formulation N stochastic variables are used. However, it is easy to see that the real part of the centre-of-mass coordinate is freely diffusing (the imaginary part is not evolving at all), since

$$\sum_a K_a(z) = 0 \qquad \Rightarrow \qquad \sum_a \dot{z}_a = \sum_a \eta_a. \tag{3.12}$$

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Since the real parts are angular degrees of freedom, this does not cause harm in terms of runaways.

Finally, we may also write the dynamics directly for the SU(N) matrix U and not in terms of the eigenvalues. After discretizing the Langevin time with stepsize ϵ, this takes the form

$$U(t+\epsilon) = \exp\left[i\lambda_a\left(\epsilon K_a + \sqrt{\epsilon}\eta_a\right)\right] U(t), \tag{3.13}$$

where λ_a (here $a = 1, \ldots, N^2-1$) are the traceless, hermitian Gell-Mann matrices, normalized as $\mathrm{Tr}\,\lambda_a\lambda_b = 2\delta_{ab}$ and the drift terms are

$$K_a = -D_a S_U = i\beta_1 \mathrm{Tr}\,\lambda_a U - i\beta_2 \mathrm{Tr}\,\lambda_a U^{-1}. \tag{3.14}$$

Note that the complex process runs in the SL($N,\mathbb{C}$) extension of SU(N) and thus, e.g. in eq. (3.13), $U \in \mathrm{SL}(N,\mathbb{C})$ and $K_a \in \mathrm{sl}(N,\mathbb{C})$. In this formulation there are N^2-1 stochastic variables, instead of $N-1$. In ref. [9] it was shown how the additional noise variables generate the correct drift for the remaining degrees of freedom when U is diagonalized after each update. This formulation was considered in refs. [8, 9, 19, 24].

3.3 Classical flow

The role of the reduced Haar measure can be seen by studying the classical flow diagrams. Since the classical flow for the SU(3) spin model with angles $\phi_{1,2}$ takes place in four real dimensions, it is hard to give a proper graphical representation. Instead we present as an illustration the classical flow for the SU(2) one-link model, in which the reduced Haar measure plays a similar stabilizing role.

Explicitly, we compare the U(1) and SU(2) case, with

$$Z_{\mathrm{U}(1)} = \int_{-\pi}^{\pi} dx\, e^{\beta\cos x}, \qquad Z_{\mathrm{SU}(2)} = \int_{-\pi}^{\pi} dx\, \sin^2 x\, e^{\beta\cos x}, \tag{3.15}$$

with complex $\beta = \beta_{\mathrm{R}} + i\beta_{\mathrm{I}}$. The real and imaginary parts of the drift K, after complexification $x \to x + iy$, are

$$K_{\mathrm{R}} = -\beta_{\mathrm{R}} \sin x \cosh y + \beta_{\mathrm{I}} \cos x \sinh y - \frac{2d\sin(2x)}{\cos(2x) - \cosh(2y)}, \tag{3.16}$$

$$K_{\mathrm{I}} = -\beta_{\mathrm{R}} \cos x \sinh y + \beta_{\mathrm{I}} \sin x \cosh y + \frac{2d\sinh(2y)}{\cos(2x) - \cosh(2y)}. \tag{3.17}$$

In the U(1) case, the contribution from the Haar measure is absent and $d = 0$; in SU(2), $d = 1$.

Let us first consider the contribution from the Haar measure. It is easy to see that when $|y|$ is large,

$$K_{\mathrm{R}} \to 0, \qquad K_{\mathrm{I}} = -2\mathrm{sgn}(y) \qquad \text{(Haar measure only)}, \tag{3.18}$$

i.e. the contribution is purely restoring. We also note that at the origin and at $(\pm\pi, 0)$ the drift force from the Haar measure becomes singular; this invalidates potentially the formal

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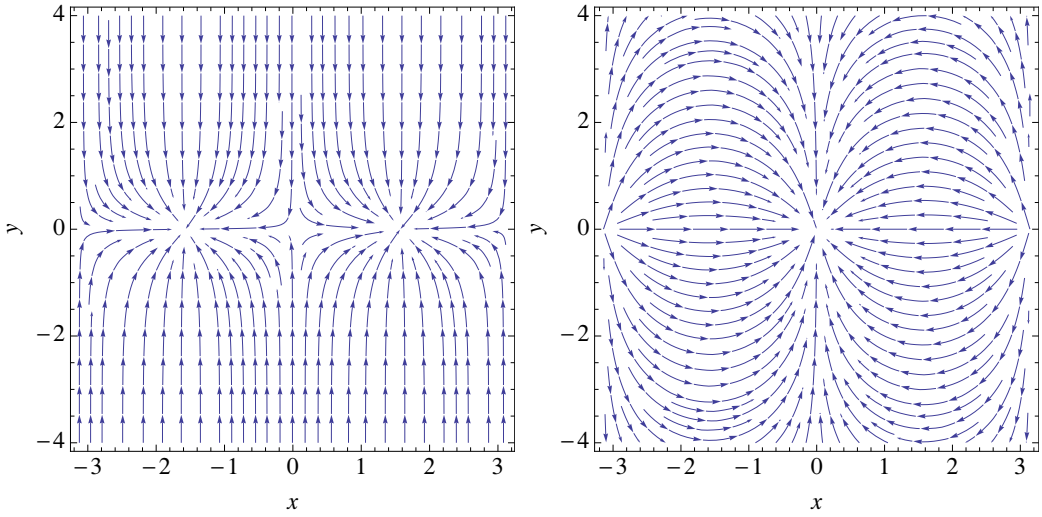

Figure 2. Classical flow diagrams: drift from the Haar measure only, in SU(2) (left); drift from the action only, in U(1) and SU(2), with $\beta = 1$ (right).

argument for correctness of the complex Langevin approach method, because it might produce boundary terms at the singularity. Practically, however, this does not seem to cause problems, as the equilibrium measure appears to vanish sufficiently strongly at the origin (although it does require the use of an adaptive stepsize algorithm in simulations [25]). Finally, there are stable fixed points at $(x, y) = (\pm\pi/2, 0)$. These findings are illustrated in figure 2 (left), where the drift from the Haar measure only is shown.

Let us now consider the contribution from the action by itself, i.e. the drift in the U(1) model ($d = 0$), see figure 2 (right). This drift has an attractive fixed point at the origin and repulsive fixed points at $(\pm\pi, 0)$. Due to these repulsive fixed points, the real manifold ($y = 0$) is unstable against small fluctuations in the y direction. Therefore even with stochastic kicks in the x direction only (real noise), fluctuations in the imaginary direction, e.g. due to a small but nonzero β_{I}, will immediately lead to an exploration of the complexified space, resulting in trajectories that may take large excursions in the y direction, due to the character of the repulsive flow around $x = \pm\pi$.

