Complex Langevin equations and their applications to quantum statistical and lattice field models

H. Gausterer
Institut für Theoretische Physik, Universität Graz, A-8010 Graz, Austria

J. R. Klauder
AT&T Bell Laboratories, Murray Hill, New Jersey 07974
(Received 21 January 1986)

We discuss the calculation of statistical averages of variables lying on S_1 or S_2 using (complex) Langevin equations. Assuming that the drift term is proportional to the gradient of a possibly complex function $S(\{x_i\})$, $x_i \in S_1$ or S_2 we give the general form of such Langevin equations. These variables cause unphysical singularities and computational problems; thus we transform them to those of the embedding Euclidean space. We show in several examples that these modified (complex) Langevin equations have good convergence properties using an improved two-stage Runge-Kutta algorithm.

I. INTRODUCTION

A variety of problems of physical interest can be formulated as multidimensional integrals involving variables that individually lie on the unit circle (S_1), or when taken in pairs, lie instead on the unit sphere (S_2). On the one hand, such problems include the partition function for classical rotors or Heisenberg models, or, on the other hand, they include the partition function for suitably formulated quantum spin systems that have applications to both statistical physics and quantum-field theory. When the integrand involves a non-negative weight function, as in classical partition-function calculation, then a standard importance-sampling Monte Carlo estimation is entirely appropriate. However, when the weight function is complex, as frequently occurs for a quantum partition function, the standard Monte Carlo approach is inapplicable. Instead an alternative approach based on the long-time average of appropriate functions of the solution of a Langevin equation with a complex drift becomes a candidate to estimate such integrals.[1-3] The Langevin method is, of course, not limited to complex weight functions and thus it is appropriate to consider its general use in the statistical estimation of many-dimensional integrals.

Although the Langevin equations are originally formulated in variables on the manifold S_1 or S_2 there are two reasons to recast them into another form. One reason has to do with the presence of trigonometric functions and the non-negligible computation time they involve. The second reason has to do with unphysical singularities in the Langevin equations and the computational problems they lead to. In this paper we shall develop and apply alternative Langevin equations that avoid both problems. For simplicity we confine attention here in Sec. I to a single integral on S_1 or S_2 reserving to Sec. II an extension to the particular many-dimensional form of interest to our examples, several of which are, in turn, discussed in Sec. III.

A. Elementary examples on S_1 and S_2

For a circle variable α, $0 \le \alpha \le 2\pi$, the integral average given by

$$\bar{a} = \int_0^{2\pi} a(\alpha) e^{-S(\alpha)} d\alpha \Big/ \int_0^{2\pi} e^{-S(\alpha)} d\alpha \,, \tag{1.1}$$

based on some periodic (action) function $S(\alpha)$, may be estimated by the quantity

$$\bar{a}_T \equiv \frac{1}{T} \int_0^T a(\alpha(\tau)) d\tau, \quad T \gg 1 \,, \tag{1.2}$$

where $\alpha(\tau)$ is a solution of the stochastic differential (Langevin) equation (SDE)

$$d\alpha(\tau) = -\frac{1}{2} \frac{\partial S}{\partial \alpha(\tau)} d\tau + dw(\tau), \quad 0 < \tau \,, \tag{1.3}$$

subject to a fairly general initial distribution at $\tau = 0$. Such equations are shorthands for their integrals, viz.,

$$\alpha(\tau) - \alpha(0) = -\frac{1}{2} \int_0^\tau \frac{\partial S}{\partial \alpha(\tau)} d\tau + w(\tau) \,. \tag{1.4}$$

Here $w(\tau)$ denotes a standard Wiener process, a normally distributed stochastic variable characterized by the fact that $w(0) = 0$, $\langle w(\tau) \rangle = 0$, and

$$\langle w(\tau_1) w(\tau_2) \rangle = \min(\tau_1, \tau_2) \,. \tag{1.5}$$

In addition we have used the shorthand

$$\frac{\partial S}{\partial \alpha(\tau)} = \left. \frac{\partial S}{\partial \alpha} \right|_{\alpha = \alpha(\tau)} \tag{1.6}$$

and shall continue to do likewise.

Remark: The foregoing scenario holds true for suitable complex actions S, which initially must satisfy

$$0 < \left| \int_0^{2\pi} e^{-S(\alpha)} d\alpha \right| \le \int_0^{2\pi} | e^{-S(\alpha)} | \, d\alpha < \infty \,. \tag{1.7}$$

Finally, we observe that if sufficiently many long-time averages actually converge, e.g., if for all real s

$$\lim_{T\to\infty}\frac{1}{T}\int_0^T e^{is\alpha(\tau)}d\tau=C(s)\ , \tag{1.8}$$

then the action S is a suitable one and

$$C(s)=\int_0^{2\pi}e^{is\alpha}e^{-S(\alpha)}d\alpha\Big/\int_0^{2\pi}e^{-S(\alpha)}d\alpha \tag{1.9}$$

as desired. For unsuitable actions, long-time averages generally fail to converge, which is an effective way to judge the suitability of an action S, albeit *a posteriori*. Thus the present working rule is to compute and let the quality of the convergence judge the suitability of the method. Examples that converge slowly can frequently be speeded up by sample averaging as well, namely, in place of (1.2) to use

$$\bar{a}_{T,J}\equiv\frac{1}{TJ}\sum_{j=1}^{J}\int_0^T a(\alpha_j(\tau))d\tau,\quad TJ\gg 1 \tag{1.10}$$

where $\{\alpha_j\}$ denotes J solutions for generally independent initial values and noise samples.

