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Ito's theorem and stochastic simulation

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Abstract. Using Ito's theorem we derive second-order formulae for the numerical integration of Langevin equations. We also show how constrained systems can be handled and hence how stochastic simulation can be applied to U(1), SU(2) and SU(3) variables.

1. Introduction

In this paper we will show that the problem of solving a set of coupled stochastic differential equations, the Langevin equations, is equivalent to evaluating multidimensional integrals of the type which occur in lattice regulated quantum field theory. Parisi and Wu (1981) have used this correspondence to postulate the so-called stochastic quantisation prescription for quantum field theory. However, our motivation is more pedestrian: we want to derive numerical methods for integrating Langevin equations and hence for evaluating functional integrals. Much work has already been done in this direction by Parisi (1981, 1982) and Drummond *et al* (1983). We will show that the use of Ito's theorem provides a simple systematic way of producing discrete versions of the Langevin equations and of handling constrained systems.

In § 2 we will state the connection between a set of Langevin equations and a multidimensional integral over a probability density. This will involve the introduction of the Fokker–Planck equation, which is also discussed (from a geometrical point of view) in the appendix. Ito's theorem is introduced in § 3 and used to derive some useful expressions from the calculus of stochastic variables. In § 4 we derive a discrete version of the Langevin equations using our previous results. In §§ 5 and 6 we show how to handle constrained systems of variables, illustrating our methods by writing down Langevin equations for U(1), SU(2) and SU(3) variables. Finally we outline how stochastic methods can be applied to the field of current interest in particle physics.

2. Langevin and Fokker–Planck equations

In this paper we are interested in the properties of the set of n coupled Langevin equations:

$$\mathrm{d}u_i = f_i(u)\,\mathrm{d}t + \sqrt{2}g_{ij}(u)\,\mathrm{d}W_j, \qquad i, j = 1, \ldots, n, \tag{2.1}$$

where the W_i are a set of independent white noise processes, having the following properties:

$$\int_{\alpha}^{\beta} \mathrm{d}W_i = (\beta-\alpha)^{1/2}\xi_i, \tag{2.2}$$

$$\langle \mathrm{d}W_i\, \mathrm{d}W_j\rangle = \delta_{ij}\, \mathrm{d}t. \tag{2.3}$$

The ξ_i are a set of independent Gaussian random variables with zero mean and unit variance.

By solving (2.1) we mean integrating an ensemble of independent sets of Langevin equations and then averaging functions of the u_i over this ensemble. As is shown in books on stochastic calculus (Ricciardi 1977, Schuss 1980), this is equivalent to solving the Fokker–Planck equation

$$\partial P/\partial t = \partial^2((gg^{\mathrm{T}})_{ij}P)/\partial u_i\, \partial u_j - \partial(f_i P)/\partial u_i, \tag{2.4}$$

associated with (2.1) for the probability density $P(u, t)$ and then performing the integration of the desired function $F(u)$ over the density

$$\langle F(u)\rangle_t = \int P(u, t)F(u)\, \mathrm{d}^n u. \tag{2.5}$$

If we choose f_i such that the Fokker–Planck equation takes the form

$$\partial P/\partial t = (\partial/\partial u_i)[(gg^{\mathrm{T}})_{ij}(\partial P/\partial u_j + P\, \partial S(u)/\partial u_j)], \tag{2.6}$$

it is easy to show (Falcioni *et al* 1983) that the probability density relaxes to the Boltzmann factor† i.e.

$$\lim_{t\to\infty} P(u, t) = \mathrm{e}^{-S(u)} \Big/ \int \mathrm{e}^{-S(u)}\, \mathrm{d}^n u, \tag{2.7}$$

and hence that

$$\lim_{t\to\infty} \langle F(u)\rangle_t = \int \mathrm{e}^{-S(u)} F(u)\, \mathrm{d}^n u \Big/ \int \mathrm{e}^{-S(u)}\, \mathrm{d}^n u. \tag{2.8}$$

Identifying $S(u)$ with the Euclidean lattice action we establish the link between the large time solution of a set of Langevin equations and lattice field theory.

