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Stochastic mechanics of Abelian lattice theories

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Abstract. A stochastic equation for lattice theories is written, which describes a Markov process on a space lattice evolving in (stochastic) time. At the cost of requiring the construction of the drift function, this reduces one dimension in numerical simulations, as compared to Monte Carlo methods. The drift can be obtained either from the asymptotic solution of an auxiliary equation or from a ground state ansatz. It is shown that for Abelian theories a drift can be constructed from ground state ansätze which are exact eigenstates of Hamiltonians with the same continuum limit as the Kogut-Susskind Hamiltonian. Lattice observables may be obtained from stochastic time correlations. In addition, a new method is obtained to measure the lowest excited state (mass gap) from the exit times of the stochastic process from a bounded region. In some cases the mass gap may be obtained at weak coupling from the theory of small random perturbations of dynamical systems.

1. Introduction

In recent years, numerical simulation of lattice systems has become increasingly popular for the study of phase diagrams, the string tension, the hadron spectrum, finite temperature phase transitions, etc. The procedure usually involves estimating expectation values of observables in a $d+1$ Euclidean spacetime lattice from averages over a subensemble of Boltzmann distributed field configurations generated by the Metropolis or heat bath algorithms.

Recently, other methods have been proposed, namely the microcanonical ensemble [1-3] and the Langevin equation [4-6] methods. The Langevin equation has been used in the stochastic quantisation [7, 8] context, where expectation values

$$\langle F(U) \rangle = \int [dU] F(U) e^{-S(U)} \left(\int [dU] e^{-S(U)} \right)^{-1} \quad (1.1)$$

are computed generating a Markov process $U(\tau)$ by a Langevin equation

$$dU(\tau) = b(U(\tau), \tau) d\tau + dW(\tau) \quad (1.2)$$

(with $b = \delta S / \delta U$ and $W(\tau)$ a Gaussian random variable) and using

$$\langle F(U) \rangle = \lim_{\tau \rightarrow \infty} \frac{1}{\tau} \int_0^\tau F(U(\tau)) d\tau \quad (1.3)$$

which holds whenever the process is ergodic. τ is an auxiliary time (computer time in actual calculations) not to be confused with physical time for the lattice system. The state space of the process $U(\tau)$ is the space of field configurations on the $d+1$ Euclidean lattice.

There is, however, another way to use the Langevin equation for lattice studies. This time one considers a lattice in d -dimensional space (not in $d + 1$ spacetime) and a process $U(s)$ defined on the space lattice and evolving in the time parameter s . $U(t)$ is a Markov diffusion obeying a stochastic differential equation as in (1.2) with a drift $b(U(s), s)$ chosen in such a way that the stationary probability density of the process coincides with the probability density of a quantum state. Furthermore the multitime correlations of the Markov process correspond to Euclidean quantum correlations, in a sense to be described below. For example, if $\phi_0 = \exp(R + iS)$ is the ground state of the Hamiltonian, a drift proportional to $E(R + S)$ (where E is the electric field operator) describes the ground state process. Let us describe briefly the stochastic formulation that we will be using, in the context of the Schrödinger equation.

Let $\phi(t, x)$ be a solution to the Schrödinger equation

$$i\hbar\partial_t\phi = -\frac{\hbar^2}{2m}\Delta\phi + V(x)\phi. \tag{1.4}$$

The position probability density $\rho(t, x) = |\phi(t, x)|^2$ obeys the equation

$$\frac{\partial\rho}{\partial t} = -\frac{\partial}{\partial x^k}\{b^k\rho\} + \frac{\hbar}{2m}\Delta\rho \tag{1.5}$$

where

$$b^k = \frac{\hbar}{2m}\frac{\partial}{\partial x^k}\ln(\phi\phi^*) + \frac{\hbar}{2im}\frac{\partial}{\partial x^k}\ln\left(\frac{\phi}{\phi^*}\right) = u(t, x) + v(t, x). \tag{1.6}$$

Associated to the (Fokker-Planck) equation (1.5) is a stochastic differential equation (SDE)

$$dX_s = b ds + (\hbar/m) dW_s. \tag{1.7}$$

The invariant probability density of the stochastic process associated to this SDE coincides with the position probability $|\phi(t, x)|^2$ for each t . Therefore the quantum mechanical (QM) expectation in the state ϕ of any function of the coordinates will coincide with the statistical expectation on the process

$$Ef(X_s) = \int f(x)\rho(x) d^n x = (\phi, f\phi). \tag{1.8}$$

When ϕ is a stationary process expectations involving multitime correlations also have a QM interpretation. Consider the two-time correlation

$$\begin{aligned} Ef(X_s)f(X_0) &= \iint f(x)P(s, x_0, dx)f(x_0)\rho(x_0) d^n x_0 \\ &= \int (T_s f)(x_0)f(x_0)\rho(x_0) d^n x_0 \\ &= \int f(x_0)\exp[-(s/\hbar)(\phi^{-1}H\phi - E)]f(x_0)\phi^2(x_0) d^n x_0 \end{aligned}$$

where $P(s, x_0, dx)$ is the transition probability for the Markov process and T_s the associated semigroup with generator $(\phi^{-1}H\phi - E)$. Hence

$$Ef(X_s)f(X_0) = e^{(s/\hbar)E}(f\phi, e^{-(s/\hbar)H}f\phi) \tag{1.9}$$

where E is the energy of the stationary state ϕ . Similar expressions hold for the general multitime correlations on the stationary process. For example

$$Ef(X_{s+s'})f(X_s)f(X_0) = e^{(E/\hbar)(s+s')} (f\phi, e^{-(s'/\hbar)H} f e^{-(s/\hbar)H} f\phi). \tag{1.10}$$

We may therefore say that the process (1.7), although formally obtained from a real-time Schrödinger equation, actually describes Euclidean evolution and Euclidean correlations in the precise sense of (1.9) and (1.10) (for a stationary ϕ).

The stochastic differential equation (1.7), related to the Schrödinger equation (1.4), is formally similar to the equation of the Fényes–Nelson [9, 10] stochastic formulation of quantum mechanics. However, at no point have we used Nelson’s quantisation procedure, nor is any identification made of the (stochastic) time s in (1.7)–(1.10) with real physical time.

The fact that the multitime correlations are associated to Euclidean-like matrix elements and not to real time correlations (nor to results of repeated physical measurements) has, in the past, been a source of confusion in the interpretation of stochastic mechanics [11, 12]. However, it is this very Euclidean nature with its time-decaying exponentials that makes the correlations perhaps even more useful to extract physical quantities like the spectrum of excitations above the state ϕ with quantum numbers controlled by f (see § 3).

