The Theory of Hybrid Stochastic Algorithms*

A. D. Kennedy

Supercomputer Computations Research Institute[†‡]
Florida State University
Tallahassee, FL 32306–4052, USA

and

Theoretical Physics Division
Fermilab
P.O. Box 500
Batavia, IL 60510, USA

November 21, 1989

SCRI preprint FSU–SCRI–89–147
Fermilab preprint FERMILAB–CONF–89/237–T

*Lectures given at the workshop on "Probabilistic Methods in Quantum Field Theory and Quantum Gravity," Cargèse, August 1989

†Supported by the US Department of Energy through contract #DE-FC05-85ER250000

‡Permanent address

Abstract

These lectures introduce the family of Hybrid Stochastic Algorithms for performing Monte Carlo calculations in Quantum Field Theory. After explaining the basic concepts of Monte Carlo integration we discuss the properties of Markov processes and one particularly useful example of them: the Metropolis algorithm. Building upon this framework we consider the Hybrid and Langevin algorithms from the viewpoint that they are approximate versions of the Hybrid Monte Carlo method; and thus we are led to consider Molecular Dynamics using the Leapfrog algorithm. The lectures conclude by reviewing recent progress in these areas, explaining higher-order integration schemes, the asymptotic large-volume behaviour of the various algorithms, and some simple exact results obtained by applying them to free field theory. It is attempted throughout to give simple yet correct proofs of the various results encountered.

1 Introduction

The problem addressed in these lectures is how to evaluate a functional integral numerically, especially in the presence of fermion fields. To be more specific, we want to evaluate the expectation value of some interesting operator Ω which depends on some fields which we shall generically denote by ϕ

$$\langle\Omega\rangle = \frac{1}{Z}\int [d\phi] e^{-S(\phi)}\Omega(\phi), \tag{1}$$

where the action is S and the measure is $[d\phi]$ (which may be Lebesgue measure for scalar fields, Haar measure for gauge fields, etc.). The partition function Z is chosen such that $\langle 1\rangle = 1$. We shall assume that the functional integral is regularized and thus well defined — throughout we shall implictly work on a finite lattice and not worry about the subtleties of taking thermodynamic and continuum limits. We shall also work from the outset in Euclidian spacetime.

2 Monte Carlo Integration

The basic technique for the numerical evaluation of infinite-dimensional integrals is that of Monte Carlo integration [1,2]. We generate a sequence of field configurations $(\phi_1, \phi_2, \ldots, \phi_t, \ldots, \phi_T)$ each chosen from the probability distribution

$$P(\phi_t)[d\phi_t] = \frac{1}{Z} e^{-S(\phi_t)}[d\phi_t]. \tag{2}$$

On each configuration in this sequence we measure the value of Ω, and we form the average

$$\bar{\Omega} \equiv \frac{1}{T}\sum_{t=1}^{T}\Omega(\phi_t). \tag{3}$$

The law of large numbers then tells us that under some very general conditions the configuration average converges to the desired expectation value, $\langle\Omega\rangle = \lim_{T\to\infty}\bar{\Omega}$, and the central limit theorem says that under only slightly more restrictive assumptions the distribution of values for $\bar{\Omega}$ tends to become

Gaussian with a variance falling as $1/T$,

$$\langle \Omega \rangle = \bar{\Omega} + O\left(\frac{V}{\sqrt{T}}\right) \qquad (T \to \infty) \tag{4}$$

These theorems are easily established. The distribution of Ω is

$$\rho_1(\omega) \equiv \int [d\phi] P(\phi)\, \delta[\omega - \Omega(\phi)] \tag{5}$$

(*i.e.*, the quantity on the left is the probability density that $\Omega(\phi)$ takes the numerical value ω when averaged over the distribution of ϕ configurations). Let us take the Fourier transform of ρ_1, and consider the quantity

$$W_1(k) \equiv \ln \int d\omega\, \rho_1(\omega) e^{ik\omega} = \ln \int [d\phi] P(\phi) e^{ik\Omega(\phi)} = \ln \left\langle e^{ik\Omega} \right\rangle \tag{6}$$

which is the generating function for the connected moments[1] of Ω:

$$\begin{aligned} W_1(k) \;=\; & (ik)\langle\Omega\rangle + \frac{(ik)^2}{2}\left\langle \big(\Omega - \langle\Omega\rangle\big)^2 \right\rangle + \frac{(ik)^3}{3!}\left\langle \big(\Omega - \langle\Omega\rangle\big)^3 \right\rangle + \\ & + \frac{(ik)^4}{4!}\left[\left\langle \big(\Omega - \langle\Omega\rangle\big)^4 \right\rangle - 3\big(\langle\Omega^2\rangle - \langle\Omega\rangle^2\big)^2 \right] + \cdots, \end{aligned} \tag{7}$$

where we assume that the distribution is sufficiently well behaved that this expansion is convergent.

The distribution of the average $\bar{\Omega}$ is

$$\rho_T(\bar{\omega}) \equiv \int [d\phi_1] \cdots [d\phi_T] P(\phi_1) \cdots P(\phi_T)\, \delta\left[\bar{\omega} - \frac{1}{T}\sum_{t=1}^{T} \Omega(\phi_t)\right], \tag{8}$$

so we may define the connected generating function

$$\begin{aligned} W_T(k) \;&\equiv\; \ln \int d\bar{\omega}\, \rho_T(\bar{\omega}) e^{ik\bar{\omega}} \\ &=\; \ln \int [d\phi_1] \cdots [d\phi_T] P(\phi_1) \cdots P(\phi_T) \exp\left(\frac{ik}{T}\sum_{t=1}^{T} \Omega(\phi_t)\right) \\ &=\; \ln \left[\int [d\phi] P(\phi) e^{\frac{ik}{T}\Omega(\phi)}\right]^T \\ &=\; T \ln \left\langle e^{ik\Omega/T} \right\rangle = T W_1(k/T). \end{aligned} \tag{9}$$

[1] Also known as *cumulants*.