By choosing the matrix g we can consider cases where there exist constraints between the variables u_i, as is shown in §§ 5, 6 and the appendix.

3. Ito's theorem and stochastic calculus

If the time evolution of the u_i is given by the Langevin equation (2.1) the differential change in a function $y = y(u, t)$ of the u_i is given (Schuss 1980) by Ito's theorem:

$$\mathrm{d}y = \left(\frac{\partial y}{\partial t} + f_i \frac{\partial y}{\partial u_i} + (gg^{\mathrm{T}})_{ij} \frac{\partial^2 y}{\partial u_i\, \partial u_j}\right) \mathrm{d}t + \sqrt{2} g_{ij} \frac{\partial y}{\partial u_i}\, \mathrm{d}W_j. \tag{3.1}$$

The presence of the second derivative term should be noted; it arises from the fact that

$$\mathrm{O}(\mathrm{d}W_i\, \mathrm{d}W_j) = \mathrm{O}(\mathrm{d}t).$$

† For gauge theories this proof breaks down because the normalisation factor in (2.7) is infinite; however, Floratas and Iliopoulos (1983) showed by perturbation theory that (2.8) still held for gauge invariant functions.

Ito's theorem is central to the calculus of stochastic variables and enables us to derive formulae for integration by parts and hence for Taylor series, as is shown in the rest of this section.

Consider the extended set of stochastic differential equations, in block form:

$$\begin{pmatrix} \mathrm{d}u_i \\ \mathrm{d}\tilde{u}_i \end{pmatrix} = \begin{pmatrix} f_i \\ 0 \end{pmatrix} \mathrm{d}t + \begin{pmatrix} \sqrt{2}g_{ij} & 0 \\ \delta_{ij} & 0 \end{pmatrix} \begin{pmatrix} \mathrm{d}W_j \\ \mathrm{d}\tilde{W}_j \end{pmatrix}. \tag{3.2}$$

By applying Ito's theorem for this extended system to the products $(\beta-t)y$ and $(W_j(\beta)-W_j(t))y$ we easily derive the formula for integration by parts of y with respect to t and W. In particular

$$\mathrm{d}(\beta-t)y = \left[-y+(\beta-t)\left(f_i\frac{\partial y}{\partial u_i}+(gg^{\mathrm{T}})_{ij}\frac{\partial^2 y}{\partial u_i\,\partial u_j}\right)\right]\mathrm{d}t+\sqrt{2}(\beta-t)\frac{\partial y}{\partial u_i}g_{ij}\,\mathrm{d}W_j, \tag{3.3}$$

which on integration gives

$$\int_\alpha^\beta y\,\mathrm{d}t = (\beta-\alpha)y(\alpha)+\int_\alpha^\beta(\beta-t)\left(f_i\frac{\partial y}{\partial u_i}+(gg^{\mathrm{T}})_{ij}\frac{\partial^2 y}{\partial u_i\,\partial u_j}\right)\mathrm{d}t + \sqrt{2}\int_\alpha^\beta(\beta-t)\frac{\partial y}{\partial u_i}g_{ij}\,\mathrm{d}W_j. \tag{3.4}$$

Similarly we have

$$\int_\alpha^\beta(\beta-t)y\,\mathrm{d}t = \tfrac{1}{2}(\beta-\alpha)^2y(\alpha)+\tfrac{1}{2}\int_\alpha^\beta(\beta-t)^2\left(f_i\frac{\partial y}{\partial u_i}+(gg^{\mathrm{T}})_{ij}\frac{\partial^2 y}{\partial u_i\,\partial u_j}\right)\mathrm{d}t + \frac{1}{\sqrt{2}}\int_\alpha^\beta(\beta-t)^2\frac{\partial y}{\partial u_i}g_{ij}\,\mathrm{d}W_j, \tag{3.5}$$

$$\int_\alpha^\beta y\,\mathrm{d}W_j = y(\alpha)(\beta-\alpha)^{1/2}\xi_j+\int_\alpha^\beta(W_j(\beta)-W_j(t))\left(f_i\frac{\partial y}{\partial u_i}+(gg^{\mathrm{T}})_{ij}\frac{\partial^2 y}{\partial u_i\,\partial u_j}\right)\mathrm{d}t, \tag{3.6}$$