As a second basic example consider the integral average

$$\bar{a}=\int_{S_2}a(\theta,\phi)e^{-S(\theta,\phi)}\sin\theta\,d\theta\,d\phi \times\left[\int_{S_2}e^{-S(\theta,\phi)}\sin\theta\,d\theta\,d\phi\right]^{-1} \tag{1.11}$$

in terms of the usual angular variables θ and ϕ on S_2. In this case the average may be estimated by

$$\bar{a}_T\equiv\frac{1}{T}\int_0^T a(\theta(\tau),\phi(\tau))d\tau,\quad T\gg 1\ , \tag{1.12}$$

where $\theta(\tau)$ and $\phi(\tau)$ satisfy the coupled stochastic differential equations

$$d\theta(\tau)=-\frac{1}{2}\frac{\partial}{\partial\theta(\tau)}\{S-\ln[\sin\theta(\tau)]\}d\tau+dw_1(\tau)\ , \tag{1.13a}$$

$$\sin\theta(\tau)d\phi(\tau)=-\frac{1}{2}\frac{\partial\{S-\ln[\sin\theta(\tau)]\}}{\sin\theta(\tau)\partial\phi(\tau)}d\tau+dw_2(\tau)\ . \tag{1.13b}$$

In obtaining these equations we have used the fact that the effective action is $S-\ln(\sin\theta)$, and also that the metric on the sphere has the form $d\theta^2+\sin^2\theta\,d\phi^2$. As $d\theta$ and $\sin\theta\,d\phi$ are orthogonal vectors it follows that w_1 and w_2 should be taken as two independent standard Wiener processes. Equation (1.13) may then be rewritten as

$$d\theta(\tau)=\frac{1}{2}\cot\theta(\tau)d\tau-\frac{1}{2}\frac{\partial S}{\partial\theta(\tau)}d\tau+dw_1(\tau)\ , \tag{1.14a}$$

$$d\phi(\tau)=-\frac{1}{2[\sin\theta(\tau)]^2}\frac{\partial S}{\partial\phi(\tau)}d\tau+\frac{1}{\sin\theta(\tau)}dw_2(\tau)\ , \tag{1.14b}$$

which is essentially the form previously given.[1,3] These equations exhibit both the trigonometric functions and the coordinate singularities mentioned earlier.

B. Itô calculus

To properly carry out the transformation of variables we have in mind we shall rely on the so-called Itô calculus.[4] This will ensure that we obtain an Itô-type SDE for which suitable Runge-Kutta integration routines for multiplicative noise have been found.[5] Thus a few words on the Itô calculus are in order. If $w(\tau)$ is a standard Wiener process it is straightforward to show that

$$\left\langle[w(\tau+\Delta\tau)-w(\tau)]^2\exp\left[\int_0^\tau s(t)w(t)dt\right]\right\rangle =\Delta\tau\left\langle\exp\left[\int_0^\tau s(t)w(t)dt\right]\right\rangle+O(\Delta\tau^2) \tag{1.15}$$

for $\Delta\tau>0$ and $s(t)$ a general smooth function. For infinitesimal $\Delta\tau$ it follows, therefore, that

$$dw(\tau)^2\equiv[w(\tau+d\tau)-w(\tau)]^2=d\tau \tag{1.16}$$

holds with probability one. Other differential products of interest are

$$dw(\tau)d\tau=0\ , \tag{1.17a}$$

and, for two independent Wiener processes,

$$dw_1(\tau)dw_2(\tau)=0\ . \tag{1.17b}$$

The differential of a function of a Wiener process needs to be taken to second order, viz.,

$$df(w(\tau))=f'(w(\tau))dw(\tau)+\tfrac{1}{2}f''(w(\tau))dw(\tau)^2 =f'(w(\tau))dw(\tau)+\tfrac{1}{2}f''(w(\tau))d\tau\ , \tag{1.18}$$

where the first term is defined as a stochastic integral by the limit

$$J_I=\int f'(w(\tau))dw(\tau)\equiv\lim_{\epsilon\to 0}\sum f'(w_k)(w_{k+1}-w_k)\ , \tag{1.19}$$

with $w_k\equiv w(k\epsilon)$, $\epsilon>0$.

Remark: It is worth noting that a common alternative definition of stochastic integral exists: the Stratonovich rule,[4] defined by the limit

$$J_S\equiv\int f'(w(\tau))\circ dw(\tau) \equiv\lim_{\epsilon\to 0}\sum\tfrac{1}{2}[f'(w_{k+1})+f'(w_k)](w_{k+1}-w_k)\ . \tag{1.20}$$

That these limits are generally unequal is just a reflection of (1.16) since

$$J_S-J_I=\lim_{\epsilon\to 0}\sum\tfrac{1}{2}[f'(w_{k+1})-f'(w_k)](w_{k+1}-w_k) =\lim_{\epsilon\to 0}\sum\tfrac{1}{2}f''(w_k)(w_{k+1}-w_k)^2 =\tfrac{1}{2}\int f''(w(\tau))d\tau\ . \tag{1.21}$$

This relation implies the simpler-looking relation

$$df(w(\tau))=f'(w(\tau))\circ dw(\tau)\ , \tag{1.22}$$

but such equations are harder to deal with in higher-order Runge-Kutta numerical integration schemes (see Refs. 5 and 6).

C. Euclidean space reformulation

The transformation of variables we have in mind is to those of the embedding Euclidean space. For S_1 we introduce

$$x=\cos\alpha,\quad y=\sin\alpha \tag{1.23}$$

subject to the constraint $x^2+y^2=1$. It follows that

$$dx=-\sin\alpha\,d\alpha-\tfrac{1}{2}\cos\alpha(d\alpha)^2\,, \tag{1.24a}$$

$$dy=\cos\alpha\,d\alpha-\tfrac{1}{2}\sin\alpha(d\alpha)^2 \tag{1.24b}$$

or, in other words,

$$dx=-\tfrac{1}{2}x\,d\tau-\frac{1}{2}y\left[y\frac{\partial S}{\partial x}-x\frac{\partial S}{\partial y}\right]d\tau-y\,dw\,, \tag{1.25a}$$

$$dy=-\tfrac{1}{2}y\,d\tau+\frac{1}{2}x\left[y\frac{\partial S}{\partial x}-x\frac{\partial S}{\partial y}\right]d\tau+x\,dw\,. \tag{1.25b}$$