Expanding in powers of k we obtain

$$W_T(k) = (ik)\langle\Omega\rangle + \frac{(ik)^2}{2T}\left\langle\left(\Omega - \langle\Omega\rangle\right)^2\right\rangle + \frac{(ik)^3}{3!T^2}\left\langle\left(\Omega - \langle\Omega\rangle\right)^3\right\rangle + \cdots; \quad (10)$$

and upon taking the inverse Fourier transform we find

$$\begin{aligned}
\rho_T(\bar{\omega}) &= \frac{1}{2\pi}\int dk\, e^{W_T(k)} e^{-ik\bar{\omega}} \\
&= \frac{1}{2\pi}\int dk\, \exp\left(ik\langle\Omega\rangle + \frac{(ik)^2}{2T}\left\langle\left(\Omega - \langle\Omega\rangle\right)^2\right\rangle + O\left(\frac{1}{T^2}\right)\right) e^{-ik\bar{\omega}} \\
&= \frac{1}{2\pi}\int dk\, e^{-ik\left(\bar{\omega}-\langle\Omega\rangle\right)} e^{-k^2V/2T}\left[1 + O\left(\frac{1}{T^2}\right)\right] \\
&= \frac{\exp\left\{-\frac{\left(\bar{\omega}-\langle\Omega\rangle\right)^2}{2V/T}\right\}}{\sqrt{2\pi V/T}}\left[1 + O\left(\frac{1}{T^2}\right)\right]. \qquad (11)
\end{aligned}$$

The distribution of $\bar{\Omega}$ thus tends to $\delta(\bar{\Omega} - \langle\Omega\rangle)$ as $T \to \infty$, and to the next order in $1/T$ it is the Gaussian distribution of Eq. (11) which has variance V/T.

3 Fermion Fields

Fermion fields are somewhat different entities from boson fields because they are Grassmann-valued. This means that e^{-S} is not positive definite, and thus if we were to try to carry out a Monte Carlo integration directly on the Grassmann-valued fields by keeping track of all the necessary signs large cancellations would occur and the result would have a huge variance. To avoid this problem we make use of the fact that fermion fields occur only quadratically in four dimensional renormalizable field theories and thus we can carry out the Grassmann integrations explicitly in favour of a non-local determinant:

$$\begin{aligned}
\langle\Omega\rangle &= \frac{1}{Z}\int [d\phi][d\bar{\psi}][d\psi] e^{-S(\phi,\bar{\psi},\psi)}\Omega(\phi,\bar{\psi},\psi) \\
&= \frac{1}{Z'}\int [d\phi] e^{-S_B(\phi)} \det(\mathcal{M})\Omega'(\phi), \qquad (12)
\end{aligned}$$

where

$$S = S_B(\phi) + \bar{\psi}\mathcal{M}(\phi)\psi \qquad (13)$$

and the operator Ω has been expressed solely in terms of the bosonic fields

$$\Omega' = \Omega\left(\phi, \frac{\delta}{\delta\eta}, \frac{\delta}{\delta\bar{\eta}}\right) e^{\eta\mathcal{M}\eta}\Big|_{\eta=\bar{\eta}=0} \tag{14}$$

One way to proceed would be to include the obnoxious fermion determinant as part of the operator being measured

$$\langle\Omega\rangle = \frac{\frac{1}{Z}\int[d\phi]e^{-S_B(\phi)}[\det(\mathcal{M})\Omega'(\phi)]}{\frac{1}{Z}\int[d\phi]e^{-S_B(\phi)}[\det(\mathcal{M})]}. \tag{15}$$

Unfortunately this approach fails, for unless the effects of the fermions are so small that we do not care about them anyhow this ratio of "quenched" expectation values will have an intolerably large variance, as $\det(\mathcal{M})$ is an extensive quantity. To put it another way, if the fermion determinant is not negligible then selecting configurations using the "quenched" action is not an adequate form of importance sampling.

It is usual, therefore, to eliminate the fermion determinant in favour of a functional integral over some new bosonic "pseudofermion" fields

$$\langle\Omega\rangle = \frac{1}{Z''}\int[d\phi][d\chi][d\chi^*]\exp\left[-S_B(\phi) - \chi^*\mathcal{M}^{-1}(\phi)\chi\right]\Omega'(\phi). \tag{16}$$

For this transformation to be valid all the bosonic Gaussian integals must converge, so all the eigenvalues λ_i of the fermion kernel $\mathcal{M}$ must be positive (that is, $\mathrm{Re}\,\lambda_i > 0$). If they are not, we shall replace $\mathcal{M}$ with $\mathcal{M}^\dagger\mathcal{M}$, thereby doubling the number of fermion flavours [3,4]. We shall use $\mathcal{M}^\dagger\mathcal{M}$ as the pseudofermion kernel from here on.

4 Markov Processes

The general Monte Carlo method solves the problem of evaluating infinite-dimensional integrals in an effective manner, but it leaves open one crucial question — how do we generate a sequence of configurations from some messy distribution like $[d\phi]e^{-S(\phi)}/Z$?

Suprisingly, there is a very simple method of doing this. Start from some arbitrary configuration ϕ_i and by some stochastic procedure generate a new configuration ϕ_f with probability $P(\phi_i \to \phi_f)$. Such a stochastic procedure,

in which a new configuration depends only upon its predecessor,[2] is called a *Markov process*, and it is *ergodic* if

$$\inf_{\phi_i,\phi_f} P(\phi_i \to \phi_f) > 0. \tag{17}$$

A distribution $Q(\phi)$ is a *fixed point* if the Markov process if

$$\int [d\phi] Q(\phi_i) P(\phi_i \to \phi_f) = [d\phi_f] Q(\phi_f). \tag{18}$$

The reason why Markov processes are useful is revealed by the following fundamental theorem: If a Markov process P is ergodic then

- $\exists$ a unique fixed point Q,
- the distribution of configurations will converge to this fixed point regardless of the starting distribution,
- the convergence rate is exponential.