In this paper and elsewhere we have used the stochastic process (1.7) merely to compute Euclidean correlations and eigenvalues. In this way all quantities that are computed have exactly the same interpretation as in conventional quantum mechanics.

In addition to operator matrix elements and Euclidean correlations from time averages the stochastic process associated to the SDE (1.7) also provides a way to determine eigenvalues from the distribution of exit times from a bounded region (§ 3).

Construction of the process (1.7) is straightforward if an eigenstate of the Hamiltonian is known. If this is not the case it is possible to construct the drift directly from the interaction potential. This is relatively easy in the case of the ground state process. Let $\phi_E(t, x)$ be a solution to the Euclidean Schrödinger equation

$$\partial_t \phi_E = \frac{\hbar}{2m} \Delta \phi_E - \frac{1}{\hbar} V(x) \phi_E \tag{1.11}$$

corresponding to an initial condition $f(x)$. If $f(x)$ is not orthogonal to the ground state ϕ_0 , then the limit

$$\lim_{t \rightarrow \infty} e^{(t/\hbar)E_0} \phi_E(t, x)$$

is proportional to $\phi_0(x)$. Consider now the following quantities associated to the Euclidean solution

$$u_E(t, x) = \frac{\hbar}{2m} \nabla \ln |\phi_E|^2 \tag{1.12a}$$

$$v_E(t, x) = \frac{\hbar}{2im} \nabla \ln \left(\frac{\phi_E}{\phi_E^*} \right). \tag{1.12b}$$

They obey the equations

$$\frac{\partial u_E}{\partial t} = \frac{1}{2} \nabla (u_E^2 - v_E^2) + \frac{\hbar}{2m} \nabla (\nabla u_E) - \frac{1}{m} \nabla V(x) \tag{1.13}$$

$$\frac{\partial v_E}{\partial t} = \frac{\hbar}{2m} \nabla (\nabla v_E) + \nabla (u_E \cdot v_E). \tag{1.14}$$

From the asymptotic form of the solutions one obtains the drift of the ground state process

$$b(x) = u_0(x) + v_0(x)$$

where

$$\lim_{t \rightarrow \infty} u_E(t, x) = u_0(x) \tag{1.15a}$$

$$\lim_{t \rightarrow \infty} v_E(t, x) = v_0(x). \tag{1.15b}$$

Similarly one obtains equations that, given the interaction potential, determine the drift for a stationary process at positive temperature T [13].

In the next section we discuss the stochastic formulation of lattice gauge theories and in § 3 the measurement and estimates of lattice observables using this formalism.

2. The stochastic formulation of lattice theories

One writes the lattice gauge theory Hamiltonians as

$$H = \frac{g^2}{2a} \sum_l E_l^2 - \frac{1}{ag^2} \sum_p M_p \tag{2.1}$$

where M_p is a function of the plaquette variables and the electric field operators E_l^α are defined by their commutation relations with the link variables U_l

$$[E_l^\alpha, U_l] = \delta_{ll'} U_l \xi^\alpha \tag{2.2a}$$

$$[E_l^\alpha, U_l^\dagger] = -\delta_{ll'} \xi^\alpha U_l^\dagger \tag{2.2b}$$

ξ^α being an element of the Lie algebra of the gauge group G .

If $G = U(1)$ one may use the representation $E_l = -i\partial/\partial\theta_l$, $U_l = e^{i\theta_l}$. From the Schrödinger equation

$$i \frac{\partial}{\partial t} \psi(t, U_l) = H\psi(t, U_l) \tag{2.3}$$

and its adjoint, one obtains a (Fokker-Planck) equation for the probability density $\rho(s, U_l) = |\phi|^2$.

$$\frac{\partial}{\partial s} \rho = \frac{\nu^2}{2} \sum_l \frac{\partial^2}{\partial \theta_l^2} \rho - \sum_l \frac{\partial}{\partial \theta_l} \{ \rho b_l \} \tag{2.4}$$

with $\nu = g/\sqrt{a}$ and a drift

$$b_l = \frac{g^2}{a} \frac{\partial}{\partial \theta_l} \{ \log |\psi| + \arg \psi \}. \tag{2.5}$$

From this one deduces the stochastic differential equation

$$d\theta_l = b_l ds + \nu dW_l \tag{2.6}$$

with the normalisation $\langle dW_l dW_l \rangle = \delta_{ll'} ds$ for the Wiener process.

For $G = SU(N)$ one may use the representation

$$E_l^\alpha \sim \sum_{ab} \left\{ (U_l \xi^\alpha)_{ab} \frac{\partial}{\partial (U_l)_{ab}} - (U_l \xi^\alpha)_{ab}^* \frac{\partial}{\partial U_{lab}^*} \right\}$$

to deduce the Fokker-Planck equation for $\rho = |\phi(t, U_i)|^2$

$$\frac{\partial}{\partial s} \rho = -\frac{g^2}{2a} \sum_{l,\alpha} E_l^\alpha E_l^\alpha \rho + \sum_{l,\alpha} E_l^\alpha \{ \rho b_l^\alpha \} \tag{2.7}$$

with drift

$$b_l^\alpha = \frac{g^2}{a} E_l^\alpha \{ \log|\psi| + \arg \psi \}. \tag{2.8}$$

The resulting stochastic equation is

$$U_l^{-1} dU_l = -\left\{ \sum_{\alpha} \xi^\alpha b_l^\alpha + \frac{g^2}{2a} \frac{N^2 - 1}{2N} \right\} ds + \frac{g}{\sqrt{a}} i \sum_{\alpha} \xi^\alpha dW_l^\alpha \tag{2.9}$$

with

$$\langle dW_l^\alpha dW_l^\beta \rangle = \delta^{\alpha\beta} \delta_{ll'} ds$$

and

$$\text{Tr}(\xi^\alpha \xi^\beta) = \delta^{\alpha\beta} / 2.$$

Once the drift function b_l is known the lattice theory is completely determined by (2.6) or (2.9), from which information on the physical observables may be extracted by stochastic methods (§ 3).

One is now left with the problem of finding a drift for the stochastic equations in such a way that the generator of the process coincides or, at least approximates, the Hamiltonian. Our main concern will be the ground state process. As described in § 1 there are two ways to obtain a drift for this process. In the first, one uses an Euclidean version of the dynamical equations that determine the drift and the asymptotic solution to these equations tends to the exact drift associated to the assumed Hamiltonian. The second method consists in using an exact or approximate eigenstate of the theory.