Note that coordinate transformations typically result in multiplicative noise equations, the rules for which (here Itô rules) need to be specified. If the constraint is satisfied at $\tau=0$ then it is preserved by the equations for all τ since

$$\begin{aligned}\tfrac{1}{2}d(x^2+y^2)&=x\,dx+y\,dy+\tfrac{1}{2}(dx^2+dy^2)\\&=x\,dx+y\,dy+\tfrac{1}{2}(x^2+y^2)d\tau\,,\end{aligned} \tag{1.26}$$

and, according to (1.25), the right side vanishes. This change of variables clearly eliminates all coordinate-based trigonometric functions since

$$e^{\pm in\alpha}=(x\pm iy)^n \tag{1.27}$$

for all $n\geq 0$. It does not eliminate those in the example $S=\sin[\sin(\alpha)]=\sin y$, however.

The analysis of the variable change for S_2 is qualitatively similar only algebraically more complicated. We first introduce

$$x=\sin\theta\cos\phi,\quad y=\sin\theta\sin\phi,\quad z=\cos\theta \tag{1.28}$$

subject to the constraint $x^2+y^2+z^2=1$. It follows that

$$\begin{aligned}dx=&\cos\theta\cos\phi\,d\theta-\sin\theta\sin\phi\,d\phi\\&-\tfrac{1}{2}\sin\theta\cos\phi(d\theta^2+d\phi^2)-\cos\theta\sin\phi\,d\theta\,d\phi\end{aligned} \tag{1.29}$$

plus similar equations for dy and dz. The Itô rules tell us that

$$\begin{aligned}&d\theta^2=dw_1{}^2=d\tau\,,\\&d\phi^2=(\sin\theta)^{-2}dw_2{}^2=(\sin\theta)^{-2}d\tau,\quad d\theta\,d\phi=0\,.\end{aligned} \tag{1.30}$$

When these relations are combined it follows that

$$dx=-x\,d\tau-\frac{1}{2}\left[(1-x^2)\frac{\partial S}{\partial x}-xy\frac{\partial S}{\partial y}-xz\frac{\partial S}{\partial z}\right]d\tau+dv_1\,, \tag{1.31a}$$

$$dy=-y\,d\tau-\frac{1}{2}\left[-xy\frac{\partial S}{\partial x}+(1-y^2)\frac{\partial S}{\partial y}-yz\frac{\partial S}{\partial z}\right]d\tau+dv_2\,, \tag{1.31b}$$

$$dz=-z\,d\tau-\frac{1}{2}\left[-xz\frac{\partial S}{\partial x}-yz\frac{\partial S}{\partial y}+(1-z^2)\frac{\partial S}{\partial z}\right]d\tau+dv_3\,, \tag{1.31c}$$

where

$$dv_1=\frac{xz}{(1-z^2)^{1/2}}dw_1-\frac{y}{(1-z^2)^{1/2}}dw_2\,, \tag{1.32a}$$

$$dv_2=\frac{yz}{(1-z^2)^{1/2}}dw_1+\frac{x}{(1-z^2)^{1/2}}dw_2\,, \tag{1.32b}$$

$$dv_3=(1-z^2)^{1/2}dw_1\,. \tag{1.32c}$$

With the notation $(x_1,x_2,x_3)=(x,y,z)$, and assuming the constraint $\sum x_i{}^2(\tau)=1$, it follows that

$$dv_j{}^2(\tau)=[1-x_j{}^2(\tau)]d\tau\,. \tag{1.33}$$

Thus it readily follows that

$$\begin{aligned}\tfrac{1}{2}d\left[\sum x_j{}^2\right]&=\sum x_j dx_j+\tfrac{1}{2}\sum dx_j{}^2\\&=\sum x_j dx_j+\tfrac{1}{2}\sum dv_j{}^2\\&=\sum x_j dx_j+\tfrac{1}{2}\sum(1-x_j{}^2)d\tau\\&=\sum x_j dx_j+d\tau\,,\end{aligned} \tag{1.34}$$

which vanishes according to (1.31) and (1.32).

Equations (1.31) have eliminated any dependence of trigonometric coordinates, but the noises seem to contain points of difficulty when $z\approx\pm 1$. It is not hard to eliminate these potential problems as well. It follows, for $i\neq j$, that

$$dv_i(\tau)dv_j(\tau)=-x_i(\tau)x_j(\tau)d\tau\,, \tag{1.35}$$

while $\langle dv_j(\tau)\rangle=0$ and $dv_j(\tau)dv_k(\tau')=0$ if $\tau\neq\tau'$. All representations of dv_j with the indicated properties are stochastically equivalent to each other, i.e., just a reshuffling of the ensemble of random functions. One alternative choice is provided by

$$dv_1=y\,dw_3-z\,dw_2\,, \tag{1.36a}$$

$$dv_2=z\,dw_1-x\,dw_3\,, \tag{1.36b}$$

$$dv_3=x\,dw_2-y\,dw_1\,, \tag{1.36c}$$

expressed in terms of three independent, standard Wiener processes, which is easily seen to satisfy the proper conditions and furthermore is singularity-free.

Thus we are led to the final form for the S_2 reformulation given by

$$\begin{aligned}dx=&-x\,d\tau-\frac{1}{2}\left[(1-x^2)\frac{\partial S}{\partial x}-xy\frac{\partial S}{\partial y}-xz\frac{\partial S}{\partial z}\right]d\tau\\&+y\,dw_3-z\,dw_2\,,\end{aligned} \tag{1.37a}$$

$$\begin{aligned}dy=&-y\,d\tau-\frac{1}{2}\left[-xy\frac{\partial S}{\partial x}+(1-y)^2\frac{\partial S}{\partial y}-yz\frac{\partial S}{\partial z}\right]d\tau\\&+z\,dw_1-x\,dw_3\,,\end{aligned} \tag{1.37b}$$

$$dz=-z\,d\tau-\frac{1}{2}\left[-xz\frac{\partial S}{\partial x}-yz\frac{\partial S}{\partial y}+(1-z^2)\frac{\partial S}{\partial z}\right]d\tau$$

$$+x\,dw_2-y\,dw_1\ . \tag{1.37c}$$

As noted these equations preserve the constraint $x^2+y^2+z^2=1$, and are free of singularities and have no trigonometric coordinates. They do involve multiplicative noise terms, which are necessary to stay on the manifold S_2.