In the nonabelian case, one has to add the contribution of the Haar measure to that of the action. The resulting flow is shown in figure 3 (left) for real $\beta = 1$. The singular flow at the origin and at $(\pm\pi, 0)$ remains. We observe that the repulsive fixed points have moved away from the real manifold to $(\pm\pi, \pm y_*)$, while the attractive fixed points remain on the real manifold at $(x_*, 0)$, where

$$\cos x_* = -\frac{d}{\beta} + \sqrt{1 + \frac{d^2}{\beta^2}}, \qquad \cosh y_* = \frac{d}{\beta} + \sqrt{1 + \frac{d^2}{\beta^2}}, \tag{3.19}$$

(for $\beta = 1$ this yields $x_* = \pm 1.14$, $y_* = \pm 1.53$). Note that the presence of the reduced Haar measure ($d = 1$) is essential. Since the repulsive fixed points have moved away, the real axis is stable in SU(2) for β values that are not too large. This can be seen by a linear

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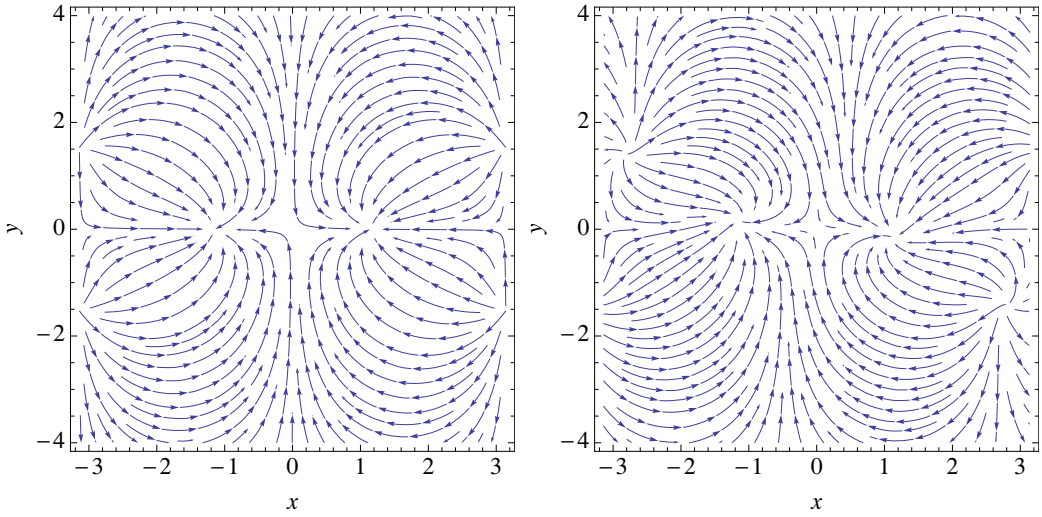

Figure 3. Classical flow diagrams for SU(2) for $\beta = 1$ (left) and $\beta = 1 + 0.5i$ (right).

stability analysis, which yields (for real β)

$$\dot{y} = -\lambda y, \qquad \lambda = \beta \cos x + \frac{4d}{1 - \cos(2x)}. \tag{3.20}$$

This is stable ($\lambda > 0$), as long as $\beta/d \lesssim 5.196$. In fact, in the entire strip bounded by $\pm y_*$, the flow is directed towards the real manifold.

Let us now see how a complex coupling changes the flow, see figure 3 (right) for $\beta = 1+0.5i$. Even though the stable fixed points move away from $y = 0$ [to $\pm(1.12, -0.158)$] and the unstable ones from $x = \pm\pi$ [to $\pm(2.79, -1.41)$], we note that in the region around $y \sim 0$ the flow is still directed to the real axis. This means that if initial conditions are chosen close to $y = 0$, the complex stochastic process will take place in a strip around $y = 0$. The probability distribution $P(x, y)$ will be strictly zero outside this strip and the theoretical foundation of the complex Langevin method is justified [15, 16]. For larger (complex) β the stable fixed points will move out further into the complex plane and the dynamics will eventually no longer be confined to a strip. The stability analysis as carried out here is then no longer applicable.

In the SU(3) case similar conclusions hold. The presence of the reduced Haar measure is essential in stabilizing the real manifold (for nearly real dynamics, i.e. when $\beta_{\rm I}, \mu \ll 1$). Instead of showing four-dimensional flow diagrams, we look at the linear stability of the real manifold in the case that $h = 0$ and β is real. We write $\phi_a \to \phi_a^{\rm R} + iy_a$ and expand to linear order in y_a ($a = 1, 2$). We find

$$\begin{pmatrix} \dot{y}_1 \\ \dot{y}_2 \end{pmatrix} = -A \begin{pmatrix} y_1 \\ y_2 \end{pmatrix}, \qquad A = \begin{pmatrix} A_1 & A_o \\ A_o & A_2 \end{pmatrix}. \tag{3.21}$$

The contributions from the action and the reduced Haar measure are denoted with U resp. H and we write $A = A^U + A^H$. We find

$$A_a^U = 2\beta \left[\cos(\phi_a^{\rm R}) + \cos(\phi_1^{\rm R} + \phi_2^{\rm R})\right], \qquad A_o^U = 2\beta \cos(\phi_1^{\rm R} + \phi_2^{\rm R}), \tag{3.22}$$

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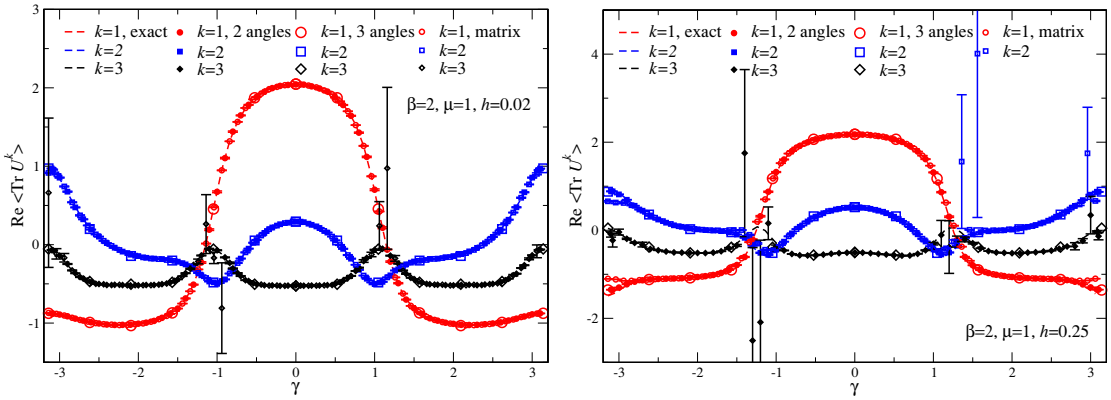

Figure 4. SU(3) one-link model: $\langle \mathrm{Tr}\, U^k \rangle$ vs. γ for $k = 1, 2, 3$, at $\beta_{\mathrm{eff}} = 2, \mu = 1$ and $h = 0.02$ (left) and 0.25 (right), using the two- and three-angle and the matrix formulations. At $h = 0.02$, agreement with the exact results is seen for all γ in the two- and three-angle case; in the matrix case there is poor convergence at specific values of γ. At larger $h = 0.25$, there is poor or wrong convergence also in the two- and three-angle case.

and

$$
\begin{aligned}
A_a^H &= \frac{1}{2}\csc^2\left(\frac{\phi_1^{\mathrm{R}} - \phi_2^{\mathrm{R}}}{2}\right) + 2\csc^2\left(\frac{2\phi_a^{\mathrm{R}} + \phi_b^{\mathrm{R}}}{2}\right) + \frac{1}{2}\csc^2\left(\frac{\phi_a^{\mathrm{R}} + 2\phi_b^{\mathrm{R}}}{2}\right), \\
A_o^H &= -\frac{1}{2}\csc^2\left(\frac{\phi_1^{\mathrm{R}} - \phi_2^{\mathrm{R}}}{2}\right) + \csc^2\left(\frac{2\phi_1^{\mathrm{R}} + \phi_2^{\mathrm{R}}}{2}\right) + \csc^2\left(\frac{\phi_1^{\mathrm{R}} + 2\phi_2^{\mathrm{R}}}{2}\right),
\end{aligned}
\tag{3.23}
$$

where $b \neq a$ and $\csc z = 1/\sin z$.

It is easy to see that the eigenvalues of A^H by itself are positive for all values of $\phi_{1,2}^{\mathrm{R}}$: the real manifold is stable when only this contribution to the drift is considered. On the other hand, the sign of the eigenvalues of A^U depends on $\phi_{1,2}^{\mathrm{R}}$, leading to unstable regions. In the combined linearized drift, with $A = A^U + A^H$, inspection shows that the real manifold is stable for $\beta \lesssim 1.75$, and (linearly) unstable for larger β. We note that this bound covers most of the parameter space indicated in figure 1, except deep in the ordered phase, where β can be larger (note that this β refers to $\beta_{\mathrm{eff}} = 6\beta|u|$ in figure 1). Here we remark that the linear stability analysis is probably too restrictive, since no problems were encountered in this region. In fact, in the ordered phase complex Langevin dynamics was seen to perform very well [14].