In general, given a lattice Hamiltonian, it is very hard to find a good analytic approximation to the ground state ψ_0 , so that the drift can be recovered from $\nabla\{\log|\psi_0| + \arg \psi_0\}$. For example, if H_{KS} is the usual Kogut-Susskind [14] lattice Hamiltonian, a variational approach to find ψ_0 seems to fare poorly. In particular, a variational calculation of the mass gap [15] indicates that independent plaquette ansätze minimising $\langle H_{KS} \rangle$ seem to be far from the scaling region. Furthermore, for an exponential ansatz that minimises $\langle H_{KS} \rangle$, the reconstruction algorithm [16] has been used to find the Hamiltonian H_R for which the ansatz becomes an exact eigenstate. The conclusion is that, as coupling constant functions, H_R and H_{KS} belong to distinct functional classes. Hence they, most probably, belong to different universality classes.

Lattice gauge theory, considered as a regularisation device for the continuum fields, is, however, in the particular situation that instead of a fixed Hamiltonian, one deals with a whole family of Hamiltonians which are, in principle, equally good provided they reduce in the classical continuum limit to the QED or QCD forms. By classical continuum limit we mean here not only the ($a \rightarrow 0, g$ fixed) limit, but also the limit that takes into account the renormalisation group a dependence of the coupling constants ($a \rightarrow 0, g(a) \rightarrow g^*$).

Convergence of a lattice Hamiltonian to the continuum in one of these limits does not guarantee, of course, that the whole physical content of the continuum theory is recovered. That would require convergence of the Green functions as well.

Using the freedom of choice for the lattice Hamiltonian one may turn the variational argument around and, given, for example, an independent plaquette ansatz $\phi(\gamma) = \prod_p f_p(\gamma(g))$, instead of looking for the set of parameters $\gamma(g)$ that minimises $\langle H_{KS} \rangle$, look for parameters $\tilde{\gamma}(g)$ such that the Hamiltonian $H(\tilde{\gamma})$ reconstructed [16] from $\phi(\tilde{\gamma})$ has the same continuum limit as H_{KS} . For $H(\tilde{\gamma})$, the state $\phi(\tilde{\gamma})$ would then be an exact eigenstate and the drift that one computes from $\nabla\{\log|\phi(\tilde{\gamma})| + \arg \phi(\tilde{\gamma})\}$ an exact drift of a process for which the generator $= H(\tilde{\gamma})$ has the desired classical continuum limit.

In this method, to obtain a drift for the stochastic equation (2.6) we would attempt to find a state ψ which is an exact zero-energy eigenstate of a Hamiltonian of the form (2.1) reducing to

$$\frac{1}{2} \sum_l a^d \varepsilon_l^2 + \frac{1}{2} \sum_p a^d B_p^2 + O(a^{d+1}) \tag{2.10}$$

under the replacement

$$\theta_p \rightarrow a^{(d+1)/2} g B_p \tag{2.11a}$$

$$E_l \rightarrow a^{(d+1)/2} g^{-1} \varepsilon_l \tag{2.11b}$$

θ_p being the sum of oriented angle variables on the boundary of the plaquette p and d the (space) dimensionality of the lattice.

When the classical ($a \rightarrow 0$) limit is taken, one should beware of the behaviour of g -dependent contributions in the $O(a^{d+1})$ term of (2.10), because in asymptotically free theories $g \rightarrow 0$ as $a \rightarrow 0$.

We discuss here only the U(1) case. For simplicity, one looks for a state of the independent plaquette product form

$$\psi = \prod_p e^{\phi(\cos \theta_p)} \tag{2.12}$$

From the reconstruction algorithm [16], one knows that ϕ is a zero-energy eigenstate of the Hamiltonian

$$H_R = \frac{g^2}{2a} \sum_l \{E_l^2 - i[E_l, L_l] + L_l^2\} \tag{2.13a}$$

where

$$L_l = \frac{-iE_l \psi}{\psi} = \sum_{p(l)} \eta_p^l \sin \theta_p \phi'(\cos \theta_p). \tag{2.13b}$$

The sum is over the plaquettes that contain the link l and η_p^l is a + or - sign which depends on the orientation of the link l in the plaquette p .

We analyse now the small- a behaviour of the terms L_l^2 and $[E_l, L_l]$ in (2.13). With the replacement (2.11a) one obtains for $(g^2/2a)(L_l^2)$,

$$\frac{g^2}{2a} L_l^2 = \frac{a^d g^4}{2} \left\{ \sum_{p(l)} \eta_p^l B_p \phi'(1) \right\}^2 + O(a^{2d+1}). \tag{2.14}$$

Because of the signs η_p^l the sum is over terms of the form $a(\partial B/\partial x)$ for small a and if the space derivatives of the (magnetic) field B are finite the leading contribution is $O(a^{d+2})$ and vanishes in the continuum limit. However, if one requires $\phi'(1) = 0$, no assumption is required on the local finiteness of $\partial B/\partial x$. Also this procedure is more

satisfactory because one avoids inverse powers of g coming from the function ϕ (see below) which hinder the convergence for theories where $g(a) \rightarrow 0$ as $a \rightarrow 0$.

For $(-ig^2/2a)[E_l, L_l]$ one obtains

$$\begin{aligned}
 -i \sum_l \frac{g^2}{2a} [E_l, L_l] &= -\frac{g^2}{2a} \sum_l \sum_{\rho(l)} \{ \phi'(\cos \theta_\rho) \cos \theta_\rho - \phi''(\cos \theta_\rho) \sin^2 \theta_\rho \} \\
 &= -\frac{2g^2}{a} \sum_\rho \phi'(1) + g^4 \sum_\rho a^d B_\rho^2 \{ 3\phi''(1) + \phi'(1) \} + O(a^{2d+1}).
 \end{aligned}
 \tag{2.15}$$

Hence, one can recover the form (2.10) by requiring $\phi'(1) = 0$, $\phi''(1) = 1/6g^4$. The simplest state that satisfies these requirements is

$$\psi = \prod_\rho \exp\{ \sin^4(\frac{1}{2}\theta_\rho) / 3g^4 \}.
 \tag{2.16}$$

It is an exact zero-energy eigenstate of the Hamiltonian

$$H_R = \frac{g^2}{2a} \sum_l E_l^2 - \frac{1}{3ag^2} \sum_\rho (\cos 2\theta_\rho - \cos \theta_\rho) + \frac{1}{72ag^6} \sum_l \left\{ \sum_{\rho(l)} \eta_\rho^l \sin \theta_\rho (\cos \theta_\rho - 1) \right\}^2
 \tag{2.17}$$

which has the same (naive) continuum limit as the standard [14] U(1) lattice Hamiltonian (see appendix 1).