To understand why this is true we construct the following metric on the space of probability distributions[3]

$$d(Q_1, Q_2) \equiv \int [d\phi] \left| Q_1(\phi) - Q_2(\phi) \right|. \tag{19}$$

We shall show that the Markov process is a contraction mapping with respect to this metric,

$$d(PQ_1, PQ_2) \leq (1 - \alpha) d(Q_1, Q_2) \qquad \text{with } \alpha > 0, \tag{20}$$

so the sequence $(Q, PQ, P^2Q, \ldots)$ is Cauchy. This, together with the completeness of the space of probability distributions, suffices to prove the claims made above.

[2] This is not really a restriction on the nature of the stochastic process as we can always make memory of the "past history" part of the "current state" of the system.

[3] *For pedants:* this is really a metric on the quotient space of probability distributions modulo the equivalence relation of equality almost everywhere.

The basic argument for P to be a contraction mapping is trivial,

$$\begin{aligned} d(PQ_1, PQ_2) &= \int [d\phi] \left| \int [d\phi'] \{Q_1(\phi') - Q_2(\phi')\} P(\phi' \to \phi) \right| \\ &\leq \int [d\phi][d\phi'] |Q_1(\phi') - Q_2(\phi')| P(\phi' \to \phi) \\ &= \int [d\phi'] |Q_1(\phi') - Q_2(\phi')| \\ &= d(Q_1, Q_2) \end{aligned} \tag{21}$$

since by conservation of probability $\int [d\phi] P(\phi' \to \phi) = 1$. Unfortunately, this is not quite good enough to establish that the sequence is Cauchy, so we have to be just a little more sophisticated.

Let $S_\pm \equiv \{\phi | Q_1(\phi) \gtrless Q_2(\phi)\}$, then the distance considered before can be expressed as follows

$$\begin{aligned} d(PQ_1, PQ_2) &= \int [d\phi] \left| \int_{S_+} [d\phi'] \{Q_1(\phi') - Q_2(\phi')\} P(\phi' \to \phi) + \right. \\ &\qquad \left. + \int_{S_-} [d\phi'] \{Q_1(\phi') - Q_2(\phi')\} P(\phi' \to \phi) \right| \end{aligned}$$

$$\begin{aligned} &= \int [d\phi] \left\{ \int [d\phi'] |Q_1(\phi') - Q_2(\phi')| P(\phi' \to \phi) - \right. \\ &\qquad \left. - 2 \min_{\pm} \int_{S_\pm} [d\phi'] |Q_1(\phi') - Q_2(\phi')| P(\phi' \to \phi) \right\} \end{aligned} \tag{22}$$

where we have used the simple identity $|x - y| = x + y - 2\min(x, y)$ where $x, y \geq 0$. Since we are working with normalized probability distributions we have $\int [d\phi] Q_1(\phi) = \int [d\phi] Q_2(\phi) = 1$, so

$$\begin{aligned} \int_{S_+} [d\phi] |Q_1(\phi) - Q_2(\phi)| &= \int_{S_-} [d\phi] |Q_1(\phi) - Q_2(\phi)| \\ &= \frac{1}{2} \int [d\phi] |Q_1(\phi) - Q_2(\phi)| = \frac{1}{2} d(Q_1, Q_2), \end{aligned} \tag{23}$$

and thus

$$d(PQ_1, PQ_2) \leq d(Q_1, Q_2) \left[1 - \inf_{\phi, \phi'} P(\phi' \to \phi) \right]. \tag{24}$$

5 Detailed Balance and the Metropolis Algorithm

All that is left is to construct an ergodic Markov process which has the desired distribution $[d\phi]Q(\phi) \equiv [d\phi]e^{-S(\phi)}/Z$ as its fixed point.

A sufficient (but not necessary) condition is to make it satisfy *detailed balance*

$$[d\phi]Q(\phi)P(\phi \to \phi') = [d\phi']Q(\phi')P(\phi' \to \phi), \tag{25}$$

as is easily verified by integrating both sides with respect to ϕ'. One simple way of implementing detailed balance is the *Metropolis Algorithm*[4] [5]

$$P(\phi \to \phi') = \min\left[1, \frac{Q(\phi')}{Q(\phi)}\right]. \tag{27}$$

If we naïvely follow the Metropolis procedure we select a candidate new configuration ϕ' at random, and we either accept ϕ' with the probability of Eq. (27) or keep the old configuration ϕ as the new one. The only constraints are that the probability of selecting ϕ' as a candidate starting from ϕ must be the same as the probability of selecting ϕ starting from ϕ'; and that we must have some non-vanishing chance of reaching any configuration, at least after some fixed number of steps, in order to ensure ergodicity.

Suppose we choose candidate configurations a characteristic "distance" Δ away from the starting point. If Δ is large then most likely $\exp[-S(\phi') + S(\phi)]$ will be tiny and the step will almost always be rejected. Successive configurations will thus be highly correlated: in fact they will be the same. If Δ is small then the acceptance rate will be near to unity, but the system will take a random walk through configuration space and the autocorrelation time will still be long ($\sim 1/\Delta^2$).

[4]There is nothing magic about this particular form, an equally valid alternative is

$$P(\phi \to \phi') = \frac{Q(\phi')}{Q(\phi) + Q(\phi')}, \tag{26}$$

which has a slightly lower acceptance rate but is sometimes easier to handle analytically.

6 The Hybrid Algorithm

We wish to introduce a trick which allows large steps through configuration space, thus producing more-or-less independent configurations, whilst maintaining a large acceptance rate.

We enlarge the space of field configurations by adding a set of "fictitious" momenta $\pi(x)$ (one for each dynamical variable $\phi(x)$); on this fictitious phase space let us generate the joint (product) distribution

$$P(\phi,\pi)[d\phi][d\pi] = \frac{1}{Z}[d\phi][d\pi]e^{-H(\phi,\pi)} \tag{28}$$

where

$$H(\phi,\pi) \equiv \frac{1}{2}\pi^2 + S(\phi). \tag{29}$$

In order to update the (ϕ,π) variables we may use the *Hybrid Algorithm* [6,7,8,9], which alternates the following two steps:

- *Momentum Refreshment*: choose π from a Gaussian distribution
- *Molecular Dynamics* [10,11,12,13,14]: move around a contour of constant H according to Hamilton's equations for some period of fictitious time τ_0

$$\left.\begin{aligned} \dot{\pi} &= -\frac{\partial H}{\partial \phi} = -\frac{\partial S}{\partial \phi} \\ \dot{\phi} &= \frac{\partial H}{\partial \pi} = \pi \end{aligned}\right\} \tag{30}$$

Each of these steps has $P(\phi,\pi)[d\phi][d\pi]$ as a fixed point, and combined they are ergodic. We shall delay a proof that Molecular Dynamics has e^{-H} as a fixed point until we consider the Hybrid Monte Carlo algorithm.