The Euclidean form of the Langevin equations will be extended in Sec. II to many coupled variables appropriate to integral representations of classical and quantum partition functions. Numerical solutions of such equations will be discussed in Sec. III.

II. LANGEVIN EQUATIONS FOR MANY-DIMENSIONAL S_1 AND S_2 VARIABLES

As a first example we study the example of many coupled S_1 variables given by

$$\bar{a}=\frac{\int a(\alpha_1,\ldots,\alpha_M)e^{-S(\alpha_1,\ldots,\alpha_M)}d\alpha_1\cdots d\alpha_M}{\int e^{-S(\alpha_1,\ldots,\alpha_M)}d\alpha_1\cdots d\alpha_M}\ . \tag{2.1}$$

The generalization of (1.3) and (1.25) is straightforward, and we content ourselves with a statement of the latter. The relevant Langevin equations read

$$\dot{x}_m=-\tfrac{1}{2}x_m-\frac{1}{2}y_m\left[y_m\frac{\partial S}{\partial x_m}-x_m\frac{\partial S}{\partial y_m}\right]-y_m\xi_m\ , \tag{2.2a}$$

$$\dot{y}_m=-\tfrac{1}{2}y_m+\frac{1}{2}x_m\left[y_m\frac{\partial S}{\partial x_m}-x_m\frac{\partial S}{\partial y_m}\right]+x_m\xi_m\ , \tag{2.2b}$$

where $1\le m\le M$, and $\{\xi_m\}$ denotes M independent standard Gaussian white-noise sources for which

$$\langle\xi_m(\tau)\rangle=0\ , \tag{2.3a}$$

$$\langle\xi_m(\tau)\xi_{m'}(\tau')\rangle=\delta_{mm'}\delta(\tau-\tau')\ . \tag{2.3b}$$

These Langevin equations are to be interpreted according to the rules laid out in Sec. I. The solution is subject to the initial condition that $x_m{}^2+y_m{}^2=1$ for all m, and the statistical estimate for $\bar{a}$ is given by

$$\bar{a}_T=\frac{1}{T}\int_0^T\tilde{a}(x_1(\tau),y_1(\tau),\ldots,x_M(\tau),y_M(\tau))d\tau,\ T\gg 1 \tag{2.4}$$

in terms of the suitably transformed function $\tilde{a}$.

These equations apply also to the Euclidean time formulation of a U(1) lattice gauge theory. For this example we choose the $d=2$ Wilson action:[7]

$$S=-\frac{\beta}{2}\sum_{\square}(U_{\square}+U_{\square}^{*})\ . \tag{2.5}$$

We will use the temporal gauge. In the temporal gauge the action has a very simple form in the Euclidean representation.

$$S=-\beta\sum_{m,n=1}^{M,N}(x_n^{m+1}x_n^m+y_n^{m+1}y_n^m)\ , \tag{2.6}$$

$$(x_n^{M+1},y_n^{M+1})=(x_n{}^1,y_n{}^1) \tag{2.7}$$

with $U_{m,n}=x_n{}^m+iy_n{}^m$. One has to be aware that using the temporal gauge implies making a slight error due to the boundary condition [Eq. (2.7)]; i.e., closed paths with $U_p=1$ are existing for all configurations. Because of the analytical solubility of this model[8] we are able to test the convergence properties of such a system and to have an idea about the effects of the finite size superposed by the effects of the temporal gauge. The numerical results we discuss in Sec. III.

For variables on S_2 statistical averages for a classical Heisenberg problem may be generally written in the form

$$\bar{a}=\int a(\theta_1,\phi_1,\ldots,\theta_M,\phi_M)e^{-S(\theta_1,\phi_1,\ldots,\theta_M,\phi_M)}\times\prod\sin\theta_m d\theta_m d\phi_m/Z\ , \tag{2.8a}$$

$$Z=\int e^{-S(\theta_1,\phi_1,\ldots,\theta_M,\phi_M)}\prod\sin\theta_m d\theta_m d\phi_m\ . \tag{2.8b}$$

The Euclidean-form Langevin equations are direct extensions of (1.37), and are given by

$$\dot{x}_m=-x_m-\frac{1}{2}\left[(1-x_m{}^2)\frac{\partial S}{\partial x_m}-x_my_m\frac{\partial S}{\partial y_m}-x_mz_m\frac{\partial S}{\partial z_m}\right]+y_m\xi_m-z_m\eta_m\ , \tag{2.9a}$$

$$\dot{y}_m=-y_m-\frac{1}{2}\left[-y_mx_m\frac{\partial S}{\partial x_m}+(1-y_m{}^2)\frac{\partial S}{\partial y_m}-y_mz_m\frac{\partial S}{\partial z_m}\right]+z_m\xi_m-x_m\xi_m\ , \tag{2.9b}$$

$$\dot{z}_m=-z_m-\frac{1}{2}\left[-z_mx_m\frac{\partial S}{\partial x_m}-z_my_m\frac{\partial S}{\partial y_m}+(1-z_m{}^2)\frac{\partial S}{\partial z_m}\right]+x_m\eta_m-y_m\xi_m\ , \tag{2.9c}$$

for $1\le m\le M$, subject to the initial condition $x_m{}^2+y_m{}^2+z_m{}^2=1$ for all m.