From the state (2.16) one computes the drift

$$b_l = \frac{1}{3ag^2} \sum_{\rho(l)} \eta_\rho^l \sin \theta_\rho \sin^2 \frac{\theta_\rho}{2}
 \tag{2.18}$$

which will be used in the computations of § 3.

Until now, we have referred to the ψ state simply as a zero-energy eigenstate of H_R . Can one guarantee that it is the ground state of H_R ? If the domain of self-adjointness of L_l is the whole of L^2 , then

$$H_R = \frac{g^2}{2a} \sum_l \{ E_l + iL_l \} \{ E_l - iL_l \}
 \tag{2.19}$$

being a positive operator, ψ must be a lowest-energy eigenstate. If the domain of L_l is a proper subspace of L^2 , H_R may have eigenstates of energy lower than ψ^\dagger . For a finite lattice with N links, L_l of (2.13b) is a bounded operator in $L^2(\mathbb{R}^N)$. Therefore, barring pathologies in the $N \rightarrow \infty$ limit, ψ is indeed a ground state for H_R . On the other hand, in the $a \rightarrow 0$ limit, the constant term in the right-hand side of (2.15) vanishes. Up to terms of order a^{d+1} , the Hamiltonian H_R converges to a positive operator. This is a necessary condition for convergence of ψ to the ground state of the continuum theory.

We have used a ground state ansatz to construct the drift of a stochastic equation, from which physical information is then obtained using the methods described in the next section. One might wonder whether this the most efficient way to extract physical

† The reader who doubts the need for these precautions should convince himself by reconstructing a Hamiltonian H' from the first excited state of the harmonic oscillator. The result is

$$H' = -\frac{1}{2}(d^2/dx^2) + (x^2/2) - \frac{3}{4}$$

but the domain of L is spanned by the odd eigenvalues only. In this subspace H' is a positive operator, but of course in L^2 , H' has an eigenstate ψ_0 of smaller energy ($H'\psi_0 = -\psi_0$).

information from the ground state and whether having the ground state one has not already the exact solution to the theory.

In quantum mechanics, given the ground state ψ_0 , one may always reconstruct the potential from $V(x) = \hbar^2 \Delta \psi_0 / (2m\psi_0) - E_0$. On the other hand, for sufficiently well behaved potentials, one may prove the existence of a unique ground state. In this sense, to have the interaction potential or the ground state is, in principle, the same. An exception is, of course, the case where the field algebra is such that all eigenvectors of the Hamiltonian can be obtained from the ground state by application of the appropriate raising operators, as in the case of non-interacting harmonic oscillator modes. This is not the case for the lattice Hamiltonians, and one should think of the exact ground state construction as just another way to define the interaction.

The stochastic differential equation (2.6) and the drift (2.18) define a stochastic model for U(1) lattice gauge fields. This model is not unique because there are states, other than (2.16), which by reconstruction lead to Hamiltonians with the same classical continuum limit as H_{KS} .

3. Stochastic methods for the measurement of lattice observables

Consider a stochastic process X_s constructed from an eigenstate ϕ of the Hamiltonian. If the drift obtained from ϕ is such that the process is positively recurrent, then $|\phi|^2$ is the stationary probability distribution of the process.

Of particular interest to us here is the probabilistic identification of time averages and $\phi^2 d^n x$ averages. This means that a matrix element of an operator or a Euclidean time correlation may be obtained from

$$\langle \phi | f | \phi \rangle = \lim_{T \rightarrow \infty} \frac{1}{T} \int_0^T f(X_s) ds \tag{3.1}$$

$$\langle \phi | f(\tau) g(0) | \phi \rangle = \lim_{T \rightarrow \infty} \frac{1}{T} \int_0^T f(X_{\tau+s}) g(X_s) ds \tag{3.2}$$

where the equality signs should be interpreted in a probabilistic sense.

Because our main interest is the ground state process, we will not deal with cases where ϕ is the wavefunction (with zeros) of an excited state of energy E_n . In such a case the singularities in the drift require careful mathematical treatment [17] and, the zeros of ϕ acting as barriers for the process, one may decompose this one into separate ergodic components.

In this paper we consider only the ground state process. The computation of lattice observables from a stochastic model (in the sense of § 2) is made by applying (3.1) or (3.2). For example for the Wilson loop, because in the Hamiltonian temporal gauge time-like links carry the unit element of the group, one obtains simply a (Euclidean) time correlation of two string operators.

$$W(L, \tau) = \lim_{T \rightarrow \infty} \frac{1}{T} \int_0^T U_L^-(\tau) \dots U_1^-(\tau+s) U_1 \dots U_L(s) ds. \tag{3.3}$$

Mass gaps may likewise be obtained from the decay of the time correlations of the appropriate lattice functions. In general, everything that can be computed in Euclidean quantum mechanics (using, for example, a spacetime lattice and the Monte Carlo method) can also be computed here from large time averages over the evolving stationary process.

In addition there is at least one useful new tool that is brought to these problems. This is the evaluation of mass gaps from the technique of exit times. This is a consequence of the probabilistic characterisation of the smallest positive eigenvalue of elliptic operators. In special cases the theory of small random perturbations of dynamical systems [18, 19] may also be applied to estimate the weak coupling behaviour of the mass gap.

New methods to measure the mass gap in lattice theories are welcome because in the time correlation technique one must use very large times to eliminate the contamination from the excited states. For large coupling constants this is not a serious difficulty. For small couplings, however, the exponential decrease of the energy levels makes the large-time slope, in the correlation function, very hard to extract from the noise.

In the remainder of this section we will concentrate in the description of the method of exit times to measure the mass gap and in its application to the U(1) stochastic model derived in § 2.

Consider a stochastic differential equation (SDE)

$$dX_s = b(X_s) ds + \sigma(X_s) dW_s.$$

There is a very useful relation between SDE of the diffusion type and elliptic operators. Let G be the generator of the Markov process associated to the SDE

$$Gu(x) = \lim_{s \downarrow 0} \frac{E_x u(X_s) - u(x)}{s}. \tag{3.4}$$

If $u(x)$ is a smooth function, G has a differential representation. Computing the stochastic differential $du(X_s)$ by Ito's formula one obtains

$$G = \frac{1}{2} \sum_{i,j=1}^n a^{ij}(x) \frac{\partial^2}{\partial x^i \partial x^j} + \sum_{i=1}^n b^i(x) \frac{\partial}{\partial x^i} \tag{3.5}$$

where

$$a^{ij}(x) = \sum_k \sigma_k^i \sigma_k^j = (\sigma \sigma^T)^{ij}.$$

The symmetric matrix (a^{ij}) is non-negative definite;

$$\sum_{i,j} a^{ij}(x) \lambda_i \lambda_j \geq 0$$

for any real λ .

