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RANDOM PATHS AND RANDOM SURFACES ON A DIGITAL COMPUTER

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ABSTRACT

We describe a local stochastic process that generates statistical ensembles of paths (or surfaces) with a Boltzmann probabilistic weight. The method is expected to be applicable to Monte Carlo simulations of field theories that contain fermions, to the roughening transition and to a reformulation of gauge theories in terms of random surfaces.

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1. Although Monte Carlo methods have been used in the past to study spin systems, gauge systems or both systems in interaction and systems as complicated as liquids, we believe that there is one distinct type of problem that has not been treated so far - random paths and random surfaces, very special systems that are of a purely geometrical nature^{*)}. These systems are sufficiently different from the more standard gauge and spin systems to require a Monte Carlo procedure of their own.

There are various motivations for the Monte Carlo generation of random paths and random surfaces:

- i) in many field theories of interest, fermions occur only quadratically, with quartic couplings being absent. Now it is well known¹⁾ that a free field theory in an external background corresponds to a statistical ensemble of non-interacting random paths. This is seen most clearly in the case of spinless bosons on a lattice where we have

$$\int D\phi^\dagger D\phi e^{-\phi^\dagger(1-\Gamma)\phi} = \frac{1}{\det(1-\Gamma)} = \exp -\text{Tr} \log(1-\Gamma)$$

$$= \exp \text{Tr} \sum_{N=0}^{\infty} \frac{\Gamma^N}{N} \quad (1)$$

The random path interpretation follows immediately from the local nature of Γ , say $\Gamma_{x,x'} = C \sum_{\mu} \{\delta_{x,x'-\mu} + \delta_{x,x'+\mu}\}$ on a hypercubic lattice. We may also give a random path interpretation to the variation of the fermionic determinant required in the simulation of QCD²⁾:

$$\delta \det[1-\Gamma(u)] = -\det[1-\Gamma(u)] \text{Tr} \delta \Gamma \frac{1}{1-\Gamma(u)} \quad (2)$$

with

$$\Gamma_{x,x'}(u) = \kappa \sum_{\mu, \pm} \delta_{x,x' \mp \mu} (1 \pm \gamma_{\mu}) u_{x,x \pm \mu} \quad (3)$$

taken from Wilson's formulation of QCD on a lattice³⁾. Since the U matrices are modified only one link at a time in a Monte Carlo simulation,

^{*)} The generation of random paths we describe here has nothing to do with the trivial random motion of a point on a lattice.

$(\delta\Gamma)_{xx}$, is a local operator and the right-hand side of Eq. (2) represents the current of the fermions induced by the gauge field. Clearly, the fermionic propagator $1/(1-\Gamma)$ involves extra spin and gauge factors, but a weight $\exp - \beta(\text{length})$ per path may be extracted:

$$\text{Tr } \delta\Gamma \frac{1}{1-\Gamma(u)} = \sum_{C: x \rightarrow x+\mu} \text{Tr} [\text{Spin factors}(C)] \text{Tr} [\text{Yang Mills factors}(C)] \times e^{-\beta \text{length}(C)} \quad (4)$$

$$e^{-\beta} = k$$

Here $(x, x+\mu)$ is the link where $\delta\Gamma$ differs from zero and one must sum over all paths C that connect x and $x + \mu$. The method to be described below samples paths with a weight $e^{-\beta \text{length}(C)}$ and should therefore be useful in computing $\text{Tr } \delta\Gamma/1-\Gamma$.

- ii) Recently there has been some renewed interest in the roughening transition⁴⁾, a transition that occurs in crystal growth⁵⁾, interfaces⁶⁾ and gauge theories⁷⁾. Only very idealized models of this transition are tractable analytically whereas our methods, suitably extended to random surfaces, may elucidate the structure of the roughening transition in an arbitrary space dimension $d \geq 3$.
- iii) On a more speculative level, $U(N)$ gauge theories in the limit of $N \rightarrow \infty$ may possibly be completely reformulated as a statistical ensemble of random surfaces⁸⁾. The methods to be described below would then enable us to compute quantities of interest in the reformulated gauge theory via random surfaces.

2. In this letter we shall focus on random paths of two different types. Consider

$$Z_{B(F)} = \sum_{C_{B(F)}: x \rightarrow x} e^{-\beta \text{length}(C)} \quad (5)$$

where we are thinking of a hypercubic lattice in d dimensions, x is a fixed lattice point and C stands for a path starting from, and returning to x . When we include all possible lattice paths we append the suffix 'B' (for bosonic) to Z whereas Z_F denotes the partition function with paths that don't have any 'spikes', e.g., a step in direction $\hat{x}$ may not be followed by a step in direction $-\hat{x}$. 'F' stands for 'fermions' and, indeed, if one uses Wilson's $\Gamma(u)$ from Eq. (3) then only paths without spikes contribute.