These equations also apply to statistical averages for quantum-spin systems. To see this let us first derive an integral representation for the partition function

$$Z=\mathrm{Tr}(e^{-\beta H})\ , \tag{2.10}$$

where the Hamiltonian $H=H(\{\mathbf{S}_n\})$ is a function of N independent sets of spin operators which obey the usual commutation relations

$$[S_{n,1},S_{n',2}]=i\delta_{nn'}S_{n,3} \tag{2.11}$$

plus cyclic permutations. We assume $\sum_i S_{n,i}{}^2=s(s+1)\mathbb{1}$ independent of n (although that is not necessary). In the spin-$\frac{1}{2}$ case $S_{n,i}$ is given by

$$S_{n,i}=\tfrac{1}{2}\sigma_i(n)\ , \tag{2.12a}$$

where we have

$$\sigma_i(n)=\bigotimes_{k=1}^{n-1}\mathbb{1}\otimes\sigma_i\bigotimes_{k=n+1}^{N}\mathbb{1}\ . \tag{2.12b}$$

σ_i are the standard Pauli matrices. For a given spin value s let us introduce the spin coherent states:[1,3,9]

$$|\{\theta,\phi\}\rangle=\bigotimes_{n=1}^{N}|\theta_n,\phi_n\rangle\ , \tag{2.13a}$$

$$|\theta_n,\phi_n\rangle=e^{-i\phi_nS_3}e^{-i\theta_nS_2}|\omega\rangle\ , \tag{2.13b}$$

$$S_3|\omega\rangle=s|\omega\rangle\ . \tag{2.13c}$$

S_i are the generators of the irreducible representations of the SU(2). These states admit a resolution of unity in the form

$$\mathbb{1}=\int_{S_2^N}|\{\theta,\phi\}\rangle\langle\{\theta,\phi\}|\,d\mu(\{\theta,\phi\})\ , \tag{2.14a}$$

$$d\mu(\{\theta,\phi\})\equiv\left[\frac{2s+1}{4\pi}\right]^N\prod_{n=1}^{N}\sin\theta_n d\theta_n d\phi_n\ , \tag{2.14b}$$

and, moreover, admit a similar representation for a general operator such as the Hamiltonian

$$H=\int_{S_2^N}\mathcal{H}(\{\theta,\phi\})|\{\theta,\phi\}\rangle\langle\{\theta,\phi\}|\,d\mu(\{\theta,\phi\})\ . \tag{2.15}$$

If H is a sum of multilinear terms,

$$H=\sum a_{n_1i_1,\ldots,n_pi_p}S_{n_1i_1}\cdots S_{n_pi_p}\ , \tag{2.16}$$

then the function $\mathcal{H}$, for $s=\frac{1}{2}$, is given by

$$\mathcal{H}=\sum a_{n_1i_1,\ldots,n_pi_p}(\tfrac{3}{2})^pT_{n_1i_1}\cdots T_{n_pi_p}\ , \tag{2.17}$$

where

$$\mathbf{T}_n=(x_n,y_n,z_n)\ . \tag{2.18}$$

Now with M a positive integer and $\epsilon\equiv\beta/M$, then

$$e^{-\epsilon H}=\int_{S_2^N}e^{-\epsilon\mathcal{H}(\{\theta,\phi\})}|\{\theta,\phi\}\rangle\langle\{\theta,\phi\}|\,d\mu+O(\epsilon^2)\ . \tag{2.19}$$

It follows that

$$Z=\mathrm{Tr}(e^{-\epsilon H}\cdots e^{-\epsilon H})\ , \tag{2.20a}$$

$$Z=\int_{S_2^{N\times M}}\prod_{m=1}^{M}\langle\{\theta,\phi\}^{m+1}|\{\theta,\phi\}^m\rangle\times e^{-\epsilon\mathcal{H}(\{\theta,\phi\}^m)}d\mu(\{\theta,\phi\}^m)+O(\epsilon)\ , \tag{2.20b}$$

where $\{\theta,\phi\}^{M+1}\equiv\{\theta,\phi\}^1$. For M sufficiently large so that the term $O(\epsilon)$ may be neglected we have achieved our goal of an integral representation over $(S_2)^{N\times M}$ of a quantum-spin partition function. While $\mathcal{H}$ is real for a self-adjoint operator H, the coherent-state overlap is complex. In particular,

$$\langle\{\theta,\phi\}^{m+1}|\{\theta,\phi\}^m\rangle=\prod_{n=1}^{N}\left[\cos\frac{\theta_n^{m+1}-\theta_n^m}{2}\cos\frac{\phi_n^{m+1}-\phi_n^m}{2}+i\cos\frac{\theta_n^{m+1}+\theta_n^m}{2}\sin\frac{\phi_n^{m+1}-\phi_n^m}{2}\right]^{2s}. \tag{2.21}$$

The variable m labels a lattice space of thermal time, an extra parametrization needed in rendering the quantum problem into a c-number (path-) integral representation.

It is clear that quantum statistical average can be put into the form (2.8), where

$$S=-\sum_{m=1}^{M}[\ln\langle\{\theta,\phi\}^{m+1}|\{\theta,\phi\}^m\rangle-\epsilon\mathcal{H}(\{\theta,\phi\}^m)]\ ; \tag{2.22}$$

thus, it falls into the class of problems covered by (2.9). After some straightforward algebra taking into account the explicit form of (2.21), it follows that the Euclidean form of the complex Langevin equations is given by

$$\begin{aligned}\dot{x}_n^m=&-x_n^m+\frac{s}{D}\{(1-z_n^{m+1})z_n^mx_n^m(1-z_n^{m-1})-(x_n^{m+1}+iy_n^{m+1})z_n^mx_n^m(x_n^{m-1}-iy_n^{m-1})\\&+(1-z_n^{m+1})[1-x_n^m(x_n^m+iy_n^m)](x_n^{m-1}-iy_n^{m-1})\\&+(x_n^{m+1}+iy_n^{m+1})[1-x_n^m(x_n^m-iy_n^m)](1-z_n^{m-1})\}\\&-\tfrac{1}{2}\{[1-(x_n^m)^2]A-x_n^my_n^mB-x_n^mz_n^mC\}+y_n^m\zeta_n^m-z_n^m\eta_n^m\ ,\end{aligned} \tag{2.23a}$$