Conversely if a non-negative matrix $a^{ij}(x)$ and a vector field $b^i(x)$ with sufficiently smooth properties are given, one can construct a diffusion process. In particular, a representation of the form $a^{ij}(x) = (\sigma \sigma^T)^{ij}$ with $\sigma_j^i(x)$ satisfying a Lipschitz condition is possible whenever the a^{ij} are twice continuously differentiable or if $\det(a^{ij}(x)) \neq 0$ it suffices that they satisfy a Lipschitz condition. Consequently there is a large class of operators of type (3.5) which have a corresponding diffusion process. The diffusion process is determined essentially uniquely by its differential generator in the sense that any two processes with a common differential generator induce the same distribution in the space of trajectories (also called sample paths). It means that although the trajectories may not be the same, expectation values of observable quantities will coincide.

The relation between diffusion processes and elliptic operators leads to many useful results and is the main reason why stochastic methods are a useful tool in quantum theory.

The characterisation of eigenvalues of the elliptic operator G is related to the stochastic representation of the solutions to the Dirichlet problem

$$G\phi(x) + c(x)\phi(x) = f(x) \tag{3.6}$$

on a bounded domain D with boundary condition $\phi(x)|_{x \in \partial D} = \chi(x)$. $c(x), f(x)$ and $\chi(x)$ are bounded continuous functions and $c(x) \leq 0$. For G one assumes $\Sigma a^{ij}(x)\lambda_i\lambda_j \geq k\Sigma\lambda_i^2, k > 0$ plus a Lipschitz condition on the coefficients. Then the unique solution to (3.6) is

$$\phi(x) = -E_x \int_0^\tau f(X_t) \exp\left(\int_0^t c(X_s) ds\right) dt + E_x \chi(x) \exp\int_0^\tau c(X_s) ds \tag{3.7}$$

where $\tau = \tau(\omega \in \Omega) = \inf\{t : X_t \notin D\}$ is the first exit time of the process from the domain D . When $c(x) = \lambda, f(x) = \chi(x) = 0$ one is led to the eigenvalue problem

$$-G\phi(x) = \lambda\phi(x) \quad \phi(x)|_{x \in \partial D} = 0. \tag{3.8}$$

From (3.7) it follows that the smallest positive eigenvalue λ_0 of $-G$ is

$$\lambda_0 = \sup\{\lambda \geq 0; \sup_{x \in D} E_x e^{\lambda\tau} < \infty\}. \tag{3.9}$$

Consider now an Hamiltonian H_R of the form (2.19) associated to the ground state ψ (i.e. $L_l = -iE_l\psi/\psi$). We perform the transformation $H_R \rightarrow \psi^{-1}H_R\psi$ which makes sense because ψ in (2.16) has no zeros. This is a unitary transformation from an operator defined in $L^2(\Pi_l d\theta_l)$ to one defined in $L^2(\psi^2\Pi_l d\theta_l)$. One obtains

$$\psi^{-1}H_R\psi = -\sum_l \frac{\nu^2}{2} \frac{\partial^2}{\partial \theta_l^2} - b_l \frac{\partial}{\partial \theta_l} \tag{3.10}$$

where the coefficients are precisely the diffusion and the drift of the stochastic equation (2.6). Comparing with (3.5) one concludes that $-\psi^{-1}H_R\psi$ is the generator of the Markov process and one may use (3.9) to obtain the lowest positive eigenvalue of the Hamiltonian (mass gap).

One way to use this equation is by direct numerical simulation of the SDE (2.6). In numerical simulations, because sizes are necessarily small, it is useful to have periodic boundary conditions to avoid contamination from boundary effects. Our simulations were on $20^2, 14^3$ and 10^3 (space) lattices with periodic boundary conditions.

For the application of (3.9), there are two suprema to consider. First there is the $\sup_{x \in D} E_x e^{\lambda\tau}$. Clearly, the expectation value grows when a large number of long exit times are obtained. Therefore we have replaced the actual finding of this supremum, which would be very time consuming, by the choice of the most stable fixed point of the classical evolution as the initial point in each measurement. This is fixed, assigning each link a value $\pm\pi/4$ (in $d = 2$) or $\pm\pi/4$ for x, y links and $\pm\pi/2$ for z links (in $d = 3$) in such a way that all plaquette angles are $\pm\pi$. Such a point is in $d = 2$ the only stable fixed point of the classical system and for $d = 3$ is also the maximum of the ground state wavefunction ψ .

The boundary ∂D of the Dirichlet problem is fixed in a symmetrical way around the fixed point, i.e. when during the course of time evolution, $|\theta_p(t) - \theta_p(0)| > \pi$ in any one of the plaquettes, a boundary hit is counted and the lattice is reset. Running until around 1000 hits ($d = 2$) or between 500–1000 depending on $g(d = 3)$ are counted, one obtains a distribution of exit times as in figure 1. The λ supremum is estimated by finding the coefficient of the exponential decay of the distribution upper tail. The

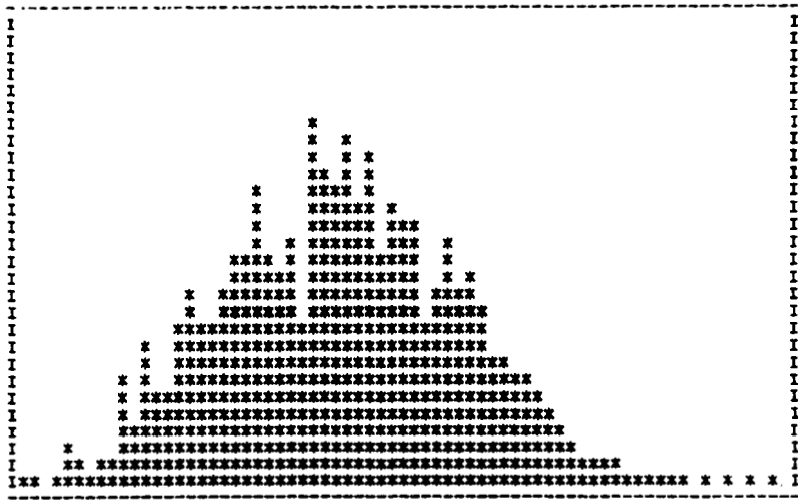


Figure 1. Exit time distribution at $g=0.8$, $d=2$; 1000 events (* = two events).

results are shown in figures 2 and 3. The error bars reflect not only the statistical error in the χ^2 fits but also an estimate of systematic errors obtained by analysing the data with different cuts of the upper tail.

