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Spurious solutions of the complex Langevin equation ☆

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The origin of the wrong equilibrium solutions of the complex Langevin equation is analyzed. We find that the Fokker–Planck equation allows in general for several equilibrium solutions in the space of distributions. They are induced by the zeros of the probability density in the complex plane. We show that a kernel allows sometimes to choose among the different distributions or can itself introduce new spurious solutions.

1. Introduction

The use of the Langevin equation to simulate complex probabilities [1,2], although very promising, has been successful in practice in only a few cases [3,4]. This is due to two kinds of problems: instabilities in the random walk and convergence to the wrong equilibrium solution [4–7]. An extreme example of the latter would be the segregation theorem for a real but non-positive definite probability: the random walk gets trapped in a positive or a negative probability region [8]. In very particular cases this problem can be circumvented, as was done in ref. [9] in a simple model for SU(2) lattice gauge theory, if only a restricted set of observables is considered.

A more general method to attack both problems is the use of a kernel in the stochastic differential equation [10,11]. Some progress has recently been made in this direction in refs. [11,12]. In this paper we will analyze the nature of the stable spurious solutions of a complex Langevin equation and its relation to the structure of the probability function in the complex plane.

Let us review the justification of the complex Langevin algorithm [10,5]. Let $P(x)$ be the D-dimensional complex probability distribution to be sampled and $P(z)$ its analytical extension in the complex plane, and let us consider the following random walk in $\mathbb{C}^D$:

$$dz^i = P^{-1}\frac{\partial}{\partial z^j}(G^{ij}P)dt + V^i_\alpha\, d\eta_\alpha\,,\qquad i=1,\dots,D\,, \tag{1}$$

where $d\eta_\alpha$, $\alpha=1,\dots,N$ are real random variables normalized to $\langle d\eta_\alpha\, d\eta_\beta\rangle = 2\, dt\, \delta_{\alpha\beta}$, $V^i_\alpha(z)$ are a set of analytical but otherwise arbitrary functions and $G^{ij}(z)=V^i_\alpha(z)V^j_\alpha(z)$ is the so-called kernel of the Langevin equation. The standard Langevin equation corresponds to $V^i_\alpha=\delta_{i\alpha}$. The real and positive probability distribution of $z(t)$ in the complex plane $\mathbb{C}^D$, $p(z,z^*,t)$ satisfies the following Fokker–Planck evolution equation [13]:

$$\frac{\partial p}{\partial t} = \left(-H_{\rm FP} - H^*_{\rm FP} + 2\frac{\partial}{\partial z^i}\frac{\partial}{\partial z^{*j}} V^i_\alpha V^{*j}_\alpha\right)p\,, \tag{2}$$

where $H_{\rm FP} = -(\partial/\partial z^i)G^{ij}P(\partial/\partial z^j)P^{-1}$ is the Fokker–Planck operator and $\partial/\partial z^i$, $\partial/\partial z^{*i}$ act as derivative operators on everything to its right, including p. One can then define an analytical projection of p on the real axis by

$$(K_{\rm R}\,p)(x) = Q(x) = \int d^D y \exp\left(-iy^j\frac{\partial}{\partial x^j}\right)p(x,y) \tag{3}$$

(note that here p is expressed as a function of x, y instead of z, z^*), so that

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$$\langle f(z)\rangle_p = \int \mathrm{d}^D x\, \mathrm{d}^D y\, p(x,y) f(z)$$
$$= \int \mathrm{d}^D x\, Q(x) f(x)$$
$$= \langle f(x)\rangle_Q \tag{4}$$

for an analytical function f, and p such that integration by parts is allowed. By construction the projection operator is linear and satisfies (here $g(z)$ is an analytical function acting as a multiplicative operator)

$$K_R g(z) = g(x) K_R ,$$
$$K_R \frac{\partial}{\partial z^i} = \frac{\partial}{\partial x^i} K_R , \quad K_R \frac{\partial}{\partial z^{*i}} = 0 . \tag{5}$$

Therefore, by applying K_R on both sides of the evolution equation one finds

$$H_{FP}(x) Q(x,t) = \frac{\partial Q(x,t)}{\partial t} . \tag{6}$$

When $p(x, y)$ is an equilibrium distribution of the random walk, so is $Q(x)$, i.e.