3.4 Numerical results

We have solved the complex Langevin equations numerically for a number of parameter values, using the two- and three-angle and the matrix formulations. Here we give a brief summary, illustrating the analytical findings discussed above.

Firstly, we find that, although they imply different processes, the two- and three-angle formulations give identical results (within the statistical error) and agree with the exact results for small values of β and h, see e.g. figure 4 (left) for $\beta = 2, h = 0.02, \mu = 1$. Since $\mu \neq 0$, the dynamics does not take place on the real manifold but in the complexified

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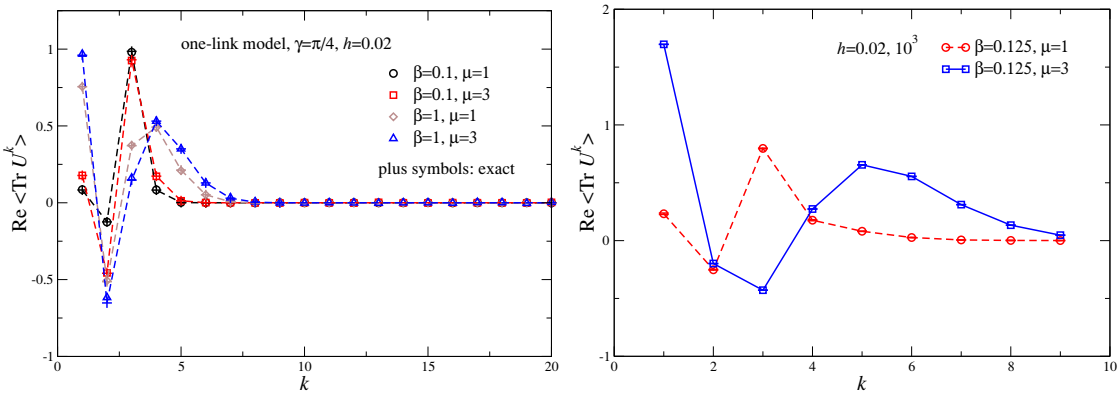

Figure 5. Expectation values $\langle \mathrm{Tr}\, U^k \rangle$ as a function of k for various values of β and μ in the SU(3) one-link model (left) and in the three-dimensional model on a 10^3 lattice. On the left, exact results are indicated with plus symbols; these can hardly be distinguished from the complex Langevin results.

configuration space. Nevertheless, the drift from the reduced Haar measure has a stabilizing effect, which constrains the dynamics. For larger values of the effective couplings $\beta_{1,2}(\mu)$ (which can be achieved by increasing β, h or μ), we find that the dynamics may break down for a range of γ values. This is illustrated in figure 4 (right) for $\beta = 2, h = 0.25, \mu = 1$. A breakdown can be characterized by large fluctuations (e.g. around $\gamma \sim \pm 1.25$) or by convergence to the wrong result (around $\gamma \sim \pm\pi$). This happens at parameter values where the dynamics is not clearly dominated by a stable fixed point in the complexified field space. Interestingly, when the one-link model is viewed as an effective model for the three-dimensional SU(3) spin model (or full QCD), the combination of parameter values where the dynamics breaks down appears to be in a region of parameter space which is less relevant for those; recall the discussion around figure 1. Therefore this breakdown does not undermine the results obtained in the three-dimensional case.

In the matrix formulation, we observe that the dynamics is more subtle and can break down earlier. This process is distinct from the previous ones in that a different complexified field space is explored, with apparently more possibilities for unstable trajectories. This is visible in figure 4 already at $h = 0.02$ for $k = 3$ at specific γ values and more so at larger $h = 0.25$ (here the result at $k = 3$ is not shown). It is of course mandatory to control the dynamics in this formulation in the context of gauge theories and this can be partly achieved using gauge cooling [26].

The mathematical foundation for complex Langevin dynamics to converge to the correct result is that the distribution in the complexified field space falls off rapidly. In ref. [14] it was found that in the three-dimensional SU(3) spin model the distribution in the imaginary direction ϕ^{I} drops exponentially, $P(\phi^{\mathrm{I}}) \sim e^{-b|\phi^{\mathrm{I}}|}$, with $b \sim 35 - 45$. This left open the question what happens to expectation values of the form $\langle \mathrm{Tr}\, U^k \rangle$ with k large. These observables contain terms of the form $e^{\pm k\phi^{\mathrm{I}}} \cos(k\phi^{\mathrm{R}})$ and the presence of the rapidly oscillating cosines should be taken into consideration. This is demonstrated in figure 5 where $\langle \mathrm{Tr}\, U^k \rangle$ is shown as a function of k in the one-link model (left) and in the three-dimensional

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model on a 10^3 lattice (right). In the one-link model, exact results are shown as well; agreement between the Langevin and exact results is observed. We conclude therefore that the higher moments decrease rapidly and that the falloff of the distribution in the imaginary direction is sufficient to achieve this.

Our conclusion from the numerical experiments with two and three angles is that the Langevin dynamics is controlled and yields the correct results when the contribution from the reduced Haar measure is not overpowered by the contribution from the action itself. This is achieved by taking the effective couplings not too large. For larger β or h values however, the real manifold is no longer stable and this implies problems for the complex Langevin process. Fortunately, this happens for parameter values in the effective one-link model, which do not seem to be relevant for the three-dimensional (or four-dimensional) original model.

Above the one-link model was used as an effective model for the SU(3) spin model. However, we can also see it as an effective model for lattice QCD in the heavy dense approximation, cf. refs. [22–24, 26]. In this case the effective coupling β represents the contributions from the staples attached to a link, and instead of eq. (2.3) the heavy dense determinant itself appears in the three-dimensional effective action:

$$S_F = -\sum_x \ln\left[\det\left(1+he^{\mu/T}\mathcal{P}_x\right)^2 \det\left(1+he^{-\mu/T}\mathcal{P}_x^{-1}\right)^2\right], \tag{3.24}$$

with $h = (2\kappa)^{N_t}$ and $\mathcal{P}_{\mathbf{x}}^{(-1)}$ the (conjugate) Polyakov loops. Using the determinant in the corresponding one-link model appears to have a stabilizing effect and the two- and three-angles simulations are even better behaved.

4 Stabilization via generalizations of the CLE

A general possible route for stabilization uses the fact that there is a wide range of possibilities to modify the complex Langevin equation (CLE). Such a modification, if chosen appropriately, can improve the falloff of the equilibrium distribution, which was identified in refs. [15, 16] as the essential prerequisite for a correct CLE process. Some of those modifications, like kernels, were known already in the 1980s [27–29], others such as variable transformations, were encountered just recently. In fact the reduction to the Cartan subgroup discussed in the previous section falls into this general category. In the present section we analyze the possible modifications more generally and find an equivalence between the approaches using a kernel and coordinate transformations.

The crucial point is that we apply the CLE only for averaging *holomorphic* functions. Different distributions in the complexified configuration space can give the same expectation values for those holomorphic functions; this is true for the probability density evolving under the Fokker-Planck equation as well as the stationary equilibrum distribution. In appendix A we give general classes of processes and equilibrium measures which are equivalent in this sense. In addition there is the well-known freedom of using different processes having the same equilibrium measure.

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Let us first describe the use of coordinate transformations. We have to distinguish two kinds of transformations:

(a) transforming the CLE process, i.e. the description of the trajectories;

(b) transforming the variables in the functional integral.

The first possibility does not change anything essential, since it is only a transformation of the description; the second choice, however, leads to a modified process due to the appearance of a Jacobian. It turns out that after changing the description of this modified process back to the original coordinates one has in fact introduced a kernel.