In a different run, we also obtained $\langle \cos \theta_p \rangle$ in a statistically stabilised lattice evolving according to the Langevin equation (2.6) (figures 4 and 5). This clearly shows

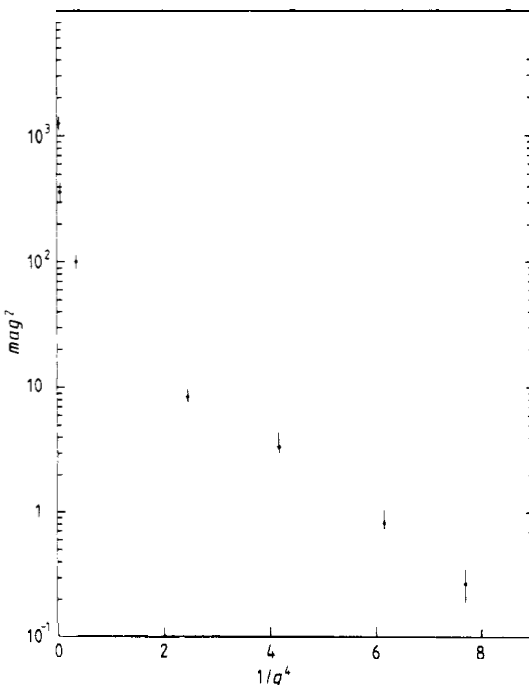


Figure 2. Lowest eigenvalue (mass gap) estimated from the exit times; $d=2$.

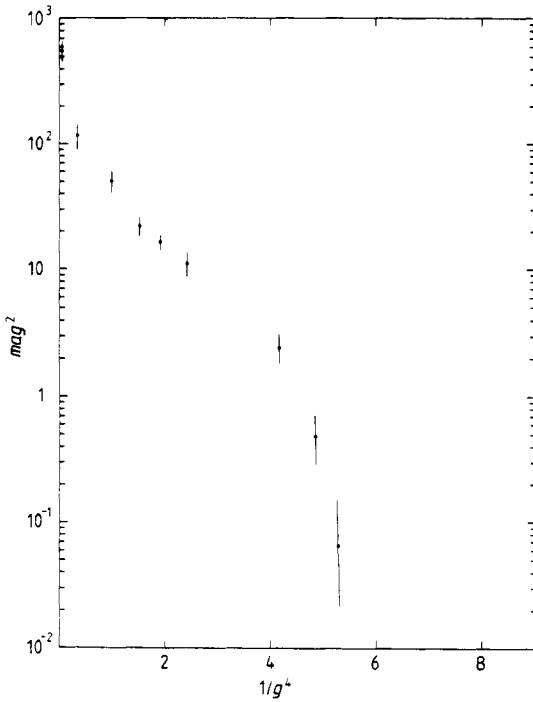


Figure 3. Lowest eigenvalue (mass gap) estimated from the exit times; $d = 3$.

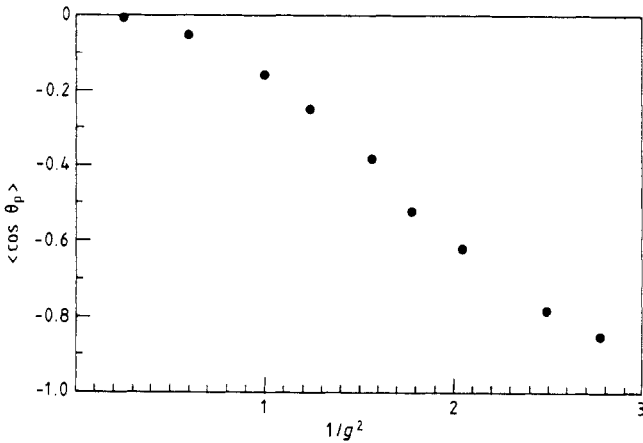


Figure 4. Average plaquette angle cosine; $d = 2$, $a = 1$.

the crossover from the strong to the weak coupling regimes, which should be compared with the behaviour of the mass gaps in figures 2 and 3.

At weak coupling the diffusion coefficient $\nu = g/\sqrt{a}$ in the stochastic differential equation (2.6) becomes small. This implies that one may use the theory of small random perturbations of dynamical systems [18-21] which, through the stochastic mechanics formulation, becomes a tool to deal with non-perturbative effects in quantum mechanics. (For a nice application to tunnelling problems, see [22].)

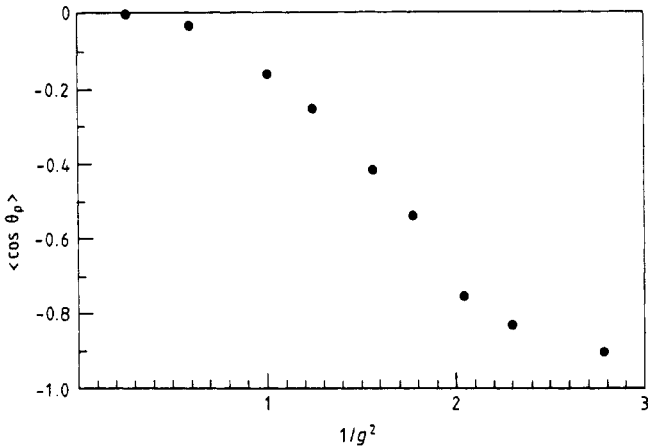


Figure 5. Average plaquette angle cosine; $d = 3, a = 1$.

To apply the theory of small random perturbations as developed in [19] one needs an elliptic operator where the coefficient of $\partial/\partial\theta_i$ is independent of the small parameter (g in this case) (cf equation (4.1) of [19]). Because the drift obtained in (2.18) is proportional to g^{-2} , we consider, instead of H_R , the operator ag^2H_R and the eigenvalue problem

$$(\psi^{-1}ag^2H_R\psi)u = \lambda u \tag{3.11}$$

in a domain D in R^{n_l} ($n_l =$ number of links) with C^2 boundary ∂D and a boundary condition $u = 0$ in ∂D .