7 The Hybrid Monte Carlo Algorithm

It is hard to integrate Hamilton's equations exactly, but we can be yet more devious. Instead of Molecular Dynamics we can choose *any* mapping on "phase space" which is

- *Reversible*:[5] $f : (\phi, \pi) \mapsto (\phi', \pi') \Rightarrow f : (\phi', -\pi') \mapsto (\phi, -\pi)$;
- *Area preserving*: $[d\phi][d\pi] = [d\phi'][d\pi']$.

Following f by a Metropolis accept/reject step we have a *discrete* procedure which has $e^{-H}[d\phi][d\pi]/Z$ as a fixed point, as it satisfies detailed balance:

$$[d\phi][d\pi]e^{-H(\phi,\pi)} \min\left(1, e^{-\delta H}\right) = [d\phi'][d\pi']e^{-H(\phi',\pi')} \min\left(1, e^{\delta H}\right) \qquad (31)$$

where $\delta H \equiv H(\phi', \pi') - H(\phi, \pi)$. This is the *Hybrid Monte Carlo algorithm* [15,16].

If f conserves energy then $\delta H = 0$ and the acceptance rate will be unity. Classical mechanics is just such a reversible, area preserving (Liouville's theorem), and energy conserving mapping, so we have also just given a proof of the validity of the Hybrid algorithm.

The Hybrid algorithm generates exactly the correct distribution of configurations only if we integrate Hamilton's equations exactly, if we integrate them approximately using some discrete time step $\delta\tau$ then errors will be introduced, so a correct Hybrid computation must also involve extrapolating to the zero step size limit.

8 Leapfrog Integration

Somewhat miraculously there are simple discrete integration schemes for Hamilton's equations which are both reversible and area preserving. The simplest is the *leapfrog* scheme:

$$\left.\begin{array}{rcccl} \pi(\delta\tau) & = & \pi(0) + \dot{\pi}(0)\,\delta\tau & = & \pi(0) - \dfrac{\partial S}{\partial \phi}(0)\,\delta\tau \\ \phi(2\delta\tau) & = & \phi(0) + \dot{\phi}(\delta\tau)2\,\delta\tau & = & \phi(0) + \pi(\delta\tau)2\,\delta\tau \\ \pi(2\delta\tau) & = & \pi(\delta\tau) + \dot{\pi}(2\delta\tau)\,\delta\tau & = & \pi(\delta\tau) - \dfrac{\partial S}{\partial \phi}(2\delta\tau)\,\delta\tau \end{array}\right\} \qquad (32)$$

[5] The change of sign of the momenta is of no fundamental significance; if we consider the mapping produced by following f with a momentum reversal then we have an operation which is reversible in the usual sense.

The Jacobian is

$$\det\left[\frac{\partial(\phi_{2\delta\tau},\pi_{2\delta\tau})}{\partial(\phi_0,\pi_0)}\right] = \det\left[\frac{\partial(\phi_{2\delta\tau},\pi_{2\delta\tau})}{\partial(\phi_{2\delta\tau},\pi_{\delta\tau})}\frac{\partial(\phi_{2\delta\tau},\pi_{\delta\tau})}{\partial(\phi_0,\pi_{\delta\tau})}\frac{\partial(\phi_0,\pi_{\delta\tau})}{\partial(\phi_0,\pi_0)}\right]$$
$$= \det\left[\begin{pmatrix} 1 & 0 \\ \bullet & 1 \end{pmatrix}\begin{pmatrix} 1 & \bullet \\ 0 & 1 \end{pmatrix}\begin{pmatrix} 1 & 0 \\ \bullet & 1 \end{pmatrix}\right] = 1 \qquad (33)$$

just from the structure of the leapfrog equations.

Using the leapfrog equations in the Hybrid Monte Carlo algorithm yields a method with

- no step size errors for any $\delta\tau > 0$ (in this sense it is an "exact" method);
- long trajectories through phase space ($\tau_0 = N\,\delta\tau \approx 1$);
- large acceptance rates

$$\delta H = \begin{cases} O(\delta\tau^3) & \text{for one leapfrog step} \\ O(\delta\tau^2) & \text{for a trajectory of length } \tau_0 = 1; \end{cases} \qquad (34)$$

- τ_0 and $\delta\tau$ are independent parameters.

The "Hamiltonians" H_{MC} used in the Metropolis step and H_{MD} used in the leapfrog equations can be different, *e.g.*, to take advantage of the "renormalization" of the parameters in the action caused by finite step size effects.

8.1 Gauge Fields

So far we have assumed that it is obvious what the dynamical variables are, and how to write down Hamilton's equations for them. When there are constraints, such as for the non-linear σ-model or gauge theories things are a little more complicated. We can impose the constraints using Lagrange multipliers [11,8], but this is awkward in practice, and it is best where possible to write the fictitious equations of motion explicitly. For gauge theories this is possible [17], and furthermore one can even construct discrete leapfrog equations which respect the constraints [18,12,19,20]. For instance, for an

$SU(n)$ gauge theory we may use the following leapfrog equations

$$\left.\begin{aligned} \pi(\delta\tau) &= \pi(0) - T\left[\frac{\partial S}{\partial U}(0)U(0)\right]\delta\tau \\ U(2\delta\tau) &= e^{\pi(\delta\tau)2\delta\tau}U(0) \\ \pi(2\delta\tau) &= \pi(\delta\tau) - T\left[\frac{\partial S}{\partial U}(2\delta\tau)U(2\delta\tau)\right]\delta\tau, \end{aligned}\right\} \tag{35}$$

where the link variables $U \in SU(n)$, their conjugate fictitious momenta $\pi \in T_*SU(n)$, the corresponding Lie Algebra, and T projects onto the space of traceless antihermitian matrices.