$$\int_\alpha^\beta(\beta-t)y\,\mathrm{d}W_j = \tfrac{1}{2}(\beta-\alpha)^{3/2}y(\alpha)\xi_j + \int_\alpha^\beta(W_j(\beta)-W_j(t))(\beta-t)\left(f_i\frac{\partial y}{\partial u_i}+(gg^{\mathrm{T}})_{ij}\frac{\partial^2 y}{\partial u_i\,\partial u_j}\right)\mathrm{d}t. \tag{3.7}$$

By taking $\beta-\alpha=\Delta t$ we can use formulae (3.4)–(3.7) to build up a power series expansion of the integral

$$\int_t^{t+\Delta t} y\,\mathrm{d}t'$$

in terms of $\sqrt{\Delta t}$. This will be very useful when we come to discretise the set of Langevin equations (2.1) in § 4. Also we can use formulae (3.4)–(3.7) to derive Taylor series for $y(u(t+\Delta t))$:

$$y(u(t+\Delta t)) = y(u(t))+\int_t^{t+\Delta t}\mathrm{d}y, \tag{3.8}$$

$$y(u(t+\Delta t)) = y(u(t))+\int_t^{t+\Delta t}\left(f_i\frac{\partial y}{\partial u_i}+(gg^{\mathrm{T}})_{ij}\frac{\partial^2 y}{\partial u_i\,\partial u_j}\right)\mathrm{d}t+\sqrt{2}\int_t^{t+\Delta t}\frac{\partial y}{\partial u_i}g_{ij}\,\mathrm{d}W_j \tag{3.9}$$

$$= y(u(t))+(2\Delta t)^{1/2}\left(\frac{\partial y}{\partial u_i}g_{ij}\right)_t\xi_j+\Delta t\left(f_i\frac{\partial y}{\partial u_i}+(gg^{\mathrm{T}})_{ij}\frac{\partial^2 y}{\partial u_i\,\partial u_j}\right)_t+-+. \tag{3.10}$$

4. Discretisation of Langevin equation

Consider the simple set of Langevin equations

$$\mathrm{d}u_i = f_i \,\mathrm{d}t + \sqrt{2}\,\mathrm{d}W_i. \tag{4.1}$$

This can be converted into the equivalent set of integral equations

$$u_i(+\Delta t) = u_i(t) + \int_t^{t+\Delta t} f_i \,\mathrm{d}t' + \sqrt{2}\int_t^{t+\Delta t} \mathrm{d}W_i. \tag{4.2}$$

Using the definition of the white noise process the second integral can be immediately performed giving

$$u_i(t+\Delta t) = u_i(t) + \int_t^{t+\Delta t} f_i \,\mathrm{d}t' + (\Delta t)^{1/2}\xi_i. \tag{4.3}$$

We can approximate the remaining integral, using the results of § 3, as a power series in $\sqrt{\Delta t}$. To first order (i.e. $\mathrm{O}(\Delta t^{3/3})$) we have

$$u_i(t+\Delta t) = u_i(t) f_i + \Delta t f_i + (2\Delta t)^{1/2}\xi_i + \mathrm{O}(\Delta t^{3/2}), \tag{4.4}$$

while to second order (i.e. $\mathrm{O}(\Delta t)^{5/2})$)

$$u_i(t+\Delta t) = u_i(t) + (\delta_{ij} + \tfrac{1}{2}\Delta t\, \partial f_i/\partial u_j)[f_j \Delta t + (2\Delta t)^{1/2}\xi_j] + \tfrac{1}{2}(\Delta t)^2\, \partial^2 f_i/\partial u_j\, \partial u_j + \mathrm{O}(\Delta t^{5/2}). \tag{4.5}$$

It is interesting to note that using Taylor series the second-order formula (4.5) can be simplified to

$$u_i(t+\Delta t) = u_i(t) + \tfrac{1}{2}\Delta t(f_i(t) + f_i(t+\Delta t)) + (2\Delta t)^{1/2}\xi_i \tag{4.6}$$

which would be the result obtained if the integral in (4.3) was naively approximated using the trapezium rule.