$$\dot{y}_n^m = -y_n^m + \frac{S}{D}\{(1-z_n^{m+1})z_n^m y_n^m(1-z_n^{m-1}) - (x_n^{m+1}+iy_n^{m+1})z_n^m y_n^m(x_n^{m-1}-iy_n^{m-1})$$
$$+(1-z_n^{m+1})[i-y_n^m(x_n^m+iy_n^m)](x_n^{m-1}-iy_n^{m-1})$$
$$-(x_n^{m+1}+iy_n^{m+1})[i+y_n^m(x_n^m-iy_n^m)](1-z_n^{m-1})\}$$
$$-\tfrac{1}{2}\{-x_n^m y_n^m A+[1-(y_n^m)^2]B-y_n^m z_n^m C\}+z_n^m\xi_n^m-x_n^m\xi_n^m , \tag{2.23b}$$

$$\dot{z}_n^m = -z_n^m - \frac{S}{D}\{(1-z_n^{m+1})[1-(z_n^m)^2](1-z_n^{m-1}) - (x_n^{m+1}+iy_n^{m+1})[1-(z_n^m)^2](x_n^{m-1}-iy_n^{m-1})$$
$$+(1-z_n^{m+1})z_n^m(x_n^m+iy_n^m)(x_n^{m-1}-iy_n^{m-1})$$
$$+(x_n^{m+1}+iy_n^{m+1})z_n^m(x_n^m-iy_n^m)(1-z_n^{m-1})\}$$
$$-\tfrac{1}{2}\{-x_n^m z_n^m A-y_n^m z_n^m B+[1-(z_n^m)^2]C\}+x_n^m\eta_n^m-y_n^m\xi_n^m , \tag{2.23c}$$

where we have

$$D\equiv(x_n^{m+1}+iy_n^{m+1})(1+z_n^m)(x_n^{m-1}-iy_n^{m-1})$$
$$+(1-z_n^{m+1})(x_n^m+iy_n^m)(x_n^{m-1}-iy_n^{m-1})$$
$$+(x_n^{m+1}+iy_n^{m+1})(x_n^m-iy_n^m)(1-z_n^{m-1})$$
$$+(1-z_n^{m+1})(1-z_n^m)(1-z_n^{m-1}) , \tag{2.24a}$$

$$A\equiv\frac{\partial\mathcal{H}}{\partial x_n^m},\quad B\equiv\frac{\partial\mathcal{H}}{\partial y_n^m},\quad C\equiv\frac{\partial\mathcal{H}}{\partial z_n^m} . \tag{2.24b}$$

ξ_n^m, η_n^m, and ζ_n^m denote $3NM$ independent standard white-noise sources.

Although these equations may appear rather complicated, they have the distinct advantage that they are free of unphysical coordinate singularities and involve only rational expressions without any coordinate-based trigonometric functions.

We have used these equations to discuss several model problems.[3] In particular, we will discuss here a free relativistic fermion system in $d=2$. As an example for an interacting fermion model we choose the Thirring model[10] in the lattice formulation.

A system of free relativistic fermions in $d=2$ can be described by the following Hamiltonian:[11]

$$H=\sum_{n=1}^{N}\left[-\frac{1}{2a}(c_n^\dagger c_{n+1}+c_{n+1}^\dagger c_n)+mc_n^\dagger c_n(-1)^n\right] . \tag{2.25}$$

[$N=4(k-1)+2$, $k\in\mathbb{N}$, implies antiperiodic boundary conditions.] Via a Jordan-Wigner transformation[12] every Hamiltonian of N fermions can be mapped onto a multi-spin problem [# denotes † or nothing (no †)]:

$$c_n^{\#}=\left[\prod_{j=1}^{n-1}[-\sigma_3(j)]\sigma^-(n)\right]^{\#},\quad \forall n>1 , \tag{2.26a}$$

$$c_1^{\#}=[\sigma^{-1}(1)]^{\#} , \tag{2.26b}$$

$$\sigma^-(n)=\tfrac{1}{2}[\sigma_1(n)-i\sigma_2(n)] . \tag{2.26c}$$

For our Hamiltonian we end up with the XX model with a space-dependent external field:

$$H=\sum_{n=1}^{N}\left[-\frac{1}{4a}[\sigma_1(n)\sigma_1(n+1)+\sigma_2(n)\sigma_2(n+1)]+\frac{m}{2}[\sigma_3(n)+1](-1)^n\right] . \tag{2.27}$$

Using spin coherent states we obtain a complex action, which reads, in the x,y,z representation,

$$S=\sum_{n,m=1}^{N,M}[-\ln\langle x_n^{m+1},y_n^{m+1},z_n^{m+1}\,|\,x_n^m,y_n^m,z_n^m\rangle$$
$$-\tfrac{9}{4}(x_n^m x_{n+1}^m+y_n^m y_{n+1}^m)+\overline{m}\tfrac{3}{2}(-1)^n z_n^m] \tag{2.28}$$

with $M=\beta/a$ and $\overline{m}=ma$.