From the asymptotic results in the theory of small random perturbations of dynamical systems one has bounds on the behaviour of the smallest positive eigenvalue λ_0 at weak coupling (theorem 11.1 of [19])

$$\overline{\lim}_{g \rightarrow 0} \{-2g^4 \log \lambda_0(g)\} \leq V^* \tag{3.12a}$$

$$\underline{\lim}_{g \rightarrow 0} \{-2g^4 \log \lambda_0(g)\} \geq V_* \tag{3.12b}$$

where $V^* = \max\{V_1, \dots, V_r\}$, $V_* = \min\{V_1, \dots, V_r\}$, r being the number of stable limit sets $\{K_i, i = 1, \dots, r\}$ of the classical deterministic system

$$d\theta = ag^2b dt \tag{3.13}$$

and $V_i = I(x, \partial D)$ the infimum of the functional

$$I = \int_{t_1}^{t_2} \left| \frac{d\theta(t)}{dt} - ag^2b(\theta(t)) \right|^2 dt \tag{3.14}$$

taken over all paths from the neighbourhood of the classical equilibrium set K_i to the boundary of the domain D . In simple cases all these quantities can actually be computed. Their meaning will become clear in the application described below.

A basic assumption in the theory is that for the deterministic system (3.13) there exists a finite number of disjoint compact sets K_1, \dots, K_r in D such that the ω -limit set of each solution of (3.13) with $\theta(0)$ in $D \setminus (\bigcup_{i=1}^r K_i)$ is contained in one of the sets K_i .

To check this condition and determine the set $\{K_i\}$ in the $2+1$ $U(1)$ theory we do a maximal gauge fixing. In the two-dimensional space lattice one fixes to the identity ($\theta_l = 0$) all group elements attached to horizontal links and also those along a particular fixed vertical line. It is easy to see that this can be achieved by a time-independent gauge transformation in any finite open $N \times N$ lattice. With this choice, the drift (2.18) becomes

$$b_n = \frac{1}{6} \{ \sin(\theta_n - \theta_{n-1}) [1 - \cos(\theta_n - \theta_{n-1})] - \sin(\theta_{n+1} - \theta_n) [1 - \cos(\theta_{n+1} - \theta_n)] \} \tag{3.15}$$

where θ_n, θ_{n+1} denote the angle variables in two vertical links separated by one lattice spacing along the horizontal direction. For the open $N \times N$ lattice that we are considering, (3.15) holds for all vertical links except for those in column N which contain only one term in b_N (the links in column 0 were gauge fixed to zero and are not dynamical variables).

The classical equilibrium sets are the fixed points of (3.13) defined by $\mathbf{b} = 0$. In particular, $b_N = 0$ implies $\theta_N - \theta_{N-1} = 0, \pm\pi$. Using (3.15) for the other links and the condition $\theta_0 = 0$ implies that one has fixed points of (3.13) for all vectors $\boldsymbol{\theta}$ for which the components are $\theta_n = 0$ or π (defined conventionally in the range $(0, \pi)$). They will be stable fixed points only if all eigenvalues of the matrix $|\partial \mathbf{b} / \partial \boldsymbol{\theta}|$ are negative at that point. It is easy to see from (3.15) that whenever $\theta_n = \theta_{n+1}$ the matrix has a zero eigenvalue which second-order analysis reveals to be associated to an unstable direction. The only stable fixed point $\bar{\boldsymbol{\theta}}$ for which all eigenvalues are strictly negative turns out to be the point for which the components alternate between 0 and π , i.e., $\Delta_n = \theta_n - \theta_{n-1} = \pm\pi$. When there is only one stable fixed point in the deterministic system (3.13) we are in a situation where the inequalities of (3.12) become an equality (corollary 11.2 of [19])

$$\lim_{g \rightarrow 0} \{-2g^4 \log \lambda_0(g)\} = V = I(\bar{\boldsymbol{\theta}}, \partial D). \tag{3.16}$$

Although there is only one stable fixed point one should take notice that the unstability directions of the other fixed points are degenerate. This means that in a numerical measurement of relaxation times, for example, trajectories with initial conditions near such a fixed point will take a long time to move away, mainly when the diffusion is weak (weak coupling).

From (3.11) it follows for the smallest positive eigenvalue m_g of H_R (mass gap)

$$am_g \sim g^{-2} \exp(-V/2g^4) \tag{3.17}$$

at weak coupling.

To try to estimate the constant V , one should define the domain and the boundary for the eigenvalue problem. This we do in a maximally symmetric way around the stable fixed point $\bar{\boldsymbol{\theta}} = \{\boldsymbol{\theta} : |\theta_n - \theta_{n-1}| = \pi \forall n\}$, in the sense that when moving away from $\bar{\boldsymbol{\theta}}$, one hits the boundary ∂D whenever any one of the differences $\theta_n - \theta_{n-1}$ reaches zero (mod 2π).

V is the infimum of the functional (3.14) for paths between the attractive fixed point and the boundary. The Euler-Lagrange equation for this variational problem is

$$\ddot{\theta}_l - ag^2 b_l = - \sum_r (\dot{\theta}_l - ag^2 b_l) \frac{\partial}{\partial \theta_l} (ag^2 b_l). \tag{3.18}$$

Consider a path parametrised in such a way that $\dot{\theta}_l = \pm ag^2 b_l$, i.e. a path composed of pieces along which one either follows the classical flow or exactly opposes this flow.

In the first case (3.18) is automatically satisfied and in the second one obtains

$$-2 \frac{\partial}{\partial t} b_l = -2 \sum_r \frac{\partial \theta_r}{\partial t} \frac{\partial}{\partial \theta_l} b_l = -2 \sum_r \frac{\partial \theta_r}{\partial t} \frac{\partial}{\partial \theta_r} b_l = -2 \frac{\partial}{\partial t} b_l$$

where the second equality follows from the fact that $b_l \sim (\partial/\partial \theta_l) \ln \psi$. The conclusion is that a path where $\dot{\theta}_l = \pm b_l(\theta)$ is a stationary point of the functional I .

In the case that we are studying we consider a path against the classical flow from the attractive fixed point to the boundary and obtain

$$V = \inf 4 \sum_l \int a g^2 b_l(\theta) d\theta_l = \min 4g^2 \{ \ln \psi(\bar{\theta}) - \ln \psi(\partial D) \}. \tag{3.19}$$

In $d = 2$ the minimum is obtained when $\bar{\theta}$ and $\theta \in \partial D$ differ by one plaquette, hence

$$V^{(2)} = \frac{4}{3} \tag{3.20}$$

a result which together with (3.17) is quite consistent with the results of our numerical simulations, namely $V_{\text{num}}^{(2)} = 1.32 \pm 0.07$.

A similar analysis is possible for the three-dimensional case. Given an arbitrary field configuration \mathcal{L} on a three-dimensional lattice it is always possible by a gauge transformation to make $U_l = 1$ ($\theta_l = 0$) in all links along the z -axis. Now we pick a particular xy plane and in this plane one uses the remaining gauge freedom to transform to the identity all links along the x direction and also those of a particular fixed line parallel to the y axis.