In one variable this works as follows: let

$$x = x(u) \tag{4.1}$$

be an invertible smooth variable transformation. To avoid confusion we rename the action $S(x)$ when considered as function of u by

$$\tilde{S}(u) \equiv S(x(u))\,. \tag{4.2}$$

We have

$$Z = \int dx\, e^{-S(x)} = \int du\, e^{-\tilde{S}_{\text{eff}}(u)}, \tag{4.3}$$

with

$$\tilde{S}_{\text{eff}}(u) = \tilde{S}(u) - \ln J(u), \qquad J(u) = \frac{dx(u)}{du}. \tag{4.4}$$

The new drift becomes

$$K(u) = -\tilde{S}'_{\text{eff}}(u) = -\tilde{S}'(u) + J'(u)/J(u),$$

and the new CLE

$$\dot{u} = -\tilde{S}'(u) + J'(u)/J(u) + \eta(t). \tag{4.5}$$

Let us first study the stability of the real manifold under small imaginary fluctuations in the original formulation. We write $x \to z = x + iy$ and linearize in y to find

$$\dot{y} = -\lambda(x)y, \qquad \lambda(x) = S''(x). \tag{4.6}$$

Only if $\lambda(x) > 0$ for all x is the real axis stable against complex perturbations.

By choosing a clever transformation one can stabilize a situation which is unstable due to a nonpositive $\lambda(x)$ or a repulsive fixed point. After the change of variables to u and writing $u \to u + iv$, one finds, to first order in v,

$$\dot{v} = -\tilde{\lambda}(u)v, \tag{4.7}$$

where now

$$\tilde{\lambda}(u) = \tilde{S}''_{\text{eff}}(u) = \tilde{S}''(u) - J''(u)/J(u) + \left[J'(u)/J(u)\right]^2. \tag{4.8}$$

The contribution from the Jacobian may now stabilize the real manifold.

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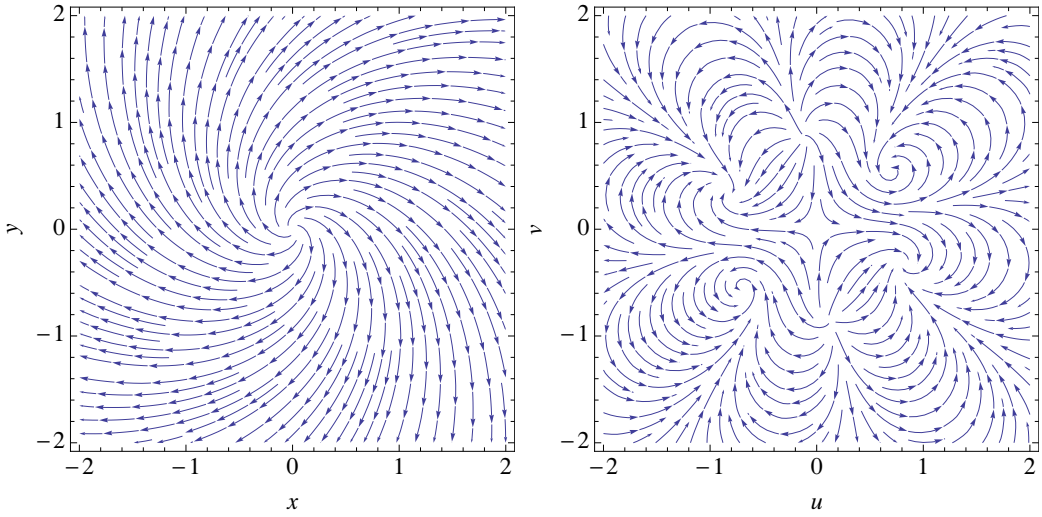

Figure 6. Classical flow diagrams in the Gaussian model with $\sigma = -1+i$ in the original formulation (left) and after the coordinate transformation $x = u^3$ (right).

A striking example is given by the Gaussian model, with the action

$$S = -\frac{1}{2}\sigma x^2, \qquad \sigma = a + ib, \tag{4.9}$$

which is well defined as long as $\mathrm{Re}\,\sigma = a > 0$. The origin is an attractive fixed point in this case. But for $a < 0$ not only does the integral become ill-defined, after complexification also the fixed point at the origin becomes repulsive, see figure 6 (left).

A simple transformation $x(u) = u^n$ (n odd) may remedy this situation, as shown in figure 6 (right) for $\sigma = -1 + i$ and $n = 3$: while the additional term in the drift, $J'(u)/J(u) = (n-1)/u$, yields a singularity at the origin, it also partly stabilizes the real axis, since

$$\tilde{\lambda}(u) = \sigma n(2n-1)u^{2(n-1)} + \frac{n-1}{u^2}, \tag{4.10}$$

and the second term is always positive. Most importantly, however, the change of variables leads to the appearance of stable fixed points in the complex plane. We find that a numerical solution of the CLE in u converges and yields for $\langle x^2\rangle = \langle u^6\rangle$

$$\langle x^2\rangle = \frac{1}{\sigma} = \frac{a+ib}{a^2+b^2}, \tag{4.11}$$

even for $a \leq 0$, see figure 7 (left). This answer is correct in the sense that it is the analytic continuation of the result valid for $a > 0$.

The same transformation also allows to evaluate the quartic 'Minkowski' integral [30, 31]

$$Z = \int_{-\infty}^{\infty} dx\, \exp\left(-\frac{i\lambda}{4!}x^4\right), \tag{4.12}$$

defined by analytic continuation, giving

$$\langle x^2\rangle = \frac{2\sqrt{3}}{\sqrt{\lambda}}\frac{\Gamma(\frac{3}{4})}{\Gamma(\frac{1}{4})}(1-i), \tag{4.13}$$

see figure 7 (right).

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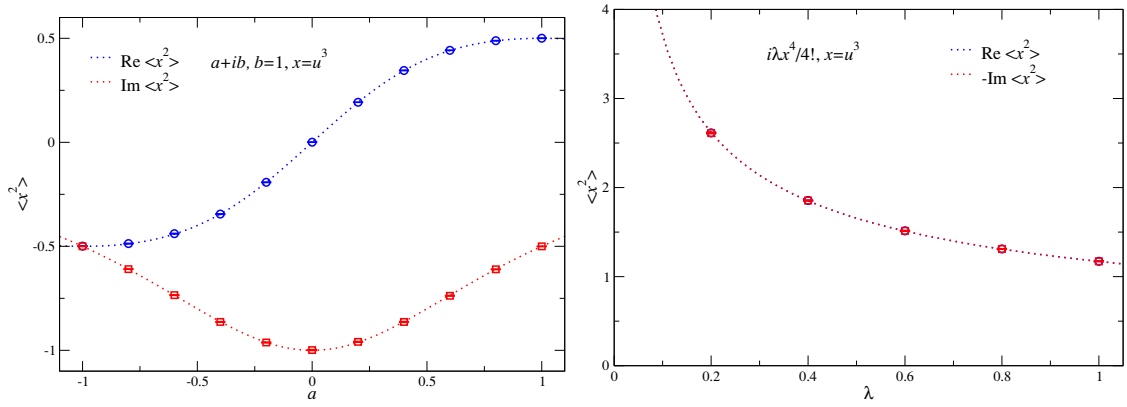

Figure 7. Complex Langevin results for the correlator $\langle x^2 \rangle$ in the Gaussian model with $\sigma = a+i$ as a function of a (left) and in the quartic model as a function of λ (right), both after the transformation $x = u^3$. The lines indicate the expected, analytically continued results.