The form of these equations obviously guarantees reversibility and the Jocobian, while no longer unity, is just that required to preserve Haar measure.

8.2 Fermion Fields

For the pseudofermion fields introduced in Eq. (16) we have the action (fictitious potential energy)

$$S = S_B(\phi) + \chi^*(\mathcal{M}^\dagger\mathcal{M})^{-1}\chi. \tag{36}$$

As the χ field occurs quadratically we can generate it using a Gaussian heatbath

$$P(\eta)[d\eta] = \frac{1}{Z}e^{-\eta^*\eta}[d\eta] \tag{37}$$

by letting $\chi = \mathcal{M}^\dagger(\phi)\eta$, as then

$$P(\chi)[d\chi] = \left\{\int [d\eta]P(\eta)\,\delta\left(\chi - \mathcal{M}^\dagger\eta\right)\right\}[d\chi] = \frac{1}{Z'}e^{-\chi^*(\mathcal{M}^\dagger\mathcal{M})^{-1}\chi}[d\chi]. \tag{38}$$

The equations of motion for the boson (gauge) field ϕ are

$$\left.\begin{aligned} \dot{\phi} &= \pi \\ \dot{\pi} &= -\frac{\partial S_B}{\partial\phi} - \chi^*\frac{\partial}{\partial\phi}(\mathcal{M}^\dagger\mathcal{M})^{-1}\chi \\ &= -\frac{\partial S_B}{\partial\phi} + \left[(\mathcal{M}^\dagger\mathcal{M})^{-1}\chi\right]^*\frac{\partial}{\partial\phi}(\mathcal{M}^\dagger\mathcal{M})\left[(\mathcal{M}^\dagger\mathcal{M})^{-1}\chi\right]. \end{aligned}\right\} \tag{39}$$

The time-consuming part of the computation is the evaluation of $(\mathcal{M}^\dagger\mathcal{M})^{-1}\chi$, which entails the solution of a large set of linear equations. This is of course much easier than evaluating the full inverse or determinant. The linear equations are usually solved using the iterative conjugate gradient method.

9 The Langevin Algorithm

Consider the Hybrid Monte Carlo algorithm when we take only one leapfrog step. Combining the leapfrog equations (32) we obtain

$$\left.\begin{aligned} \phi' &= \phi + 2\,\delta\tau\pi - \frac{1}{2}\frac{\partial S}{\partial \phi}(2\delta\tau)^2 \\ \pi' &= \pi - \left(\frac{\partial S}{\partial \phi} + \frac{\partial S'}{\partial \phi}\right)\delta\tau. \end{aligned}\right\} \tag{40}$$

If $\delta\tau \ll 1$, and hence $\delta H = O(\delta\tau^3) \ll 1$, we may approximate this *Langevin Monte Carlo* algorithm [21,22] by dropping the Metropolis step. This means we do not need the π' equation above, and we are left with precisely the usual Langevin equation [23,18,24,25,26,27] with Langevin time $\epsilon = 4\,\delta\tau^2$.

The Hybrid (Monte Carlo) method is always more efficient than the Langevin (Monte Carlo) method if the cost per independent configuration is smallest for $\tau_0 > 2\,\delta\tau$ [28,9,29,30].

An interesting observation has been made by Mackenzie [31]. If it is meaningful to think of the system as having weakly coupled modes of different frequencies then it would not be unreasonable to take τ_0 to be of the order of the period of the slowest mode of the system in order to minimize correlations between successive configurations. However, for any τ_0 larger than the period of the fastest mode there is a good chance that one Hybrid Monte Carlo trajectory will be very close to some multiple of the period of some mode of the system. We would then expect this mode to take a very large number of trajectories to relax, and thus we would not see any significant decrease in the autocorrelation time on taking $\tau_0 > 1$. Mackenzie suggests that suitably varying the trajectory length τ_0 from trajectory to trajectory should eliminate this problem.

10 Asymptotic Behaviour

The performance of the Hybrid Monte Carlo and related algorithms depends on the nature of the theory to which they are being applied, but we can learn something useful about the simplest case, where we take the lattice volume to infinity while keeping all the parameters in the action fixed [32,33,29].

The Hybrid Monte Carlo partition function is

$$Z = \int [d\phi][d\pi] e^{-H(\phi,\pi)}. \tag{41}$$

We rewrite this in terms of the variables (ϕ', π') at the end of a Molecular Dynamics trajectory, and use the fact that $[d\phi][d\pi] = [d\phi'][d\pi']$:

$$Z = \int [d\phi'][d\pi'] e^{-H(\phi',\pi')} = \int [d\phi][d\pi] e^{-H(\phi,\pi)-\delta H} \tag{42}$$

to prove that $\langle e^{-\delta H} \rangle = 1$.

Since e^x is a convex function[6] Jensen's inequality is satisfied,[7] so $\langle e^{-\delta H} \rangle \geq e^{-\langle \delta H \rangle}$, which in turn implies that $\langle \delta H \rangle \geq 0$. In other words δH cannot decrease on average; the best that can be done is to conserve energy, which is what classical mechanics does.

Expanding in powers of δH, which corresponds to a small $\delta\tau$ expansion, gives

$$\langle \delta H \rangle = \frac{1}{2} \langle \delta H^2 \rangle + O(\delta H^3). \tag{43}$$

This result will prove very useful in the sequel.

For Langevin Monte Carlo the energy change after one step is

$$\delta H = \left(2\pi \frac{\partial S}{\partial \phi} \frac{\partial^2 S}{\partial \phi^2} - \frac{2\pi^3}{3} \frac{\partial^3 S}{\partial \phi^3} \right) \delta\tau^3 + O(\delta\tau^4), \tag{44}$$

so Eq. (43) tells us that

$$\langle \delta H \rangle = \frac{1}{2} \left\langle \left(2\pi \frac{\partial S}{\partial \phi} \frac{\partial^2 S}{\partial \phi^2} - \frac{2\pi^3}{3} \frac{\partial^3 S}{\partial \phi^3} \right)^2 \delta\tau^6 \right\rangle + O(\delta\tau^8). \tag{45}$$

[6] Any function f whose second derivative is positive on an interval, $f''(x) > 0 \quad \forall x \in (a,b)$, is convex on that interval $f(x) \geq f(c) + f'(c)(x-c) \quad \forall x, c \in (a,b)$.