One denotes by $g_0(\mathcal{L})$ the gauge transformation that performs this transformation on the configuration.

Equation (3.13) being a gradient dynamical system its attractive fixed points correspond to the maxima of $\ln \psi$. They are therefore the set of points for which $\theta_p = \pm \pi$. There are many configurations $\mathcal{L}_\pi^{(i)}$ that are attractive fixed points. However it is easy to see that for any two such configurations

$$g_0(\mathcal{L}_\pi^{(1)}) \mathcal{L}_\pi^{(1)} = g_0(\mathcal{L}_\pi^{(2)}) \mathcal{L}_\pi^{(2)}$$

i.e. all attractive fixed points are gauge equivalent. Modulo a gauge transformation, the domain D for the eigenvalue problem is symmetric around the attractive fixed points in the sense that the boundary ∂D is reached whenever any one of the θ_p reaches zero (mod 2π).

Using the gauge transformation g_0 , defined above, on a boundary configuration $\mathcal{L}_{\partial D}$ it is easy to see that for $d = 3$ the minimum of (3.19) is obtained when \mathcal{L}_π and $\mathcal{L}_{\partial D}$ differ by 4 plaquettes. Therefore

$$V^{(3)} = \frac{16}{3} \tag{3.21}$$

a result which is also consistent with the numerical results in the weak coupling region.

Both the numerical results and the analytical estimates at weak coupling show the reliability of the method of exit times as a mass gap evaluation technique.

Our analysis implies that the $U(1)$ stochastic model defined by the drift (2.18) scales like $\exp(-\alpha/g^4)$ at weak coupling.

The model defined by (2.18) leads therefore to a non-trivial universality class apparently different from the one formally defined by perturbation theory. The fact that the Hamiltonian of the model has the same classical $a \rightarrow 0$ limit as QED, shows that in gauge theories there may be distinct models which, although associated to the same classical continuum limit, nevertheless belong to different universality classes.

The exploration of other models possibly associated to different universality classes is of interest to clarify the meaning and the structures underlying the gauge theories formally defined in the continuum. Some preliminary results obtained recently indicate that at least another universality class can be obtained by reconstructing the non-vanishing magnetic terms (in the $a \rightarrow 0$ limit) from the $L_l L_l$ term of (2.19), as opposed to the commutator $[E_l, L_l]$ as in the model of (2.18) (cf appendix).

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Appendix

It is instructive to compare the $a \rightarrow 0$ limit of the Hamiltonian (2.17) which has ψ of (2.16) as a zero-energy eigenstate with the $a \rightarrow 0$ limit of the usual (Kogut-Susskind [14]) lattice Hamiltonian H_{KS}

$$H_{KS} = \frac{g^2}{2a} \sum_l E_l^2 - \frac{1}{ag^2} \sum_p (\cos \theta_p - 1).$$

Under the replacement (2.11a) the relevant terms become

$$\begin{aligned} -\frac{1}{ag^2} \sum_p (\cos \theta_p - 1) &= \frac{1}{2} \sum_p a^d B_p + O(a^{d+1} g^2 \sum_p a^d) \\ -\frac{1}{3ag^2} \sum_p (\cos 2\theta_p - \cos \theta_p) &= \frac{1}{2} \sum_p a^d B_p + O(a^{d+1} g^2 \sum_p a^d) \\ \frac{1}{72ag^6} \sum_l \left\{ \sum_{p(l)} \eta_p^l \sin \theta_p (\cos \theta_p - 1) \right\}^2 &= O(a^{2(d+1)} \sum_l a^d). \end{aligned}$$

Hence the $a \rightarrow 0$ limits of H_R and H_{KS} coincide. The leading terms also coincide in the $a \rightarrow 0, g \rightarrow 0$ limit. One should be aware however of the remark made in the text that to prove convergence to the same continuum limit of the theories based on H_R and H_{KS} the agreement of the (naive) $a \rightarrow 0$ limits shown above is not enough. Something like a proof of convergence of the Green functions to the same limit would be required.

Notice also that all the magnetic terms that do not vanish in the $a \rightarrow 0$ limit of H_R come from the commutator term $[E_l, L_l]$.

References

- [1] Callaway D and Rahman A 1982 *Phys. Rev. Lett.* **49** 613
- [2] Creutz M 1983 *Phys. Rev. Lett.* **50** 1411
- [3] Creutz M and Moriarty K J M 1983 *Comp. Phys. Commun.* **30** 255
- [4] Fucito F, Marinari E, Parisi G and Rebbi C 1981 *Nucl. Phys. B* **180** 369
- [5] Guha A and Lee S-C 1983 *Phys. Rev. D* **27** 2412; 1984 *Phys. Lett.* **134B** 216

- [6] Bohr H and Katznelson E 1983 *Comp. Phys. Commun.* **30** 337
- [7] Parisi G and Wu Y-S 1981 *Sci. Sin.* **24** 483
- [8] Baulieu L and Zwanziger D 1981 *Nucl. Phys. B* **193** 163
- [9] Fényes I 1952 *Z. Phys.* **132** 81
- [10] Nelson E 1966 *Phys. Rev.* **150** 1079; 1967 *Dynamical Theories of Brownian Motion* (Princeton: Princeton University Press)
- [11] Grabert H, Hänggi P and Talkner P 1979 *Phys. Rev. A* **19** 2440
- [12] Nelson E 1986 *Stochastic Processes in Classical and Quantum Systems (Lecture Notes in Physics 262)* ed S Albeverio *et al* (Berlin: Springer)
- [13] Mendes R V 1986 *Phys. Lett.* **116A** 216
- [14] Kogut J and Susskind L 1975 *Phys. Rev. D* **11** 395
- [15] Duncan A and Roskies R 1984 *Gauge Theory on a Lattice: 1984* (Argonne National Laboratory Proc.) p 242
- [16] Mendes R V 1984 *Z. Phys. C* **24** 45
- [17] Carlen E A 1984 *Commun. Math. Phys.* **94** 293
- [18] Ventcel A D and Freidlin M I 1970 *Russian Math. Surveys* **25** 1
- [19] Friedman A 1976 *Stochastic Differential Equations and Applications* vol 2 (New York: Academic) ch 14
- [20] Ventcel A D 1972 *Sov. Mat. Dokl.* **13** 13, 65
- [21] Friedman A 1973 *Indiana Univ. Math. J.* **22** 1005
- [22] Jona-Lasinio G, Martinelli F and Scoppola E 1981 *Phys. Rep.* **77** 313; 1981 *Commun. Math. Phys.* **80** 223