As the third example, we take a more realistic case, encountered in the previous section, namely

$$Z = \int_{-\pi}^{\pi} dx\, e^{\beta \cos x} \qquad (\beta \in \mathbb{C}). \tag{4.14}$$

We would like to stabilize this by a variable transformation that casts the integral in the form of an SU(2)-like integral, see eq. (3.15). This can be achieved by the change of variables,

$$x(u) = u - \frac{1}{2}\sin(2u), \qquad -\pi < u < \pi, \tag{4.15}$$

since the Jacobian is

$$J(u) = \frac{dx(u)}{du} = 2\sin^2 u. \tag{4.16}$$

Simulations in the new formulation yield results shown in figure 8. The results are in line with the findings from above. For small $\beta = 0.3$ (left), the Jacobian indeed has a stabilizing effect and the exact results are reproduced. For larger $\beta = 1$ (right), the unstable contribution from the action takes over and exact results are only reproduced for $\gamma \sim 0, \pi$. In the three-dimensional XY model, a variable change along these lines gave only partial success, unfortunately.

We now want to show that these transformations are equivalent to the introduction of a kernel. The CLE with a kernel can be written as

$$\dot{z} = H^2(z)K(z) + 2H(z)H'(z) + H(z)\eta(t), \tag{4.17}$$

with $z = x + iy$ and a holomorphic function H (see refs. [27–29], where H^2 is called the kernel). Separating real and imaginary parts, eq. (4.17) becomes

$$\dot{x} = \hat{K}_x + \mathrm{Re}\, H\eta(t), \qquad \dot{y} = \hat{K}_y + \mathrm{Im}\, H\eta(t), \tag{4.18}$$

with

$$\hat{K} \equiv -H^2\nabla_z S + \nabla_z H^2, \qquad \hat{K}_x \equiv \mathrm{Re}\,\hat{K} \qquad \hat{K}_y \equiv \mathrm{Im}\,\hat{K}. \tag{4.19}$$

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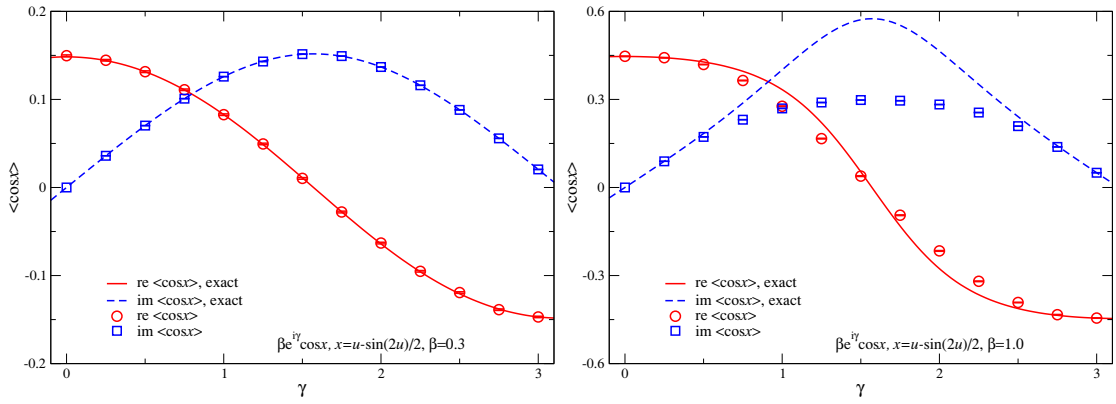

Figure 8. Complex Langevin results for the correlator $\langle \cos x \rangle$ in the U(1) model, with complex coupling $\beta e^{i\gamma}$ as a function of γ at $\beta = 0.3$ (left) and $\beta = 1.0$ (right), after the transformation $x = u - \frac{1}{2}\sin(2u)$.

Let us now change the description of the transformed process back to the original variables. This requires the use of Ito calculus and the chain rule; one obtains the process

$$\dot{z} = \left[-\frac{1}{(u')^2} S'(z) - \frac{2u''}{(u')^3} \right] + (u')^{-1} \eta(t), \tag{4.20}$$

This can be recognized as the original process modified by a kernel using $H = 1/u' = J$. The fact that H strictly speaking is not a holomorphic kernel because of its singularity at the origin is of no consequence in the cases discussed before, because the equilibrium distribution vanishes at this point.

The reduction of the SU(2) and SU(3) effective models to the Cartan subgroup discussed in section 3 is an example of singular variable transformation; the same is true about the relation between the N angle and the $(N-1)$ angle formalisms discussed there. In appendix A these issues are discussed in a more systematic way.

5 Conclusion

Complex Langevin dynamics can handle theories with a complex action, even when the sign problem is severe, but success is not guaranteed. In this paper we contrasted the apparent success in the three-dimensional SU(3) spin model, an effective model for QCD at nonzero chemical potential, with the observed failure in the three-dimensional XY model in the disordered phase, by constructing and analyzing effective one-link models.

We found that a crucial role is played by the presence of the nontrivial Haar measure in the nonabelian case. The contribution from the reduced Haar measure to the drift constrains the dynamics in the complexified field space: it is purely restoring and directed towards attractive fixed points on the real manifold. The presence of a singularity in the drift at the origin does not cause problems. On the other hand, the drift from the action yields repulsive fixed points, which can be located on or close to the real manifold and are responsible for large excursions in the complexified field space. As we have shown earlier,

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an uncontrolled exploration of the enlarged field space results in insufficient falloff of the equilibrium distribution, which causes the formal justification of the complex Langevin equation to break down and also leads to wrong results in practice.

In the nonabelian case, the contributions from the reduced Haar measure and action balance each other, resulting in a controlled Langevin process. We showed that the real manifold is stable against small complex fluctuations. This ensures analyticity of the observables in e.g. μ^2. By increasing the importance of the contribution from the action, the Langevin process can be made to break down. However, the parameter values in the effective one-link models for which this happens do not seem to be relevant for the three-dimensional SU(3) spin model. The results of this paper provide further justification for the conclusion drawn in ref. [14], in which complex Langevin was argued to be applicable in the entire phase diagram by carrying out a series of assessments, without relying on knowledge of the 'exact' result.

In the (abelian) XY model the Haar measure is trivial: hence there is no restoring component and the real manifold is unstable against small complex fluctuations. Since these fluctuations are introduced as soon as $\mu \neq 0$, simulations when $\mu \to 0$ and $\mu = 0$ do not agree. This is indeed what has been observed in the disordered phase of three-dimensional XY model and is now fully explained. Deep in the ordered phase, the theory becomes effectively real and there is no problem for complex Langevin dynamics.

The important lesson is that it is desirable for the real manifold to be stable against complex fluctuations in order for complex Langevin dynamics to work (even though strictly speaking it is neither sufficient nor necessary). This provides a useful benchmark to address, given that there is a wide range of options to modify the complex Langevin approach (some of them were discussed here). This is especially relevant for gauge theories, where the complexification leads to an extension from $\mathrm{SU}(N)$ to $\mathrm{SL}(N, \mathbb{C})$. Here it is possible to stabilize the real group manifold via gauge cooling, at least partly [26].

Acknowledgments

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A Generalizations of Langevin dynamics

In this appendix we investigate systematically possible generalizations of complex Langevin (CL) dynamics that are at least formally equivalent to the original one. For the formal equivalence (i.e. ignoring problems of slow falloff and possible boundary terms, see refs. [15,

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16]) it is sufficient to verify that the (complex) Fokker-Planck (FP) operator has $\exp(-S)$ as a zero mode. In refs. [15, 16] it is also explained how the equilibrium distribution of the real FP operator acting on functions of the complexified configuration space becomes, when evaluated on holomorphic observables, equivalent to that zero mode.