$$\frac{\partial}{\partial x^i} G^{ij}(x) P(x) \frac{\partial}{\partial x^j} P^{-1}(x) Q(x) = 0 , \tag{7}$$

which admits the solution $Q(x) = P(x)$ as expected. Therefore, as long as there is an equilibrium distribution $p(x, y)$ and $Q(x) = P(x)$ is the only normalizable solution of eq. (7), the Langevin algorithm will correctly sample the complex probability $P(x)$. In practice one can find that for a given problem the random walk is not stable and thus there is no equilibrium distribution $p(x, y)$. Sometimes this can be fixed by choosing the kernel properly [11]. Assuming that the random walk is stable, still one can find that it converges to the wrong solution. This must be related to the existence of other solutions of the equilibrium equation (7). It is important to realize that one must allow for solutions in the space of distributions and not only of ordinary functions. Let us clarify this point with an example. Consider the one-dimensional real probability distribution $P(x) = xP_0(x)$, $P_0(x)$ positive and normalizable, and $G(x) = 1$. In this case eq. (7) admits two linearly independent normalizable solutions $Q_\pm(x) = \pm\theta(\pm x) \times P(x)$ and the standard Langevin algorithm will produce a sampling of one of both distributions, which is depending on the initial conditions, in agreement with the segregation theorem. Now if we consider the same problem but shifted to the complex plane, $P(x) = (x - ia) P_0(x - ia)$, $a \in \mathbb{R}$, again there will be two independent normalizable solutions, formally given by $Q_\pm(x - ia)$, that is

$$\langle f(x)\rangle_\pm = \int_{\Gamma_\pm} \mathrm{d}z\, f(z) P(z) , \quad \Gamma_\pm = R^\pm + ia , \tag{8}$$

and the random walk will concentrate on Γ_+ or Γ_-. This is so even if in the shifted case eq. (7) has no singular points in $\mathbb{R}$ and therefore admits only one normalizable solution in the space of ordinary functions, namely $Q(x) = P(x)$.

We can generalize the above considerations and define a distribution $P_\Gamma(x)$ on the real axis associated to $P(z)$ and a path Γ by

$$\int \mathrm{d}^D x\, P_\Gamma(x) f(x) = \int_\Gamma \mathrm{d}^D z\, P(z) f(z) . \tag{9}$$

Actually P_Γ depends on Γ only through the equivalence class of paths obtained by deforming Γ without crossing singularities of $P(z)$ and keeping the boundary fixed. In the space of distributions P_Γ is a solution of $H_{FP}(x) P_\Gamma(x) = 0$ if and only if $\langle H_{FP}^T(x) \times f(x)\rangle_{P_\Gamma} = 0$ for an arbitrary test function $f(x)$, where H_{FP}^T is the transposed operator of H_{FP}. Therefore eq. (7) is equivalent to

$$0 = \int \mathrm{d}^D x\, P_\Gamma(x) H_{FP}^T f(x)$$
$$= -\int_\Gamma \mathrm{d}^D z\, P(z) P^{-1}(z) \frac{\partial}{\partial z^j} G^{ij}(z) P(z) \frac{\partial}{\partial z^i} f(z)$$
$$= -\int_{\partial\Gamma} \mathrm{d}^{D-1} S_j G^{ij}(z) P(z) \frac{\partial f(z)}{\partial z^i} , \tag{10}$$

$\mathrm{d}S$ being the surface element of the boundary of Γ. This is guaranteed if $P(z) = 0$ on $\partial\Gamma$, that is, if Γ connects zeros of $P(z)$ in the complex plane. In the example above $\Gamma_\pm$ connected the zero at $z = ia$ with that at $z = \pm\infty$. We conjecture that the general solution of the equilibrium equation will be a linear combination of pathlike solutions, i.e.

$$Q(x) = \sum_{\Gamma, P(\partial\Gamma)=0} a_\Gamma P_\Gamma(x) , \tag{11}$$

where the coefficients a_Γ will depend on the kernel chosen and perhaps on the initial conditions.

Let us illustrate the point with a one-dimensional example, $P(x)=\exp(-Ax^n/n)$, analyzed in ref. [11]. Its analytical extension $P(z)$ vanishes at infinity in n different regions. For $n=2$ there are just two zeros and essentially only one nontrivial path connecting them, therefore either the standard Langevin procedure reproduces the correct distribution on the real axis or else it is unstable, depending on A. It can always be made stable by properly choosing the kernel [11]. For n even and greater than 2, $\langle x^2\rangle = c_n A^{2/n}$ is a multivalued function of A. The various branches can be reproduced by suitable constant kernels corresponding to integrals along straight lines connecting diametrically opposed zeros of $P(z)$.