We are now able to use straightforward equations (2.23), where we have

$$A=-\tfrac{9}{4}(x_{n+1}^m+x_{n-1}^m) , \tag{2.29a}$$

$$B=-\tfrac{9}{4}(y_{n+1}^m+y_{n-1}^m) , \tag{2.29b}$$

$$C=\tfrac{3}{2}(-1)^n\overline{m} . \tag{2.29c}$$

The lattice Hamiltonian for the Thirring model in Kogut-Susskind form reads

$$H=\sum_{n=1}^{N}\left[-\frac{1}{2a}(c_n^\dagger c_{n+1}+c_{n+1}^\dagger c_n)-\frac{g^2}{4}(c_n^\dagger c_n-c_{n+1}^\dagger c_{n+1})^2\right] . \tag{2.30}$$

In a Jordan-Wigner representation this model is identical to the XXZ model:

$$H=\sum_{n=1}^{N}\left[-\frac{1}{4a}[\sigma_1(n)\sigma_1(n+1)+\sigma_2(n)\sigma_2(n+1)]+\frac{g^2}{8}[\sigma_3(n)\sigma_3(n+1)-1]\right]. \tag{2.31}$$

For the action we obtain

$$S=\sum_{n,m=1}^{N,M}\left[-\ln\langle x_n^{m+1},y_n^{m+1},z_n^{m+1}\,|\,x_n^m,y_n^m,z_n^m\rangle-\tfrac{9}{4}(x_n^m x_{n+1}^m+y_n^m y_{n+1}^m)+\frac{9\bar{g}^2}{8}(z_n^m z_{n+1}^m)\right], \tag{2.32}$$

with $\bar{g}^2=g^2a$. For C one gets

$$C=9\bar{g}^2/8(z_{n+1}^m+z_{n-1}^m)\,. \tag{2.33}$$

A and B are identical with the results of the free system given before.

III. NUMERICAL METHOD AND RESULTS

As discussed in Sec. I we choose an Itô-type SDE, for which a suitable two-stage Runge-Kutta algorithm has been found.[5] We give here a brief sketch of this algorithm for a vector Itô SDE with multiplicative noise. For the estimates of the systematical errors caused by the discretization we refer to Ref. 5.

Consider the general Itô SDE of the following form:

$$dx^i(t)=b^i(\{x^k(t)\})dt+a^{ij}(\{x^k(t)\})dw^j(t)\,,\qquad i,j,k\in I\,. \tag{3.1}$$

The two-stage algorithm with step size h is then given by

$$\omega_1^i=b^i(\{x_t^k\})\,, \tag{3.2a}$$

$$g_0^{ij}=a^{ij}(\{x_t^k\})\,, \tag{3.2b}$$

$$g_1^{ij}=a^{ij}(\{x_t^k+\sqrt{h/2}g_0^{km}z_1^m\})\,, \tag{3.2c}$$

$$g_2^{ij}=a^{ij}(\{x_t^k+h\omega_1^k+\sqrt{h/2}g_0^{km}z_1^m\})\,, \tag{3.2d}$$

$$\omega_2^i=b^i(\{x_t^k+h\omega_1^k+\sqrt{h}g_0^{km}z_0^m\})\,, \tag{3.2e}$$

$$x_{t+h}^i=x_t^i+\tfrac{1}{2}h(\omega_1^i+\omega_2^i)+\tfrac{1}{2}\sqrt{h}(g_1^{ij}+g_2^{ij})z_0^j\,. \tag{3.2f}$$

z_0 and z_1 are two independent sets of standard normal random variables:

$$\langle z_\alpha^i\rangle=0,\quad \langle z_\alpha^i z_\beta^j\rangle=\delta_{\alpha\beta}\delta_{ij},\quad \alpha,\beta=0,1\,. \tag{3.3}$$

Applying this algorithm to the U(1) problem we simulated the theory on a 20×20 lattice. For each value, we generated 4000 configurations, discarded the first 1000 of them, and measured every fifth one thereafter. As may be seen in Fig. 1 we obtained with fictitious time step size $h=0.01$ for the average of the real part of the plaquette an excellent agreement with the exact solution in the thermodynamic limit, which is given by the solid line. It can be supposed that the effects of the temporal gauge superposed by the effects of finite size are still small on a 20×20 lattice.

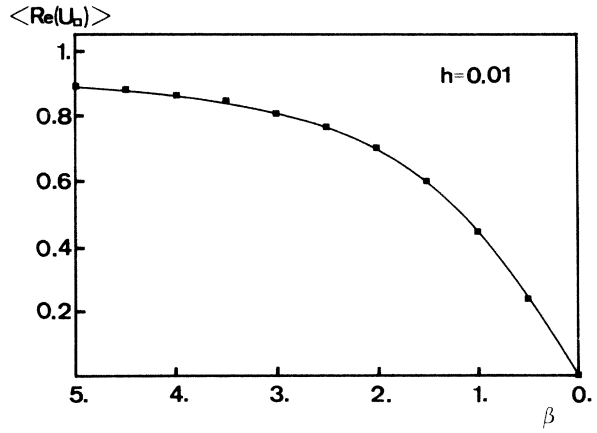

FIG. 1. $\langle \mathrm{Re}(U_\Box)\rangle$ for the pure U(1) theory on 20×20 lattice using Wilson action in temporal gauge (statistical errors are within the points); the solid line gives the exact result for the Wilson action for $\langle \mathrm{Re}(U_\Box)\rangle$ in the thermodynamic limit.

The order parameter $\langle \psi_n\sigma_3\psi_n^\dagger\rangle$ of the free relativistic fermion system in $d=2$ can be mapped according to Ref. 11 onto

$$\langle \psi_n\bar{\psi}_n\rangle\equiv\frac{2}{N}\left\langle\sum_{n=1}^{N}c_n c_n^\dagger(-1)^n\right\rangle \tag{3.4}$$

due to translation invariance.

Using the improved two-stage algorithm we calculated the order parameter on a 10×10 lattice with stepsize $h=0.01$. Reasonably good results were obtained by generating 8000 configurations again discarding the first 1000, and measuring every fifth one thereafter. Figure 2 shows the expected behavior for such a system. We also transformed the Itô equations to a Stratonovich-type Langevin equation. Using the algorithm given in Refs. 5 and 6 we simulated the free relativistic fermion system

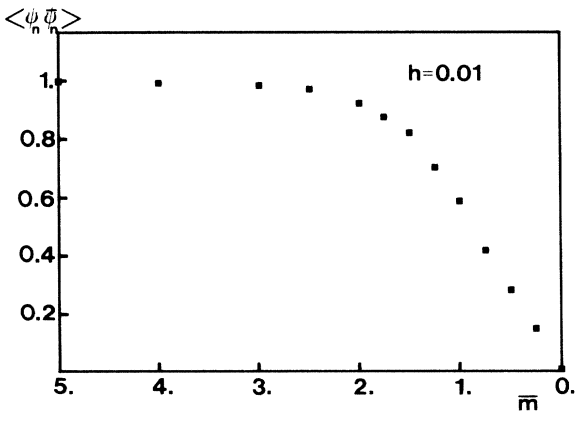

FIG. 2. The order parameter $\langle \psi_n\bar{\psi}_n\rangle$ for the free relativistic fermion theory on a 10×10 lattice (statistical errors are within the points).