Let us first describe how paths of type 'F' are generated. Examples of basic stochastic processes we need are:

In general, given a curve C , we choose a link at random (a priori probability = $1/\text{length}(C)$) and then move it perpendicularly to itself in direction λ with $2(d-1)$ possible directions λ in d dimensions:

If $\lambda = -\mu_1$ or $\lambda = +\mu_2$ or both we annihilate one or two "spikes" or both, e.g.,

The change in length of the curve therefore turns out to be:

$$\Delta \ell = +2 - 2(\delta_{\lambda, -\mu_1} + \delta_{\lambda, +\mu_2}) \quad (\lambda \neq \pm \mathbf{s}) \quad (7)$$

We are guaranteed to achieve the correct Boltzmann probabilistic weight provided the transitions $C \leftrightarrow C'$ are in one-to-one correspondence and satisfy the detailed balance condition⁹⁾

$$\frac{p_{c \rightarrow c'}}{p_{c' \rightarrow c}} = e^{-\beta [\text{length}(C') - \text{length}(C)]} \quad (8)$$

and provided the path space is sufficiently connected. We therefore choose the probabilities $(\lambda, \rho, \mu_1, \mu_2)$ for a displacement λ to depend on the change of length

$$p(\lambda; s, \mu_1, \mu_2) = p(\Delta l(\lambda; s, \mu_1, \mu_2)) \geq 0 \quad (9)$$

$$\frac{p(\Delta l)}{p(-\Delta l)} = e^{-\beta \Delta l}, \quad \Delta l = 2, 0, -2$$

$$\sum_{\lambda} p(\lambda; s, \mu_1, \mu_2) \leq 1$$

In cases where the resulting path has a spike such as

(10)

we discard the transition if we are simulating paths of class 'F' and then we go back to the curve C and choose a new link at random. Because the a priori probability of choosing a link actually involves the number of links of the curve, our stochastic process will, in fact, generate the following partition function:

$$Z_F^{\text{modified}} = \sum_{C_F: x \rightarrow x} \text{length}(C) e^{-\beta \text{length}(C)} \quad (11)$$

With the rules given here so far, paths of type F cannot be generated correctly in $d = 2$ dimensions. This is because one may define a winding number for paths without spikes on a $d = 2$ lattice. The reader may easily convince herself or himself that the processes (6) do not change the winding number for paths 'F' in $d = 2$ dimensions. To remedy this deficiency we may add a transition

to our Monte Carlo rules. Similar difficulties will occur in the simulation of random surfaces in $d = 3$ and $d = 4$ dimensions if the class of surfaces considered permits the definition of a topological invariant.

Let us now describe the modifications of the stochastic process needed to generate paths of type 'B'. In the class C_B we allow "spikes" and this is seen to cause problems, for instance we have the transition

but not its inverse:

according to our previous rules. To maintain detailed balance, Eq. (8), we must forbid transitions of the type (12). To summarize then, the simulation of paths of class 'B' with spikes admitted is slightly more complicated than for class 'F'.

The Monte Carlo method described so far depends on two parameters, $p(2)$ and $p(0)$, see Eq. (9). But it is clear that the procedure is optimized by setting

$$\sum_{\lambda} p(\lambda; \rho, \mu_1, \mu_2) = 1$$

for as many triples (ρ, μ_1, μ_2) as possible. This means that the probability for the nullevent is minimized. The reader may easily check that for paths of class 'F'

$$p(+2) = \frac{k^2}{1 + (2d-3)k^2}, \quad p(-2) = \frac{1}{1 + (2d-3)k^2}, \quad p(0) = \frac{1}{2} \frac{1+k^2}{1 + (2d-3)k^2}$$

is the optimal choice.