[7] Take the average of the convexity condition with respect to any probability measure μ: $\langle f \rangle_\mu \geq f(c) + f'(c)\langle x - c \rangle_\mu = f(\langle x \rangle_\mu)$ since $\langle 1 \rangle_\mu = 1$ and setting $c = \langle x \rangle_\mu$.

To compute the acceptance rate we need to know the size of δH on the individual configurations, rather than the average over the equilibrium ensemble. On a large enough volume, $V \gg \xi^4$ where ξ is the correlation length, the average over a single configuration behaves in a similar way to the ensemble average: to be definite we may expect

$$\langle \pi \rangle \sim \sqrt{V} \qquad \langle \pi^2 \rangle \sim V \tag{46}$$

and so forth, thus the average over a single configuration $\overline{\delta H} = C\sqrt{V}\delta\tau^3 + \frac{1}{2}C^2 V \delta\tau^6 + \cdots$. Therefore in order to keep the acceptance rate fixed as we increase the lattice volume we must take $\delta\tau \propto V^{-1/6}$.

For $\delta\tau \ll 1$ we require $O(1/\delta\tau^2)$ Langevin Monte Carlo trajectories to get uncorrelated configurations, so the cost grows as $V^{4/3}$.

The analysis for Hybrid Monte Carlo is very similar to that for Langevin Monte Carlo. The energy change per trajectory is larger, namely

$$\overline{\delta H} = C\sqrt{V}\delta\tau^2 + \cdots + \frac{1}{2}C^2 V \delta\tau^4 + \cdots, \tag{47}$$

so $\delta\tau \propto V^{-1/4}$ as $V \to \infty$ for a constant acceptance rate. If the Hybrid Monte Carlo trajectories are chosen to be of length $\tau_0 \approx 1$ each trajectory may be assumed to be fairly uncorrelated with its predecessor, but we must take $N = \tau_0/\delta\tau$ steps, so the cost grows as $V^{5/4}$.

11 Higher-Order Integration Schemes

In practice the coefficient in front of the $V^{5/4}$ dependence of cost upon volume appears to be the contraining factor on currently feasible lattices, but it is very interesting to learn how to improve the asymptotic form as well. The technique for doing this is to find a higher-order analogue to the leapfrog equations Eq. (32) [34]. A very elegant way of doing this has been found by Campostrini [35], Creutz and Gocksch [36]. The leapfrog equations may be considered as a leading approximation to the exact solution of Hamilton's equations

$$\Lambda(\Delta\tau) = e^{H\Delta\tau} + R\Delta\tau^3 + O(\Delta\tau^5), \tag{48}$$

where H is the Hamiltonian operator acting on fictitious phase space, Λ is the operator defined by the leapfrog equations, and R is an operator which is the

coefficient of the next term in the expansion in powers of $\Delta\tau$. Consider now a "wiggle" consisting of a leapfrog step forwards of size $\Delta\tau$, a step backwards of size $\sigma\Delta\tau$ where σ is a judiciously selected constant, and then another set forwards of size $\Delta\tau$. The reversibility and area-preserving properties of Λ immediately imply that the "wiggle" is also reversible and area-preserving; furthermore applying Eq. 48 to the wiggle we obtain

$$\Lambda(\Delta\tau)\Lambda(-\sigma\Delta\tau)\Lambda(\Delta\tau) = e^{H(2-\sigma)\Delta\tau} + R(2-\sigma^3)\Delta\tau^3 + O(\Delta\tau^5). \qquad (49)$$

Clearly, the wiggle has a leading error of order $\Delta\tau^5$ if we take $\sigma = \sqrt[3]{2}$. In order to ensure that the wiggle moves the same distance throught phase space as the original leap we should also take $(2-\sigma)\Delta\tau = \delta\tau$.

This procedure can be applied recursively as many times as we like, producing a method which has errors of arbitrarily high order in $\delta\tau$, although if we bear in mind that a wiggle is more than three times as much work as a single leap we may make the naïve estimate that the best asymptotic volume dependence is proportional to $V \exp\sqrt{k \ln V}$, which grows more slowly than any power of V greater than unity.

12 Exact Results for Free Field Theory

It is informative to study Hybrid Stochastic Monte Carlo algorithms for some simple models for which we can derive analytic formulæ for their behaviour [37,38]. For these models we should at least be able to make quantitative statements about the optimal choice of parameters for making specific measurements. Of course, the objection may be made that their behaviour for toy models has little bearing on what happens for non-trivial field theories but, perhaps suprisingly, a lot of interesting phenomena already show up even for these simple cases.

12.1 Uncoupled Harmonic Oscillators

We may start by considering a set of V uncoupled harmonic oscillators (in ficticious phase space) described by the Hamiltonian

$$H = \frac{1}{2}\sum_{i=1}^{V}(p_i^2 + \omega_i^2 q_i^2). \qquad (50)$$

The leapfrog equations (32) reduce to

$$\left.\begin{array}{rcl} p_i(\delta\tau) &=& p_i(0) - \omega_i^2 q_i(0)\delta\tau \\ q_i(2\delta\tau) &=& q_i(0) + p_i(\delta\tau)2\delta\tau \\ p_i(2\delta\tau) &=& p_i(\delta\tau) - \omega_i^2 q_i(2\delta\tau)\delta\tau \end{array}\right\} \tag{51}$$

for this Hamiltonian; and the change in energy for this step is

$$\begin{aligned} \delta H &\equiv H(2\delta\tau) - H(0) \qquad (52) \\ &= \sum_i \Big\{ 2\omega_i^4 q_i p_i \delta\tau^3 + 2\omega_i^4 (p_i^2 - \omega_i^2 q_i^2)\delta\tau^4 - 4\omega_i^6 q_i p_i \delta\tau^5 + 2\omega_i^8 q_i^2 \delta\tau^6 \Big\}. \end{aligned}$$