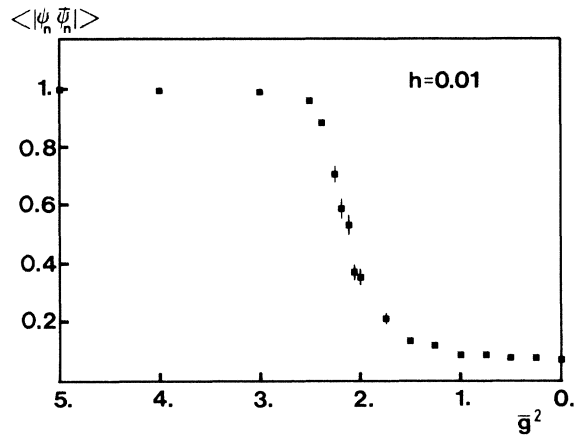

FIG. 3. $\langle\,|\,\psi_n\bar{\psi}_n\,|\,\rangle$ for the Thirring model on a 10×10 lattice (statistical errors are within the points or indicated by vertical bars).

based also on the Stratonovich-type SDE. Comparing the Stratonovich with the Itô procedure we got the same results consistent within statistical errors.

For the Thirring model one expects a degenerate ground state. Because of the finite size of the lattice the system will tunnel between the two possible ground states in the coupling region with broken symmetry. Using time averaging a direct measurement of the order parameter is nearly impossible; thus, we measured, according to Ref. 13,

$$\langle\,|\,\psi_n\bar{\psi}_n\,|\,\rangle=\frac{2}{N}\left\langle\left|\sum_{n=1}^{N}(-1)^n c_n c_n^{\dagger}\right|\right\rangle . \tag{3.5}$$

Again using $h=0.01$ we simulated the Thirring model on a 10×10 lattice. Since this system shows larger fluctuations than the free model we generated up to 10000 configurations, otherwise we proceeded as with the free system. As may be seen in Fig. 3 we obtained the expected behavior.

(1) There exists a coupling region where $\langle\,|\,\psi_n\bar{\psi}_n\,|\,\rangle$ is very small and about constant; thus one would expect a vanishing order parameter due to

$$|\,\langle\psi_n\bar{\psi}_n\rangle\,|\le\langle\,|\,\psi_n\bar{\psi}_n\,|\,\rangle . \tag{3.6}$$

(2) There is a region for which one would expect broken symmetry in the thermodynamic limit.

Surprising are the results for the imaginary parts of the expectation values of both fermion models, which are consistently of a magnitude 10^{-2}–10^{-3}. This is smaller than the statistical errors of the real parts. Within our statistical accuracy a fictitious time step size of $h=0.01$ seems to be the optimal choice, since we could not obtain a significant change in the results by going to $h<0.01$ for all systems investigated using the improved two-stage algorithm. The results for the systems investigated indicate that the Langevin approach to classical statistical systems and quantum systems and especially the complex approach to fermionic (multispin) systems show very reasonable convergence properties in an acceptable amount of C.P. time.

ACKNOWLEDGMENTS

The calculations were performed on the UNIVAC 1100/81 of the RZ Graz and on the VAX 11/750 of the EDV Center of the University Graz.

[1]J. R. Klauder, J. Phys. A **16**, L317 (1983); in *Recent Developments in High-Energy Physics,* proceedings of the XXII Schladming Conference (Acta Phys. Austriaca Suppl. 25), edited by H. Mitter and C. B. Lang (Springer, New York, 1983).

[2]G. Parisi and Wu Yong-Shi, Sci. Sin. **24**, 483 (1981); G. Parisi, Phys. Lett. **131B**, 393 (1983).

[3]H. Gausterer and J. R. Klauder, Phys. Lett. **164B**, 127 (1985); Phys. Rev. Lett. **56**, 306 (1986); H. Gausterer, in *Proceedings of Path Integrals from meV to MeV,* edited by M. Gutzwiller *et al.* (World Scientific, Singapore, to be published).

[4]L. Arnold, *Stochastic Differential Equations* (Wiley, New York, 1974); C. W. Gardiner, *Handbook of Stochastic Methods* (Springer, Berlin, 1983).

[5]J. R. Klauder and W. R. Petersen, SIAM J. Numer. Anal. **22**, 1153 (1985).

[6]P. E. Kloeden and R. A. Pearson, J. Austral. Math. Soc. **20B**, 8 (1977).

[7]K. G. Wilson, Phys. Rev. D **10**, 2445 (1974).

[8]J. M. Drouffe and C. Itzykson, Phys. Rep. **38C**, 133 (1978); A. Duncan and H. Vaidya, Phys. Rev. D **20**, 903 (1979).

[9]J. R. Klauder, J. Math. Phys. **4**, 1058 (1963); **23**, 1797 (1982).

[10]W. Thirring, Ann. Phys. (N.Y.) **3**, 91 (1958).

[11]L. Susskind, Phys. Rev. D **16**, 3031 (1977); J. Kogut and L. Susskind, *ibid.* **11**, 395 (1975).

[12]P. Jordan and E. Wigner, Z. Phys. **47**, 631 (1928).

[13]O. G. Mouritsen, *Computer Studies of Phase Transitions and Critical Phenomena* (Springer Series in Computational Physics) (Springer, Berlin, 1984).