3. We now present some of our Monte Carlo data. We have computed the average length of paths of class 'B' and 'F' in $d = 3$ and of class 'F' in $d = 4$ dimensions as a function of β . For technical reasons, we used a modified partition function

$$Z_{B(F)}^{\text{technical}} = \sum_{C_{B(F)}: X \rightarrow X} [\text{length}(C) - 1] e^{-\beta \text{length}(C)} \quad (14)$$

It is not too difficult to compute the exact analytic form of these partition functions. They are [with $Z_{B,F}$ as in Eq. (5)]

$$Z_{B,F}^{\text{technical}} = 1 - (1 + \partial_\beta) Z_{B,F} \quad (15)$$

$$Z_B = \int_{0 \leq p_i \leq 2\pi} \frac{d^d p}{(2\pi)^d} \frac{1}{1 - 2e^{-\beta} \sum_{\mu=1}^d \cos p_\mu}$$

$$Z_F = \frac{1}{2d} \int_{0 \leq p_i \leq 2\pi} \frac{d^d p}{(2\pi)^d} \sum_{\pm} \left\{ \frac{1}{1 - E_{\pm} e^{-\beta}} + \frac{d-1}{1 \pm e^{-\beta}} \right\}$$

$$E_{\pm}(p) = \sum_{\mu=1}^d \cos p_\mu \pm \left[\left(\sum_{\mu=1}^d \cos p_\mu \right)^2 - 2d + 1 \right]^{\frac{1}{2}}$$

On the basis of simple random walk arguments we expect the length of paths 'B' and 'F' to diverge at $\beta = \log(2d)$ and $\beta = \log(2d-1)$, respectively. Indeed, our Monte Carlo data for the average path length in Figs. 1 - 3 show a divergence at precisely these points. The agreement with the average path length calculated exactly is also shown in Figs. 1 - 3 and indicates that our method works.

Because our method is local and operates only on one link at a time, our procedure slows down for very large loops near the critical values of β . To achieve reasonable statistics for paths of length ~ 100 in this regime we had to perform of the order of millions of iterations. Accordingly, most of our computer time was spent near the critical points, but nonetheless the total computer time used was small in spite of the programmes not being optimal.

4. We have described a viable Monte Carlo procedure to generate random paths with a Boltzmann probabilistic weight. Work on the application of this procedure to gauge theories containing fermions and to random surfaces is now in progress (in collaboration with A. Billoire). It will also be quite interesting to compare our numerical results on random surfaces with the new analytical work of A. Polyakov on the summation over random surfaces¹⁰⁾.

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REFERENCES

- 1) K. Symanzik, Varenna Lectures (1969);
J.S. Schwinger, Phys. Rev. 82 (1951) 664.
- 2) Fermions have been included in Monte Carlo calculations by:
F. Fucito, E. Marinari, G. Parisi and C. Rebbik CERN preprint TH-2960 (1980);
D.H. Weingarten and D.N. Petcher, Indiana University preprint IUHET 61 (1980);
D.J. Scalapino and R.L. Sugar, Phys. Rev. Lett. 46 (1981) 519;
H. Nicolai and C. Lang, CERN preprint TH-3087 (1981);
A. Duncan and M. Furman, Columbia University preprint CU-TP-194;
E. Marinari, G. Parisi and C. Rebbi CERN preprint TH-3080 (1981);
A. Hasenfratz and P. Hasenfratz, Budapest preprint KFKI-1981-47.
- 3) K. Wilson, Cargèse lectures (1976).
- 4) J.D. Weeks et al., Phys. Rev. B14 (1976) 4928.
- 5) A computer generated film on roughening in crystal growth exists at Cornell University.
- 6) J.D. Weeks et al., Phys. Rev. Lett. 31 (1973) 549.
- 7) P. Hasenfratz and A. Hasenfratz, Nucl. Phys. 13 (1981) 180;
C. Itzykson, M. Peskin and J.B. Zuber, Phys. Lett. 59B (1980) 259;
M. Lüscher, G. Münster and P. Weisz, Nucl. Phys. B180 (1981) 13 and further papers in that volume.
- 8) D. Foerster, Nucl. Phys. B170 (1980) 107;
A. Migdal, Landau Institute preprint (1980), "Exact equivalence..." preliminary version.
- 9) For the Monte Carlo method see, for example, K. Binder in "Phase Transition and Critical Phenomena", ed. C. Domb and M.S. Green, Academic Press, New York, 1976 Vol. 5B.
- 10) A. Polyakov, "Quantum Geometry of Bosonic Strings", to be published in Phys. Lett. B.

FIGURE CAPTIONS

- Figure 1 : Monte Carlo data for the average path length in the ensemble $Z_B^{\text{technical}}$ in $d = 3$ and comparison with the exact results (represented by the full line).
- Figure 2 : Monte Carlo data and exact results for the average path length for $Z_F^{\text{technical}}$ in $d = 3$.
- Figure 3 : Monte Carlo data and exact results for the average path length in $d = 4$ for the ensembles Z_F and $Z_F^{\text{technical}}$.

FIG. 1

FIG. 2

FIG. 3