The equilibrium acceptance probability for Langevin Monte Carlo is thus

$$P_{acc} = \frac{1}{Z}\int d^V q\, d^V p\, e^{-H(q_i,p_i)} \min(1, e^{-\delta H}) \tag{53}$$

$$= \frac{1}{Z}\int_{-\infty}^{\infty} d\xi \min(1, e^{-\xi}) \int d^V q\, d^V p\, e^{-H} \delta(\xi - \delta H) \tag{54}$$

$$= \frac{1}{2\pi Z}\int_{-\infty}^{\infty} d\xi\, d\eta\ \min(1, e^{-\xi}) e^{i\eta\xi} F(\eta), \tag{55}$$

where

$$F(\eta) \equiv \int d^V q\, d^V p\, e^{-H - i\eta\delta H} = \int d^V q\, d^V p\, e^{-H'}. \tag{56}$$

Because this is a free theory H' is quadratic, hence

$$H' = \frac{1}{2}\begin{pmatrix} q_i & p_i \end{pmatrix} M \begin{pmatrix} q_i \\ p_i \end{pmatrix} \tag{57}$$

where M is the Hessian

$$M = \begin{pmatrix} \omega_i^2 - 4i\eta\omega_i^6\delta\tau^4(1 - \omega_i^2\delta\tau^2) & 2i\eta\omega_i^4\delta\tau^3(1 - 2\omega_i^2\delta\tau^2) \\ 2i\eta\omega_i^4\delta\tau^3(1 - 2\omega_i^2\delta\tau^2) & 1 + 4i\eta\omega_i^4\delta\tau^4 \end{pmatrix}, \tag{58}$$

which leads to

$$F(\eta) = (2\pi)^V \Big/ \sqrt{\det M} \tag{59}$$

$$= (2\pi)^V \prod_{i=1}^{V} \Big\{ \omega_i^2 \left[1 + B_i\eta(\eta + i)\right] \Big\}^{-1/2} \tag{60}$$

where $B_i = 4\omega_i^6 \delta\tau^6$.

We are thus lead to considering an integral of the form

$$P_{acc} = \frac{(2\pi)^{V-1}}{Z} \int_{-\infty}^{\infty} d\xi \, d\eta \, \min(1, e^{-\xi}) e^{i\eta\xi} \left\{ \prod_{i=1}^{V} \omega_i^2 \left[1 + B_i \eta(\eta + i) \right] \right\}^{-1/2} . \tag{61}$$

For $B_i \ll 1$ we may evaluate this integral, and we find

$$P_{acc} = \mathrm{erfc}\left(\frac{1}{\sqrt{8}} \sum_{i=1}^{V} B_i \right) . \tag{62}$$

For Langevin Monte Carlo this becomes

$$P_{acc} = \mathrm{erfc}\left(\delta\tau^3 \sqrt{V\sigma} \right) , \tag{63}$$

where we have introduced the quantity $\sigma \equiv \frac{1}{V} \sum_i \omega_i^6$.

12.2 Free Field Theory

Consider the one-dimensional free scalar field theory with action

$$S = \frac{1}{2} \sum_{x=1}^{V} \phi_x^* (-\Delta^2 + m^2) \phi_x \tag{64}$$

where Δ^2 is the lattice Laplacian

$$\Delta^2 \phi_x \equiv \phi_{x+1} + \phi_{x-1} - 2\phi_x , \tag{65}$$

For Hybrid Monte Carlo we introduce the ficticious momenta π_x and the Hamiltonian

$$H = \frac{1}{2} \sum_{x=1}^{V} \left\{ \pi_x^* \pi_x + \phi_x^* (-\Delta^2 + m^2) \phi_x \right\} . \tag{66}$$

In order to diagonalize this Hamiltonian we Fourier transform to "real" momentum space

$$\phi_x = \sqrt{\frac{1}{V}} \sum_{p=1}^{V} e^{2\pi i p x / V} \phi_p , \qquad \phi_p = \sqrt{\frac{1}{V}} \sum_{x=1}^{V} e^{-2\pi i p x / V} \phi_x , \tag{67}$$

and likewise for π_x.[8] We find

$$H = \frac{1}{2}\sum_{p=1}^{V}\left\{\pi_p^*\pi_p + \omega_p^2\phi_p^*\phi_p\right\} \tag{68}$$

where the frequency spectrum is

$$\omega_p^2 \equiv m^2 + 4\sin^2\left(\frac{\pi p}{V}\right). \tag{69}$$

The parameter σ in the acceptance rate is

$$\begin{aligned}
\sigma &\equiv \frac{1}{V}\sum_{p=1}^{V}\omega_p^6 = \frac{1}{V}\sum_{p=1}^{V}\left[m^2 + 4\sin^2\left(\frac{\pi p}{V}\right)\right]^3 && (70)\\
&\to \int_0^{2\pi}\frac{d\tilde{p}}{2\pi}\left[m^2 + 4\sin^2\left(\frac{\tilde{p}}{2}\right)\right]^3 && (71)\\
&= 20 + 18m^2 + 6m^4 + m^6 && (72)
\end{aligned}$$

as $V \to \infty$, with $\tilde{p} \equiv 2\pi p/V$.

We may repeat the preceding arguments for the the higher-order integration scheme of section 11, albeit with a lot more algebra: We find

$$\begin{aligned}
\det M &= \prod_i \omega_i^2\Big[1 + \omega_i^{10}\delta\tau^{10}\times\\
&\qquad \times\Big\{\eta(\eta+i)\tfrac{4}{243}(120 + 96\sqrt[3]{2} + 75\sqrt[3]{4}) + O(\omega_i^2\delta\tau^2)\Big\}\Big]\\
&\approx \prod_i \omega_i^2\left[1 + 5.9\omega_i^{10}\delta\tau^{10}\eta(\eta+i)\right] + O(\delta\tau^{12}), && (73)
\end{aligned}$$

which gives immediately that $B_i \approx 5.9\omega_i^{10}\delta\tau^{10}$, and hence

$$P_{acc} \approx \mathrm{erfc}\left(0.85\,\delta\tau^5\sqrt{V\sigma}\right) \tag{74}$$

where now $\sigma \equiv \frac{1}{V}\sum_i \omega_i^{10}$. For free field theory $\sigma = 252 + 350m^2 + 200m^4 + 60m^6 + 10m^8 + m^{10}$.