2. Kernel and coordinate transformations

In some cases it may be useful to view a path Γ in the complex plane z as the image of the real axis of a new complex plane w related to z by an analytical change of variable. Hence it will be interesting to study the properties of the Langevin equation under a coordinate transformation.

Let it be a real n-dimensional Langevin equation sampling $P(x)$,

$$dx^i = P^{-1}(x)\frac{\partial}{\partial x^j}(G^{ij}(x)P(x))dt + V^i_\alpha\, d\eta_\alpha\,, \qquad (12)$$

again with $G^{ij}=V^i_\alpha V^j_\alpha$ and $\langle d\eta_\alpha\, d\eta_\beta\rangle = 2\, dt\, \delta_{\alpha\beta}$. In order to write the stochastic differential equation in a new coordinate system $x'^i=f^i(x)$ one should Taylor expand dx'^i in terms of dx^j through second order to retain the terms of $O(dt)$ coming from $dx^j\, dx^k = V^j_\alpha V^k_\beta\, d\eta_\alpha d\eta_\beta + O(dt^2) = 2G^{jk}(x)dt + O(dt^{3/2})$. In this way one can check that the equation transforms covariantly with

$$P'(x)=J^{-1}(x)P(x)\,, \quad J(x)=\det\left(\frac{\partial x'^i}{\partial x^j}\right),$$

$$V'^i_\alpha(x)=\frac{\partial x'^i}{\partial x^j}V^j_\alpha(x)\,, \qquad (13)$$

$$G'^{ij}(x)=\frac{\partial x'^i}{\partial x^k}\frac{\partial x'^j}{\partial x^l}G^{kl}=V'^i_\alpha(x)V'^j_\alpha(x)\,, \qquad (13\text{ cont'd})$$

as can be seen by using the identity $\partial\log J/\partial x^i = (\partial x^j/\partial x'^k)(\partial^2 x'^k/\partial x^i\partial x^j)$. Therefore the kernel $G^{ij}(x)$ transforms as the contravariant component of a metric tensor with euclidean signature and V^i_α as a "tretad" field [14]. The same goes for the D-dimensional complex case which can be reduced to a $2D$-dimensional real problem where pairs of coordinates (x^j, y^j) transform as the real and imaginary part of complex variables under an analytical transformation. The corresponding equations can then be written as D equations for $z^j=x^j+iy^j$ and their complex conjugate, if G^{ij}, V^i_α and P are analytical functions as well.

If the associated Riemann–Christoffel curvature tensor vanishes everywhere there exists (at least locally) a coordinate system with $V^i_\alpha=\delta_{i\alpha}$, $G^{ij}=\delta_{ij}$, which gives the standard (i.e. unkernelled) Langevin equation. This is always the case in one dimension. From now on we will restrict ourselves to the one-dimensional case as it is simpler and nontrivial. Thus given a stochastic equation of the form (1) for the variable z, there is a new variable w such that $z(w)$ is analytical and

$$dw=\frac{d\log P_w(w)}{dw}dt+d\eta\,, \quad P_w(w)=\frac{dz}{dw}P(z) \qquad (14)$$

(up to finite dt corrections), with $G(z)=V^2(z)=(dz/dw)^2$. This observation can be useful in order to construct kernels to pick up particular solutions of the Langevin equation. For instance, considering again $P(x)=\exp(-Ax^n/n)$ for $n=4$, and $A>0$, the distribution P_Γ associated to the imaginary axis is obtained with $z=iw$ and eq. (14) or equivalently with eq. (1) and $G(z)=-1$, $V(z)=i$ [11]. A less trivial example is $A>0$ and $n=3$. In this case $P(z)$ vanishes at $z_k=R\hat{z}_k$, $\hat{z}_k=e^{i2\pi k/3}$, $k=0$, 1, 2, and $R\to+\infty$. One can try to sample P_Γ for Γ connecting z_i and z_j, $(i\neq j)$ by means of the path $z(w)=\hat{z}_i e^w+\hat{z}_j e^{-w}$, $w\in\mathbb{R}$, i.e. $G(z)=z^2-4\hat{z}_i\hat{z}_j$. Numerically we have checked this for $A=1$, $i=0$, $j=1$, with $dt=0.01$, $t=300$, $z(0)=1$, obtaining $\langle z\rangle = (0.35\pm0.02,\ 0.63\pm0.02)$ to be compared with the exact value (0.36, 0.63). The sampling points fall nearby Γ.