A.1 Nonuniqueness of measures for holomorphic observables

For simplicity we consider the 'flat' case of $\mathbb{R}^N$. The goal of the complex Langevin equation (CLE) is to find a probability measure on $\mathbb{C}^N$,

$$P(x,y)dxdy \qquad x,y \in \mathbb{R}^N, \tag{A.1}$$

which for holomorphic observables $\mathcal{O}$ is equivalent to a complex measure on $\mathbb{R}^N$,

$$\rho(x)dx, \tag{A.2}$$

in the sense that for all $\mathcal{O}$,

$$\int_{\mathbb{C}^N} dxdy\, P(x,y)\mathcal{O}(x+iy) = \int_{\mathbb{R}^N} dx\, \rho(x)\mathcal{O}(x). \tag{A.3}$$

The question of the existence of such a measure P was already discussed by Weingarten [32], but here we are interested in the nonuniqueness.

Clearly P is not uniquely determined by the requirement (A.3). First one has to recognize that a precise answer to this nonuniqueness depends on specifying the space of holomorphic observables for which eq. (A.3) is supposed to hold. We consider spaces $\mathcal{H}_f$ defined in terms of some growth condition

$$\sup \sigma(x,y)|\mathcal{O}(x,y)| < C < \infty, \tag{A.4}$$

for some positive weight function σ. Examples for f are $f = \exp((x^2+y^2)^\alpha)$, with $x^2 = x_1^2 + \ldots x_N^2$, etc.

Obviously P_1 and P_2 are equivalent in the sense above if and only if for all $\mathcal{O} \in \mathcal{H}_f$ $Q \equiv P_1 - P_2$ satifies

$$\int_{\mathbb{C}^N} dxdy\, Q(x,y)\mathcal{O}(x+iy) = 0. \tag{A.5}$$

In other words, Q has to be orthogonal to the intersections of the kernels of the Cauchy-Riemann operators

$$C_j \equiv \partial_{x_j} + i\partial_{y_j}. \tag{A.6}$$

Ignoring possible convergence problems or boundary terms, eq. (A.5) seems to say only that $Qdxdy$ is a signed measure satisfying

$$Q(x,y) = \sum_{j=1}^{N} C_j H_j(x,y), \tag{A.7}$$

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where the H_j are some complex-valued functions (of bounded variation), because rolling the CR operators C_j over to act on the observables would yield zero. Those conditions are satified if there are real functions $G_j(x, y)$ satisfying

$$Q(x, y) = \sum_{j=1}^{N} \Delta_j G_j(x, y) \tag{A.8}$$

with $\Delta_j = \partial_{x_j}^2 + \partial_{y_j}^2$.

The convergence problems have to be taken seriously; we are only sure that they are absent if $Q\mathcal{O}$ is absolutely integrable. Depending on the class of holomorphic observables chosen, one has to demand corresponding decay properties of the G_j.

To make use of eq. (A.7) for a cure of convergence to the wrong limit, one would need to do the following: first find a Q that is such that it improves the decay of $P + Q$ at infinity (this is of course only possible if Q shows that same rate of decay as P), then find a modified CL process having $P + Q$ as its equilibrium measure.

A.2 Neutral modification of the CL process

Next we ask how one can modify the CL process without changing the evolution of holomorphic observables under the Langevin evolution; we call this a neutral modification. If the Langevin operator is given by

$$L = [\nabla_x + K_x]\nabla_x + K_y \nabla_y, \tag{A.9}$$

we want to see if we can replace it by an operator of the general form

$$L' \equiv L + \sum_j F_j(x, y)^2 \partial_{x_j}^2 + \sum_j G_j(x, y)^2 \partial_{y_j}^2 + R_x \cdot \nabla_x + R_y \cdot \nabla_y, \tag{A.10}$$

with coefficient functions F_j, G_j, R_x, R_y $(F, G \geq 0)$ in such a way that when applied to holomorphic observables $\mathcal{O}$, L' becomes equal to L, because $\partial_{y_j}\mathcal{O} = i\partial_{x_j}\mathcal{O}$ $(j = 1, \ldots N)$.

It is not hard to see that this requires (1) $G_j^2 = F_j^2$ $(j = 1, \ldots N)$; (2) $R_x = R_y = 0$. So the modifying operator is of the form

$$L_m = \sum_j F_j^2 (\partial_{x_j}^2 + \partial_{y_j}^2), \tag{A.11}$$

corresponding to the modified CL process

$$\dot{x}_j = K_{x_j} + \sqrt{1 + F_j^2}\, \eta_j(t), \qquad \dot{y}_j = K_{y_j} + F_j\, \eta_j(t). \tag{A.12}$$

A well-known special case arises by choosing

$$F_j(x, y) = N_I, \quad j = 1, \ldots N, \tag{A.13}$$

which we refer to as 'complex diffusion'. Here we have discovered a generalization: 'configuration-dependent complex diffusion'. But it is not clear how much this can help in solving the problems of the CLE, in view of the fact that it was found that introducing 'imaginary diffusion' (or complex noise) actually tends to create problems by leading to slow decay in the imaginary directions and convergence to the wrong limit [15, 16]. So F_j should at least be chosen in such a way that it vanishes sufficiently fast for $|y_j| \to \infty$, $y = 1, \ldots, N$.

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A.3 Nonneutral modifications of the CLE: holomorphic (matrix) kernels

A way of modifying the CL process that was discussed already in the 1980s is the introduction of a so-called kernel [27–29]. It is nonneutral in the sense that it does not preserve the Langevin evolution of holomorphic observables (but is supposed to preserve the long-time averages of holomorphic observables). For one dimension it amounts to the following:

Let H be holomorphic on $\mathbb{C}$ (H corresponds to what is called $\sqrt{K}$ in the older literature). We denote

$$\operatorname{Re} H \equiv R, \qquad \operatorname{Im} H \equiv I. \tag{A.14}$$

The corresponding CLE becomes

$$\dot{x} = \hat{K}_x + R\eta(t), \qquad \dot{y} = \hat{K}_y + I\eta(t), \tag{A.15}$$

where

$$\hat{K} \equiv -H^2 S' + 2HH', \qquad \hat{K}_x \equiv \operatorname{Re} \hat{K}, \qquad \hat{K}_y \equiv \operatorname{Im} \hat{K}. \tag{A.16}$$

It is easy to find choices for the kernel that eliminate the drift force altogether or change its sign, but the resulting process suffer from steeply rising diffusion coefficients and dubious stability.

A special case that does not suffer from these problems is a constant (complex) kernel H, with $\operatorname{Re} H^2 > 0$. In this case the kernel just amounts to multiplying the time coordinate by a factor H^2 and there are no consistency problems. This simple device has been shown to improve the situation in certain cases with quadratic action in refs. [28, 29]; the stabilization occurring there is actually equivalent to the one discussed in section 4.

For more than one variable there is a more general way of introducing kernels which we call matrix kernels. In short, take a holomorphic $H_{jk}(x_1 + iy_1, \cdots, x_n + iy_n)$, then

$$\dot{x}_j = \hat{K}_{x,j} + \operatorname{Re} \sum_k H_{jk}\eta_k(t), \qquad \dot{y}_j = \hat{K}_{y,j} + \operatorname{Im} \sum_k H_{jk}\eta_k(t),$$

where

$$\begin{aligned} \hat{K}_j &\equiv \sum_k \left\{ -(H^T H)_{kj}(\nabla_{z_k} S) + \nabla_{z_k}(H^T H)_{jk} \right\}, \\ \hat{K}_{x,j} &\equiv \operatorname{Re} \hat{K}_j, \qquad \hat{K}_{y,j} \equiv \operatorname{Im} \hat{K}_j. \end{aligned} \tag{A.17}$$

To see that this is (formally) correct, note that the complex Fokker-Planck operator is

$$L_H^T = \sum_{k,j} \left\{ \nabla_j (H^T H)_{kj} \left[\nabla_k + (\nabla_k S) \right] \right\}. \tag{A.18}$$

It is manifest that $\exp(-S)$ is a (hopefully unique) zero mode of L^T.