For the more general set of Langevin equations (2.1) we easily derive the first-order formula

$$u_i(t+\Delta t) = u_i(t) + \Delta t f_i + (2\Delta t)^{1/2} g_{ij}\xi_j + \mathrm{O}(\Delta t^{3/2}). \tag{4.7}$$

The equivalent formula to (4.5) will be more complex: we do not derive it here.

In §§ 5 and 6 we show how Ito's theorem allows us to set up Langevin equations for constrained systems, that is cases where the u_i are not all independent. Section 5 treats the case of one equation of constraint, using U(1) and SU(2) variables as illustrative examples. The more complex case of several equations of constraint is handled in § 6, the example being SU(3).

5. Langevin equation for U(1) and SU(2) variables

We can write a U(1) variable as

$$U = u_1 + \mathrm{i}u_2, \tag{5.1}$$

subject to the constraint

$$u_1^2 + u_2^2 = 1. \tag{5.2}$$

Similarly we can write a SU(2) variable as

$$U = \begin{pmatrix} u_1 + \mathrm{i}u_2 & u_3 + \mathrm{i}u_4 \\ -u_3 + \mathrm{i}u_4 & u_1 - \mathrm{i}u_2 \end{pmatrix}, \tag{5.3}$$

subject to the constraint

$$u_1^2+u_2^2+u_3^2+u_4^2=1. \tag{5.4}$$

We will consider the two cases together, taking the equation of constraint to be

$$C(u)\equiv\tfrac{1}{2}u_\alpha u_\alpha=\tfrac{1}{2}. \tag{5.5}$$

We desire a Langevin equation which obeys this constraint. This will be achieved if at time zero $C(u)=\frac{1}{2}$ and for all later times

$$\mathrm{d}C(u)=0. \tag{5.6}$$

Using Ito's theorem this is equivalent to

$$(u_i f_i+(gg^{\mathrm{T}})_{ii})\,\mathrm{d}t+\sqrt{2}u_i g_{ij}\,\mathrm{d}W_j=0. \tag{5.7}$$

A suitable choice for the g_{ij} is

$$g_{ij}=\delta_{ij}-u_i u_j. \tag{5.8}$$

This choice of g_{ij} has the following properties at $C=\frac{1}{2}$:

$$u_i g_{ij}=0, \tag{5.9}$$

$$(gg^{\mathrm{T}})_{ij}=g_{ij}, \tag{5.10}$$

$$u_j(\partial/\partial u_i)(gg^{\mathrm{T}})_{ij}=-(gg^{\mathrm{T}})_{ii}, \tag{5.11}$$

$$(\partial/\partial u_i)(gg^{\mathrm{T}})_{ij}=-(\delta_{ii}-1)u_j. \tag{5.12}$$

A suitable choice of f_i is

$$f_i=-(gg^{\mathrm{T}})_{ij}\,\partial S(u)/\partial u_j+(\partial/\partial u_j)(gg^{\mathrm{T}})_{ij}. \tag{5.13}$$

The resulting Fokker–Planck equation is (see also the appendix)

$$\partial P/\partial t=(\partial/\partial u_i)[(gg^{\mathrm{T}})_{ij}(P\,\partial S/\partial u_j+\partial P/\partial u_j)], \tag{5.14}$$

whose large t solution relaxes to the Boltzmann factor (see § 2).

The choice (5.8) and (5.13) leads using (5.10) to the discrete formula

$$\Delta u_i=(\delta_{ij}-u_i u_j)\{-(\partial S/\partial u_j)\Delta t+(2\Delta t)^{1/2}\xi_j]-(\delta_{jj}-1)u_i\,\Delta t. \tag{5.15}$$