In the example just considered $P(x)$ was real on the real axis but not normalizable, nevertheless it could be given a meaning by going into the complex plane. The corresponding distribution is not real but one can take $Q(x)=\mathrm{Re}\,P_\Gamma(x)$, which is also of the form (11). This prescription gives a well-defined meaning to the corresponding bottomless action, although not in a unique way. For instance, $P_{\Gamma'}$, with Γ' connecting z_1 and z_2, is also real.

3. Solutions associated to zeros of $P(z)$

In one dimension, eq. (10) reduces to

$$G(z)P(z)\left.\frac{\mathrm{d}f(z)}{\mathrm{d}z}\right|_{\partial\Gamma}=0\,, \tag{15}$$

where $\partial\Gamma$ consists of the two end points of Γ, and is satisfied if $P(z)=0$ at $\partial\Gamma$. As an example consider $P(x)=(x-a)\exp(-\frac{1}{2}x^2)$, which vanishes at $z=a$, $\pm\infty$. There are two basic paths $\Gamma_\pm$ from a to $\pm\infty$. The real axis corresponds to $\Gamma_\mathrm{R}=\Gamma_+-\Gamma_-$. If we define $N_\pm=\pm\int_{\Gamma_\pm}z^2P(z)\mathrm{d}z$, $D_\pm=\pm\int_{\Gamma_\pm}P(z)\mathrm{d}z$, we have

$$\langle z^2\rangle_\pm=\frac{N_\pm}{D_\pm}\,,\quad \langle z^2\rangle_\mathrm{R}=\frac{N_++N_-}{D_++D_-}=1\,. \tag{16}$$

We will call $\langle z^2\rangle_\mathrm{R}$ the coherent sum of $\langle z^2\rangle_+$ and $\langle z^2\rangle_-$ as opposed to their incoherent sum $\langle z^2\rangle_\mathrm{I}=\frac{1}{2}(\langle z^2\rangle_++\langle z^2\rangle_-)$. The first case corresponds to the sampling of the distribution P_R associated to the real axis while the second one corresponds to $P_\mathrm{I}=\frac{1}{2}(P_++P_-)$.

Let us consider the unkernelled random walk, $G(z)=1$. In this case

$$\mathrm{d}z=F(z)\mathrm{d}t+\mathrm{d}\eta\,,$$

$$F(z)=\frac{\mathrm{d}\log P(z)}{\mathrm{d}z}=-z+\frac{1}{z-a}\,. \tag{17}$$

In addition we choose $a=\mathrm{i}|a|$, hence $F(-z^*)=-F(z)^*$ and the flow is symmetric about the imaginary axis. For $|a|=0$ (and $\mathrm{d}t\to0$), this symmetry is spontaneously broken, in agreement with the segregation theorem. Depending on the initial conditions, P_+ or P_- will be sampled. For small non-vanishing $|a|$, the symmetry is restored but the points are highly segregated in two regions, one sampling P_+, the other P_-. This is shown in fig. 1, for $|a|=0.5$ (upper panel). This distribution corresponds to P_I, as confirmed by the numerical results in table 1. There we can see that for $|a|$ small compared to unity, the incoherent distribution P_I is sampled while for larger $|a|$ the equilibrium distribution switches to P_R. The sampling points for $|a|=1.5$ are shown in fig. 1 (lower part). The distribution is no longer segregated in this case, although it does not lie on the real axis. This is necessary in order to correctly reproduce $\langle z\rangle_\mathrm{R}$ which is purely imaginary. We have checked that $\langle z\rangle$ follows the same trend as $\langle z^2\rangle$ for several

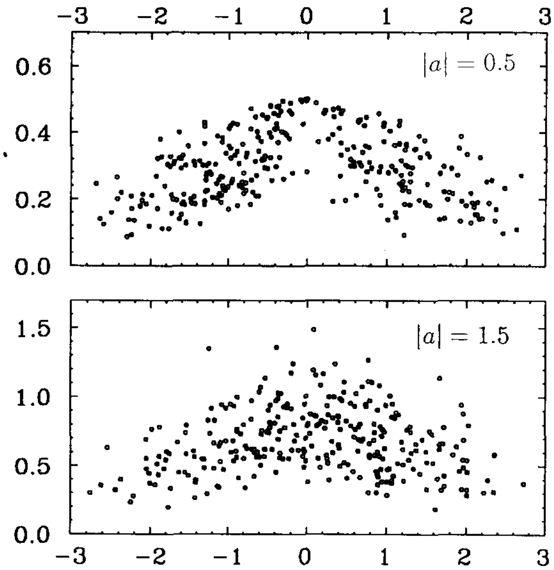

Fig. 1. Points sampling the random walk in the z complex plane, associated to $P(x)=(x-a)\exp(-\frac{1}{2}x^2)$, for $a=\mathrm{i}0.5$ (upper panel) and $a=\mathrm{i}1.5$ (lower panel).