We remark that we can actually combine the two previous modifications (kernel and imaginary diffusion). For simplicity we only describe the case of one dimension: let again H be a holomorphic function and F a real valued function on $\mathcal{M}_c$. Then the modified Langevin operator

$$L_H = \left((R^2 + F^2)\nabla_x + \hat{K}_x \right) \nabla_x + \left((I^2 + F^2)\nabla_y + \hat{K}_y \right) \nabla_y + 2RI \nabla_x \nabla_y \tag{A.19}$$

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reduces on holomorphic observables to

$$\tilde{L}_{H,F} = H^2\Delta_z + \hat{K}\nabla_z, \tag{A.20}$$

as before.

We have to find a process corresponding to these operators. This problem does not have a unique solution, but the following stochastic differential equation turns out to give the right $L_{H,F}$:

$$\begin{aligned}\dot{x} &= \hat{K}_x + \frac{R\sqrt{R^2+I^2+F^2}}{\sqrt{R^2+I^2}}\eta_1(t) - \frac{FI}{\sqrt{R^2+I^2}}\eta_2(t),\\ \dot{y} &= \hat{K}_y + \frac{I\sqrt{R^2+I^2+F^2}}{\sqrt{R^2+I^2}}\eta_1(t) + \frac{FR}{\sqrt{R^2+I^2}}\eta_2(t)\,,\end{aligned} \tag{A.21}$$

where η_1, η_2 are two independent white noises. Note that these equations reduce to the previous ones for the special case $F = 0$; for $F = N_I$ and $R = 1$, $I = 0$ one recovers the standard complex noise.

A.4 Nonneutral modifications of the CLE: coordinate transformations

As remarked in section 4, coordinate transformations are closely related to kernels. In fact they lead to a subset of the general matrix kernels discussed above, but since they are sometimes easier to handle we discuss them in some detail. To avoid heavy notation, we treat real actions and comment about the complex case in subsection A.4.6.

A.4.1 General remarks on coordinate transformations

As stated in section 4, we have to distinguish two types of coordinate transformations:

(I) Transforming the descriptions of the trajectories;

(II) Transforming the functional integral.

Choice (I) does not change the process, only its description, but choice (II) is nontrivial. The difference can be seen clearly in a simple linear one-dimensional example: let

$$u = ax \ (a \neq 0) \tag{A.22}$$

and consider the real Langevin process corresponding to the action $S(x) = S(u/a) \equiv T(u)$:

$$\dot{x} = -S'(x) + \eta(t). \tag{A.23}$$

Then (I) means

$$\text{(I)}: \quad \dot{u} = -a^2T'(u) + a\eta(t), \tag{A.24}$$

whereas (II) means replacing the measure proportional to $\exp(-S(x))dx$ by the transformed one proportional to $\exp(-T(u))du$ and setting up a Langevin process that has the transformed measure as its equilibrium measure. We find

$$\text{(II)}: \quad \dot{u} = -T'(u) + \eta(t). \tag{A.25}$$

So in this simple example the difference between (I) and (II) is just a different time scale.

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A.4.2 Nonsingular (invertible) linear transformations

We now consider a less trivial case of a Langevin process in $\mathbb{R}^N$, using vector notation:

$$\dot{x} = -\nabla S(x) + \eta(t), \tag{A.26}$$

and the transformation by a nonsingular matrix A

$$u = A\,x, \qquad T(u) \equiv S(A^{-1}\,u). \tag{A.27}$$

Scheme (I) yields, simply by acting with A on both sides of the LE,

$$\dot{u} = -A\nabla_x S(x) + Ad\eta \quad \text{for} \quad u = A\,x. \tag{A.28}$$

To re-express the drift in terms of $T(u)$, we use the chain rule

$$\nabla_x T(Ax) = A^T \nabla_u T(u) \quad \text{for} \quad u = A\,x, \tag{A.29}$$

which leads to

$$\text{(I)}: \quad \dot{u} = -AA^T \nabla T(u) + A\eta(t), \tag{A.30}$$

whereas (II) gives

$$\text{(II)}: \quad \dot{u} = -\nabla T(u) + \eta(t). \tag{A.31}$$

The two processes now no longer differ just by different times scales. It is also instructive to compare the Fokker-Planck operators for the two processes. In matrix notation

$$\text{(I)}: \quad L^T = \nabla AA^T(\nabla + (\nabla T)) \tag{A.32}$$

and

$$\text{(II)}: \quad L^T = \nabla(\nabla + (\nabla T)). \tag{A.33}$$

It obvious that both operators have the same equilibrium solution. The transition from scheme (II) to scheme (I) can be viewed as the introduction of a constant 'matrix kernel' A; in this sense it is more general than the standard introduction of scalar kernels.

A.4.3 Singular (noninvertible) linear transformations

If the action has a certain symmetry, noninvertible linear transformations can be used to reduce the number of variables to a subset; conversely one can use them to introduce a redundant set of variables, which is sometimes useful.

Here we show explicitly how this can be used to justify the process on the Cartan subgroup of SU(N), using N instead of $N-1$ angles, as discussed in section 3.2. We have to consider singular linear transformations A that map $\mathbb{R}^N$ into a lower dimensional space $\mathbb{R}^M$ (with $M < N$):

$$u = A\,x. \tag{A.34}$$

A has a null space $V_o \subset \mathbb{R}^N$ and an orthogonal complement $V_\perp$. We assume that the action is invariant under shifts in the V_0 directions, i.e.

$$S(x+u) = S(x) \quad \text{whenever} \quad u \in V_0. \tag{A.35}$$

Then the drift ∇S will leave $V_\perp$ invariant.

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Specializing now to the case of SU(3) and going from the 3 angle to the 2 angle formulation, we may think of factorizing A as

$$A = QB, \tag{A.36}$$

where B is a singular symmetric $N \times N$ matrix annihilating V_0 and mapping $V_\perp$ onto itself. Q is then a one to one mapping of V_0 onto $\mathbb{R}^M$.

In the case of eq. (3.10), with x resp. u in eq. (A.34) denoted with z resp. ϕ in section 3.2, B maps the z's onto the subspace with $\phi_1 + \phi_2 + \phi_3 = 0$ in terms of the 3 angles ϕ_1, ϕ_2, ϕ_3, so we have

$$B = \frac{1}{3}\begin{pmatrix} 2 & -1 & -1 \\ -1 & 2 & -1 \\ -1 & -1 & 2 \end{pmatrix}, \tag{A.37}$$

and Q maps onto the two independent angles ϕ_1, ϕ_2, i.e.

$$Q = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}, \tag{A.38}$$

so finally

$$A = QB = \frac{1}{3}\begin{pmatrix} 2 & -1 & -1 \\ -1 & 2 & -1 \end{pmatrix}. \tag{A.39}$$

The LE for the variables $x \in \mathbb{R}^N$ is

$$\dot{x} = -\nabla S(x) + \eta(t)\,, \tag{A.40}$$

where η consists of N independent white noises, hence does *not* leave the subspace V_0 invariant. The remainder of the analysis is almost identical to the one for nonsingular A: the LE for $u = A\,x$ (scheme (I)) can at first be written as

$$\dot{u} = -A\nabla_x S(x) + A\eta(t)\,, \tag{A.41}$$

but we have to re-express the drift $-\nabla S(x)$ in terms of the transformed variables u. First we define

$$T(u) \equiv S(x) \quad \text{whenever} \quad u = A\,x, \tag{A.42}$$

which is well defined because of the invariance of $S(x)$. By the chain rule again

$$\nabla_x T(A\,x) = A^T \nabla_u T(u), \tag{A.43}$$

so the LE for u becomes

$$\text{(I)}: \quad \dot{u} = -AA^T \nabla_u T(u) + A\eta(t)\,. \tag{A.44}$$

In scheme (II), on the other hand, the LE for u is simply

$$\text{(II)}: \quad \dot{u} = \nabla_u T(u) + \eta(t)\,, \tag{A.45}$$

where $\eta(t)$ consists now of M independent white noises. To see to which extent the two schemes are equivalent, let us look at the corresponding FP operators:

$$(\mathrm{I}): \quad L_{\mathrm{I}}^T = \nabla_u^T A A^T (\nabla_u + (\nabla_u T)) \tag{A.46}$$

and

$$(\mathrm{II}): \quad L_{\mathrm{II}}^T = \nabla_u (\nabla_u + (\nabla_u T)) \,. \tag{A.47}$$

Again it is obvious that both schemes lead again to the same equilibrium measures, but clearly the processes are quite different.