This discrete form of the Langevin equation will not obey the constraint to all orders of Δt, but we can compensate for this by renormalising the u_i after each time step:

$$u_i\to u_i/(u_\alpha u_\alpha)^{1/2}. \tag{5.16}$$

Parisi (1982) suggested that a simpler way of carrying out the stochastic simulation of U(1) and SU(2) would be to consider the unconstrained Langevin equation

$$\mathrm{d}\phi_i=-[\partial S(\phi)/\partial\phi_i]\,\mathrm{d}t+\sqrt{2}\,\mathrm{d}W_i \tag{5.17}$$

and the variable

$$u_i=\phi_i/(\phi_\alpha\phi_\alpha)^{1/2}.$$

Applying Ito's theorem to u_i and discretising gives

$$\Delta u_i=\left(-\frac{\partial u_i}{\partial\phi_j}\frac{\partial S}{\partial\phi_j}+\frac{\partial^2 u_i}{\partial\phi_j\,\partial\phi_j}\right)\Delta t+\frac{\partial u_i}{\partial\phi_j}(2\Delta t)^{1/2}\xi_j. \tag{5.18}$$

This agrees with the previous formula provided $\phi_\alpha\phi_\alpha=1$ at the start of the step, hence proving that Parisi's algorithm

$$\begin{aligned}&\phi_i(t+\Delta t)=\phi_i(t)-(\partial S/\partial\phi_i)\Delta t+(2\Delta t)^{1/2}\xi_i,\\&u_i(t+\Delta t)=\phi_i(t+\Delta t)/(\phi_\alpha(t+\Delta t)\phi_\alpha(t+\Delta t))^{1/2},\\&\phi_i(t+\Delta t)=u_i(t+\Delta t),\end{aligned}\tag{5.19}$$

will produce a sequence of SU(2) or U(1) elements with the correct limiting distribution, if the initial state obeys the constraint.

6. Langevin equation for SU(3) variables

We adopt the same approach as we did for the group SU(2). However, the greater complexity of SU(3) over SU(2) will be reflected in the resulting Langevin equation.

A general SU(3) matrix can be written

$$U=\begin{pmatrix}a_1 & a_2 & a_3\\ b_1 & b_2 & b_3\\ (\boldsymbol{a}^*\wedge\boldsymbol{b}^*)_1 & (\boldsymbol{a}^*\wedge\boldsymbol{b}^*)_2 & (\boldsymbol{a}^*\wedge\boldsymbol{b}^*)_3\end{pmatrix},\tag{6.1}$$

where

$$\boldsymbol{a}=\boldsymbol{x}+\mathrm{i}\boldsymbol{y},\qquad \boldsymbol{b}=\boldsymbol{s}+\mathrm{i}\boldsymbol{t},\tag{6.2}$$

are complex three-vectors obeying the four constraints

$$\boldsymbol{a}\cdot\boldsymbol{a}^*=1,\qquad \boldsymbol{b}\cdot\boldsymbol{b}^*=1,\tag{6.3}$$

$$\boldsymbol{a}\cdot\boldsymbol{b}^*=0\tag{6.4}$$

(the real and imaginary parts of the third equation forming two separate conditions).

We will find it more convenient to rearrange the constraints in the symmetric form

$$\begin{aligned}&C^1\equiv(1/\sqrt{8})(\boldsymbol{x}\cdot\boldsymbol{x}+\boldsymbol{y}\cdot\boldsymbol{y}+\boldsymbol{s}\cdot\boldsymbol{s}+\boldsymbol{t}\cdot\boldsymbol{t})=1/\sqrt{2},\\&C^2\equiv(1/\sqrt{8})(\boldsymbol{x}\cdot\boldsymbol{x}+\boldsymbol{y}\cdot\boldsymbol{y}-\boldsymbol{s}\cdot\boldsymbol{s}-\boldsymbol{t}\cdot\boldsymbol{t})=0,\\&C^3\equiv(1/\sqrt{2})(\boldsymbol{x}\cdot\boldsymbol{s}+\boldsymbol{y}\cdot\boldsymbol{t})=0,\qquad C^4\equiv(1/\sqrt{2})(-\boldsymbol{x}\cdot\boldsymbol{t}+\boldsymbol{s}\cdot\boldsymbol{y})=0,\end{aligned}\tag{6.5}$$

and to introduce the notation

$$u_j=(\boldsymbol{x},\boldsymbol{y},\boldsymbol{s},\boldsymbol{t}),\qquad j=1,\ldots,12.\tag{6.6}$$