Table 1
$\langle z^2\rangle$ for the distributions P_+, P_I, P_R and (unkernelled) complex Langevin simulation associated to $P(x)=(x-a)\exp(\frac{1}{2}x^2)$, $a=\mathrm{i}|a|$.

$\lvert a\rvert$	$\langle z^2\rangle_+$	$\langle z^2\rangle_\mathrm{I}$	$\langle z^2\rangle_\mathrm{R}$	$\langle z^2\rangle_\mathrm{CL}$
0.1	1.99+i0.12	1.99	1	2.01
0.5	1.85+i0.62	1.85	1	1.89
1.0	1.42+i1.16	1.42	1	1.42
1.5	0.67+i1.56	0.67	1	1.03
2.0	−0.44+i1.75	−0.44	1	1.09

values of a, hence the transition from P_I to P_R is a property of the Langevin distribution itself and not of certain particular observables. This transition between both regimes is rather sharp and it can qualitatively be understood from the flow $F(z)$ above. The linear part of $F(z)$ attracts to $z=0$, while the pole part is attractive at $z=a$ along the imaginary axis but repulsive parallel to the real axis. For small a the pole dominates and the distribution gets segregated, on the other hand for large a the region near $z=0$ becomes stable and the zero of $P(z)$ at a is just a small disturbance. This is confirmed by studying the flow associated to $P(x)=(x-a)^{-1}\exp(-\frac{1}{2}x^2)$. In this case $z=0$ is always stable and numerically P_R is obtained even for small a. Going back to $P(x)=(x-a)\exp(-\frac{1}{2}x^2)$, we must warn that the stability of a solution cannot be established numerically because it cannot be distinguished from a metastability with sufficiently long lifetime. It could very well be that only one of the solutions, P_I or P_R, is truly stable.

Attending to the form of eq. (15), one could devise a way to remove the spurious solution P_I consisting of choosing a kernel $G(z)$ with a pole at $z=a$, thereby cancelling the zero of $P(z)$, hence

$$dz=F_G(z)dt+\sqrt{G(z)}\,d\eta\,,$$
$$F_G(z)=G(z)F(z)+\frac{dG(z)}{dz}\,, \tag{18}$$

and $F(z)$ as given in eq. (17). A possibility would be $G(z)=(z-a)^{-1}$, however in this case $F_G(z)=-1-a(z-a)^{-1}$ and one finds that for large z, $dz\sim -dt$, which admits no stable equilibrium distribution. In fact no choice of $G(z)$ has proven suitable to remove the spurious solution, either because the random walk turned out to be unstable or else because new spurious solutions, introduced by the kernel, showed up. This latter phenomenon is studied in the next section. In connection with this failure let us remark that, to our knowledge, no general necessary and sufficient condition is known to decide whether for a given complex and normalizable distribution $P(x)$ on $\mathbb{R}$ there exists a real and positive definite distribution $p(x,y)$ on $\mathbb{C}$ such that $\forall n$: $\langle x^n\rangle_P=\langle z^n\rangle_p$. If there is, p is certainly not unique because its convolution with an isotropic gaussian gives a new solution. On the other hand p could simply not exist for some $P(x)$, and for those cases the complex Langevin approach cannot work.

4. Solutions associated to zeros of the kernel

By inspection of eq. (15) one can see that it can also be satisfied if $G(z)=0$ at $\partial\Gamma$, (or more generally $G(z)P(z)=0$ at $\partial\Gamma$). Therefore the kernel can itself introduce spurious solutions. An example is provided by $P(x)=\exp(-\frac{1}{2}x^2)$, for which the standard Langevin method provides a stable distribution.