A.4.4 Invertible nonlinear coordinate transformations

The treatment of nonlinear coordinate transformations is quite similar to the linear case, except that one has to use Ito's calculus (see for instance ref. [33]) in some places. Again we have to consider both schemes (I) and (II). We first consider invertible transformations of $\mathbb{R}^N$ and comment in the next subsection about singular (noninvertible) ones.

Let $f : \mathbb{R}^N \to \mathbb{R}^N$ be an invertible and continuously differentiable coordinate transformation. If (in vector notation)

$$u = f(x) \tag{A.48}$$

and $x(t)$ evolves according to the Langevin equation

$$\dot{x} = -\nabla S(x) + \eta(t), \tag{A.49}$$

we define again

$$T(u) \equiv S(f^{-1}(u)). \tag{A.50}$$

Then by the Ito calculus, u evolves according to the LE

$$\dot{u}_i = -\sum_j \left\{ \left[\frac{\partial u_i}{\partial x_j} \frac{\partial S}{\partial x_j} + \Delta_x u_j \right] + \frac{\partial u_i}{\partial x_j} \eta_j(t) \right\}. \tag{A.51}$$

To express this LE in terms of u and $T(u)$ we again use the chain rule

$$\frac{\partial S(u)}{\partial x_j} = \sum_r \frac{\partial u_r}{\partial x_j} \frac{\partial T(u(x))}{\partial u_r}. \tag{A.52}$$

If we define the matrix A by

$$A_{ij} = \frac{\partial u_i}{\partial x_j}, \tag{A.53}$$

the LE for u becomes in matrix notation

$$(\mathrm{I}): \quad \dot{u} = -A A^T \nabla_u T(u) + \Delta_x u + A\eta(t), \tag{A.54}$$

which clearly reduces to eq. (A.44) in the linear case.

In scheme (II) the transformation of the functional integral involves the Jacobian

$$J = \frac{\partial(x)}{\partial(u)} = \det A^{-1}, \tag{A.55}$$

so the action $T(u)$ receives an extra term

$$T_J \equiv -\ln J = \ln \det A. \tag{A.56}$$

With

$$T_{\rm eff} \equiv T + T_J = T + \ln \det A, \tag{A.57}$$

we get the Langevin equation for scheme (II)

$$\text{(II)}: \quad \dot{u} = -\nabla_u T_{\rm eff}(u) + \eta(t)\,, \tag{A.58}$$

with the $\eta(t)$ denoting again N independent white noises.

To see that the two schemes are equivalent as far as their equilibrium measures are concerned, we again compare the Langevin and FP operators of the two schemes. We first note a general fact (see for instance ref. [33]): if

$$\dot{x} = K(x) + A(x)\eta(t), \tag{A.59}$$

then by the Ito calculus

$$L = \sum_{i,k} (AA^T)_{ik}(x)\partial_i\partial_k + K(x)\cdot\nabla \tag{A.60}$$

and

$$L^T = \sum_{i,k} \partial_i\partial_k (AA^T)_{ik}(x) - \nabla\cdot K(x). \tag{A.61}$$

Applying this to our two Langevin equations above we find for scheme (I)

$$\text{(I)}: \quad L_I^T = \sum_{i,k} \frac{\partial}{\partial u_i}\frac{\partial}{\partial u_k}(AA^T)_{ik} - \sum_i \frac{\partial}{\partial u_i}\Delta_x u_i + \sum_{i,k}\frac{\partial}{\partial u_i}(AA^T)_{ik}\frac{\partial T}{\partial u_k} \tag{A.62}$$

and for scheme (II)

$$\text{(II)}: \quad L_{\rm II}^T = \nabla_u^T\left[\nabla_u + (\nabla_u T_{\rm eff}(u))\right]. \tag{A.63}$$

We claim that the FP operator in scheme (I) can be rewritten as

$$\text{(I)}: \quad L_{\rm I}^T = \nabla_u^T AA^T\left[\nabla_u + ([\nabla_u T_{\rm eff}(u))\right], \tag{A.64}$$

again making the equivalence of the two schemes obvious. To prove our claim we only have to show that

$$\sum_k (AA^T)_{ik}\frac{\partial}{\partial u_k}\ln\det A = -\Delta_x u_i + \sum_k \frac{\partial}{\partial u_k}(AA^T)_{ik}; \tag{A.65}$$

this follows again using the chain rule:

$$\sum_k \frac{\partial}{\partial u_k}(AA^T)_{ik} = \sum_{k,l,r}\frac{\partial x_l}{\partial u_k}\frac{\partial}{\partial x_l}\left(\frac{\partial u_i}{\partial x_r}\frac{\partial u_k}{\partial x_r}\right). \tag{A.66}$$

The last expression is equal to

$$\sum_{k,l,r}\left\{\frac{\partial x_l}{\partial u_k}\frac{\partial^2 u_i}{\partial x_l\partial x_r}\frac{\partial u_k}{\partial x_r} + \frac{\partial x_l}{\partial u_k}\frac{\partial u_i}{\partial x_r}\frac{\partial^2 u_k}{\partial x_l\partial x_r}\right\}; \tag{A.67}$$

here the first term simplifies to $\Delta_x u_i$, whereas the second term equals

$$\sum_k (AA^T)_{ik} \frac{\partial}{\partial u_i} \ln \det A, \tag{A.68}$$

so eq. (A.65) is correct.

As in the linear case the transition from scheme (II) to scheme (I) can be viewed as the introduction of a 'matrix kernel' A (see eq. (A.53)), which is a generalization of the standard introduction of scalar kernels. Again we can transform scheme (II) back to the original coordinates using scheme (I) and obtain a process with a matrix kernel A^{-1}.

But note that the matrix kernels obtained here are not as general as before, since the matrix $A^{-1}_{ij} = \partial x_i / \partial u_j$ has to satisfy an integrability condition, which was not required of the matrix H in section A.3.

A.4.5 Singular (noninvertible) nonlinear transformations

As in the case of singular linear transformations, in this case we have to require some additional symmetries of the action. A simple example is the action

$$S = -\beta \operatorname{tr} U, \tag{A.69}$$

with U an element of SU(N). The symmetry in question is the invariance of S under similarity transformations

$$U \mapsto V^{-1} U V, \tag{A.70}$$

which allows the transition to the Cartan subgroup of SU(N). The map from the $N^2 - 1$ parameters of SU(N) to the $N - 1$ Cartan angles is clearly a singular noninvertible transformation.

More generally, in a lattice gauge model gauge invariance allows to reduce the process to one remaining in a lower-dimensional gauge-fixed configuration space.

A.4.6 Remark on complex actions

If $S(x)$ is complex, at least on the formal level (ignoring possible problems with boundary terms under integration by parts) everything goes through as before.

The formal proof of correctness given in refs. [15, 16] only uses the fact that the complex FP operator annihilates the complex measure $\exp(-S)dx$. This is manifestly the case for the most general case of a holomorphic matrix kernel, see eq. (A.18).

Here in principle we have to limit ourselves to transformations that are bi-holomorphic maps from $z = x + iy$ to $w = u + iv$. In practice it seems that this restriction is too severe and certain singularities can be tolerated — provided we are lucky and the equilibrium density vanishes at those points. The formal proof of equivalence again only uses the equivalence of the complex Fokker-Planck operators — the Langevin evolutions in the 0 space are again different in the two schemes.

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