Differentiating C^1 through C^4 gives, in block form,

$$\begin{aligned}&C_j^1=(1/\sqrt{2})(\boldsymbol{x},\boldsymbol{y},\boldsymbol{s},\boldsymbol{t}),\qquad C_j^2=(1/\sqrt{2})(\boldsymbol{x},\boldsymbol{y},-\boldsymbol{s},-\boldsymbol{t}),\\&C_j^3=(1/\sqrt{2})(\boldsymbol{s},\boldsymbol{t},\boldsymbol{x},\boldsymbol{y}),\qquad C_j^4=(1/\sqrt{2})(-\boldsymbol{t},\boldsymbol{s},\boldsymbol{y},-\boldsymbol{x}).\end{aligned}\tag{6.7}$$

It is easy to see, provided the constraints are obeyed, that the C_j^α form an orthonormal set, i.e.

$$C_j^\alpha C_j^\beta=\delta^{\alpha\beta}.\tag{6.8}$$

Extending the arguments of § 5 we require a Langevin equation which makes

$$\mathrm{d}C^\alpha=0,\qquad \alpha=1,2,3,4.\tag{6.9}$$

More explicitly we want to choose g_{ij} and f_i such that

$$(f_i\, \partial C^\alpha/\partial u_i + (gg)^{\mathrm{T}}_{ij}\, \partial^2 C^\alpha/\partial u_i\, \partial u_j)\, \mathrm{d}t + \sqrt{2} g_{ij}(\partial C^\alpha/\partial u_i)\, \mathrm{d}W_j = 0. \tag{6.10}$$

A suitable choice for g_{ij} is

$$g_{ij} = \delta_{ij} - C_i^\alpha C_j^\alpha, \tag{6.11}$$

and for the f_i

$$f_i = -(gg^{\mathrm{T}})_{ij}\, \partial S/\partial u_j + (\partial/\partial u_j)(gg^{\mathrm{T}})_{ij}, \tag{6.12}$$

as can easily be verified using the properties of the C_j^α, namely

$$C_i^\gamma g_{ij} = 0 \qquad \text{for all } \gamma, \tag{6.13}$$

$$(gg^{\mathrm{T}})_{ij} = g_{ij}, \tag{6.14}$$

$$C_i^\gamma\, (\partial/\partial u_j)(gg^{\mathrm{T}})_{ij} = -(gg^{\mathrm{T}})_{ij} C_{ij}^\gamma, \tag{6.15}$$

$$(\partial/\partial u_j)(gg^{\mathrm{T}})_{ij} = -4u_i, \tag{6.16}$$

provided constraints (6.5) are obeyed. The form of Langevin equation we use for numerical work is, in discrete form,

$$\Delta u_i = (\delta_{ij} - C_i^\alpha C_j^\alpha)[-(\partial S/\partial u_j)\Delta t + (2\Delta t)^{1/2}\xi_j] - 4u_i\, \Delta t. \tag{6.17}$$

As for the SU(2) it is easy to show that the large time solution of the Fokker–Planck equation corresponding to our choice of g_{ij} and f_i converges to the desired Boltzmann factor.

Our discrete version of the constrained Langevin equation will only approximately generate a set of SU(3) matrices (to $O(\Delta t^{3/2})$). Hence it will be necessary to reimpose the constraints after each time step.

7. Stochastic methods in field theory

In quantum field theory we often wish to calculate connected Green functions of the form

$$\langle I(u)J(u)\rangle_{\mathrm{c}} \equiv \langle I(u)J(u)\rangle - \langle I(u)\rangle\langle J(u)\rangle, \tag{7.1}$$

where $\langle\ \rangle$ denotes integration over a probability density. Using stochastic methods we could evaluate (7.1) by calculating each term on the right-hand side separately (see § 2). However, there is an alternative procedure using the fluctuation–dissipation theorem.