If we take $G(z)=z-a$, $a\in\mathbb{C}$ the stochastic differential equation takes the form (18) with $F_G(z)=-z(z-a)+1$. Numerically one finds that $p(x,y)$ is distributed nearby a path Γ from $z=a$ to $z=+\infty$, fig. 2, and $\langle z\rangle=\langle z\rangle_\Gamma$ within statistical (and finite step) errors. This is understood by making a change of variable $z=z(w)$ in order to remove the kernel, that is, $\sqrt{G}=dz/dw$, with the result $z=w^2+a$. For real w, $z(w)$ describes such a path Γ. In the w variable one is sampling $P_w(w)=w\exp[-\frac{1}{2}(w^2+a^2)^2]$, which is real for a, $w\in\mathbb{R}$, and therefore the random walk is stable in this case. For complex a it is probably just metastable because if it ever reaches a large negative z, F_G will be large and negative too, and larger than the stochastic term $\sqrt{G}\,d\eta$, thus leading the random walk to $-\infty$. Starting at $\mathrm{Re}\,z>0$, we have not found any instability within the finite time of the numerical calculation.

In more than one dimension, and even for the real Langevin problem, the kernel can introduce spurious

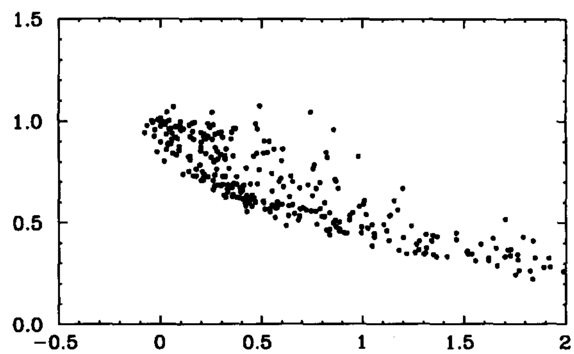

Fig. 2. Points sampling the random walk in the z complex plane, associated to $P(x)=\exp(-\frac{1}{2}x^2)$ with a kernel $G(z)=z-a$, for $a=1$.

solutions if the matrix $G^{ij}(x)$ is singular [10].

5. Solutions associated to poles of $P(z)$

This more exotic possibility follows from the observation that eq. (15) can also be satisfied if Γ is a closed curve and therefore has no boundary. For such a Γ and for $P(z)$ analytical, P_Γ defined in eq. (9) vanishes. However it may not vanish if $P(z)$ is meromorphic in a region containing Γ. As an example consider $P(x)=(x-a)^{-1}\exp(-\frac{1}{2}x^2)$. We already mentioned that the unkernelled associated random walk correctly reproduces the expectation values of $P_{\mathbf{R}}$. In order to induce a solution P_C associated to a closed curve C enclosing a, consider a new variable $z=a+\exp(iw)$. For real w, $z(w)$ describes a closed curve C. If there is no kernel in the variable w, $G(z)=-(z-a)^2$ in variable z. From eq. (18), the deterministic as well as the stochastic parts of the flow vanish at $z=a$. In fact the deterministic part goes as $F_G\sim-(z-a)+\mathrm{O}((z-a)^2)$ and thus $z=a$ is an attractor of the random walk. This in agreement with $\langle f(z)\rangle_C=f(a)$ by the theorem of residues.

A numerical calculation with $a=\mathrm{i}|a|$ agrees well with these expectations. However for $|a|=2$ the region near $z=0$ is metastable, taking a long time to the random walk to reach $z=a$, and this time increases rapidly with $|a|$. For higher-order poles, $z=a$ is no longer a stable fixed point and no stable solutions were found.

6. Conclusion

We have shown how the complex Langevin equation, with or without a kernel, can present spurious stable solutions and their origin, namely the stochastic equation, seeks equilibrium solutions of the Fokker–Planck equation in the space of distributions which is larger than that of ordinary functions. Also in some cases we were able to construct a kernel to pick up a particular solution P_Γ. This was achieved by showing that the kernel transforms as a metric tensor under coordinate transformations. By this method we were also able, within the complex Langevin scheme, to assign a real and normalizable distribution to the bottomless action $S=-\frac{1}{3}x^3$, although not in a unique way.

A major problem of the complex Langevin method is still that one cannot say in advance which solution P_Γ or combinations of them will be reproduced by a given kernel. At the moment it is rather a trial and error method. It would be extremely interesting to construct some kind of effective potential functional of which the minimum were the actual result of the simulation.

As a final comment, let us point out that perhaps the spurious solutions should be regarded as different phases of the action, with the same equations of motion but different boundary conditions, and could be relevant in some situations.

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