We can add a source term $\lambda J(u)$ to the action $S(u)$ and note that

$$\langle I(u)J(u)\rangle_{\mathrm{c}} = \frac{\partial}{\partial\lambda}\left(\frac{\int \mathrm{e}^{-S(u)+\lambda J(u)} I(u)\, \mathrm{d}^n u}{\int \mathrm{e}^{-S(u)+\lambda J(u)}\, \mathrm{d}^n u}\right)\Bigg|_{\lambda=0}. \tag{7.2}$$

This suggests considering the λ dependent set of Langevin equations (initially we take the u_i to be unconstrained for simplicity)

$$\mathrm{d}u_i = (-\partial S/\partial u_i + \lambda\, \partial J/\partial u_i)\, \mathrm{d}t + \mathrm{d}W_i. \tag{7.3}$$

Expanding u_i in powers of λ (Parisi and Wu 1981),

$$u_i = u_i^{(0)} + \lambda u_i^{(1)} + \tfrac{1}{2}\lambda^2 u_i^{(2)} + \dots,$$

substituting into (7.3) and equating powers of λ we obtain

$$du_i^{(0)} - \partial S/\partial u_i + dW_i, \tag{7.4}$$

$$du_i^{(1)} = -(\partial^2 S/\partial u_i\, \partial u_i)u_j^{(1)} + \partial J/\partial u_i, \tag{7.5}$$

where the derivatives are evaluated at $u_i = u_i^{(0)}$. The large time limit of the average of $u_i^{(1)}$ over the ensemble of stochastic differential equations converges to $\langle u_i J(u)\rangle_c$. Similarly by expanding $I(u)$ as a power series in λ we can calculate $\langle I(u)J(u)\rangle_c$.

We can use the same procedure for the constrained case. Additional complications arise, however, because we must expand the matrix $g_{ij}(u)$ in powers of λ. An alternative to the above is (Parisi 1982) to simulate equation (7.3) for $\lambda = 0$ and $\lambda = a$ small value, using the same set of random numbers in each case, and then form the derivative with respect to λ numerically. Whether using the fluctuation–dissipation theorem to calculate connected Green functions is more accurate than a direct evaluation of (7.1) must be decided by numerical experiment.

In summary, we have found a means of calculating the Green functions of a quantum field theory by numerically solving a coupled set of Langevin equations. For the unconstrained case we have derived a second-order algorithm for iterating the Langevin equations, and for the constrained case a first-order algorithm. A possible way of improving the performances of the first-order algorithm is to note (Drummond *et al* 1983) that it gives an error proportional to the step size Δt when used to calculate Green functions. If the calculation was repeated for several values of Δt the results could be extrapolated to $\Delta t = 0$. At present we are testing these ideas by numerical experiment.

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Appendix. Geometrical picture of the Fokker–Planck equation

Using the divergence theorem we can gain an interesting geometrical insight into the meaning of the Fokker–Planck equation. This will be particularly illuminating for the constrained case.

Consider a volume V enclosed by a surface Ω; integrating the Fokker–Planck equation over the volume V, we have for the unconstrained case

$$(\partial/\partial t)\int_V P\, d\tau = \int_\Omega (P\, \partial S/\partial u_i + \partial P/\partial u_i)\, d\sigma_i.$$

We can interpret this as a conservation theorem for 'probability mass'. The left-hand side is the rate of change of probability mass contained in V and the right-hand side is the flux of probability mass entering V through Ω.

For the constrained case we take V to be the part of the total space which obeys the constraints. The boundary of this region is given by the surfaces defined by the equation(s) of constraint. Integrating the Fokker–Planck equation as before, we obtain

$$(\partial/\partial t)\int_V P\,\mathrm{d}\tau=\int_\Omega (gg^{\mathrm{T}})_{ij}(P\,\partial S/\partial u_j+\partial P/\partial u_j)\,\mathrm{d}\sigma_i.$$

But $\mathrm{d}\sigma_i$ is in the direction of $\partial C/\partial u_i$, hence $(gg^{\mathrm{T}})_{ij}\,\mathrm{d}\sigma_i=0$,

$$(\partial/\partial t)\int_V P\,\mathrm{d}\tau=0.$$

If an ensemble of points is set up obeying the constraint(s) they will remain trapped in the volume of space obeying the constraints for all later times.

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