[8] That is, we introduce a momentum space representation for the ficticious momenta.

12.3 Hybrid Monte Carlo

It is simple to extend these Langevin Monte Carlo results to more than one leapfrog step. For n steps we find

$$\begin{aligned}\delta H &= 2n\omega_i^4 q_i p_i \delta\tau^3 + 2n^2\omega_i^4(p_i^2 - w_i^2 q_i^2)\delta\tau^4 - \\ &\quad -\tfrac{4}{3}n(4n^2-1)\omega_i^6 q_i p_i \delta\tau^5 + \\ &\quad +\tfrac{2}{3}n^2\left[(4n^2-1)q_i^2 - (4n^2-4)p_i^2\right]\omega_i^6\delta\tau^6 + \cdots, \end{aligned} \tag{75}$$

but substituting $n = \tau_0/\delta\tau$ in this expression is not a correct procedure to obtain the Hybrid Monte Carlo formula.

For free field theory the leapfrog step (51) is a linear map on phase space:

$$\begin{pmatrix} q_i(2\delta\tau) \\ p_i(2\delta\tau) \end{pmatrix} = \begin{pmatrix} 1 - 2\omega_i^2\delta\tau^2 & 2\delta\tau \\ -2\omega_i^2\delta\tau(1-\omega_i^2\delta\tau^2) & 1 - 2\omega_i^2\delta\tau^2 \end{pmatrix} \begin{pmatrix} q_i(0) \\ p_i(0) \end{pmatrix}. \tag{76}$$

Iterating this map n times, setting $n \equiv \tau_0/\delta\tau$, and Taylor expanding in $\delta\tau$ leads to the following determinant for the Hessian M of H':

$$\begin{aligned}\det M &= \prod_i \omega_i^2\Big[1 + \omega_i^4\delta\tau^4\eta(\eta+i)\tfrac{1}{6}\Big\{3 - 3\cos(4\omega_i\tau_0) + \\ &\quad + \left(3\omega_i^2 - 3\omega_i^2\cos(4\omega_i\tau_0) + 2\tau_0\omega_i^3\sin(4\omega_i\tau_0)\right)\delta\tau^2 + \\ &\quad + O(\delta\tau^4)\Big\}\Big]. \end{aligned} \tag{77}$$

Using our previous formalism we have $B_i = \frac{1}{2}\omega_i^4\delta\tau^4[1-\cos(4\omega_i\tau_0)] + O(\delta\tau^6)$, and

$$P_{\rm acc} = \operatorname{erfc}\left(\delta\tau^2\sqrt{V\sigma/2}\right), \tag{78}$$

with $\sigma \equiv \frac{1}{8V}\sum_i \omega_i^2\{1-\cos(4\omega_i\tau_0)\}$.

Using the free field spectrum

$$\begin{aligned}\sigma &= \frac{1}{8V}\sum_{p=1}^{V}\left[m^2 + 4\sin^2\left(\frac{\pi p}{V}\right)\right]\left[1 - \cos\left(4\tau_0\sqrt{m^2 + 4\sin^2\left(\frac{\pi p}{V}\right)}\right)\right] \\ &\to \frac{1}{8}\int_0^{2\pi}\frac{d\tilde{p}}{2\pi}\left[m^2 + 4\sin^2\left(\frac{\tilde{p}}{2}\right)\right]\left[1 - \cos\left(4\tau_0\sqrt{m^2 + 4\sin^2\left(\frac{\tilde{p}}{2}\right)}\right)\right] \end{aligned} \tag{79}$$

as $V \to \infty$. For $m = 0$ the integral becomes

$$\sigma = \frac{1}{2\pi} \int_0^\pi dx \, \sin^2 x [1 - \cos(8\tau_0 \sin x)] \tag{80}$$

$$= \frac{1}{4} - \frac{1}{2} \mathrm{J}_0(8\tau_0) + \frac{1}{16\tau_0} \mathrm{J}_1(8\tau_0), \tag{81}$$

showing that there are oscillations in acceptance rate with τ_0. This phenomenon has been observed in Hybrid Monte Carlo computations for interacting four-dimensional field theories.

Notice the interesting property that the spectral sums σ all involve positive powers of the frequencies ω_i: this means that the acceptance rate is dominated by the highest frequency modes. This is a hint that very significant improvements in Hybrid Stochastic algorithms may still be found.

References

[1] John H. Halton. A retrospective and prospective survey of the Monte Carlo method. *SIAM Review*, 12:1–63, 1970.

[2] F. James. Monte Carlo in theory and practice. *Rept. Prog. Phys.*, 43:1145, 1980.

[3] Olivier Martin and Steve W. Otto. Reducing the number of flavors in the microcanonical method. *Phys. Rev.*, D31(2):435–437, January 1985.

[4] Janos Polonyi, H. W. Wyld, and John B. Kogut. Finite-temperature phase transitions in SU(3) lattice gauge theory with dynamical, light fermions. *Phys. Rev. Lett.*, 53(7):644–647, August 1984.

[5] N. A. Metropolis, M. N. Rosenbluth, A. H. Rosenbluth, E. Teller, and J. Teller. *J. Chem. Phys*, 21:1087, 1953.

[6] S. Duane. Stochastic quantization vs. the microcanonical ensemble: getting the best of both worlds. *Nucl. Phys.*, B257 [FS14]:652, 1985.

[7] Simon Duane and John B. Kogut. Hybrid stochastic differential equations applied to quantum chromodynamics. *Phys. Rev. Lett.*, 55(25):2774–2777, December 1985.

[8] Simon Duane and John B. Kogut. The theory of hybrid stochastic algorithms. *Nucl. Phys.*, B275:398, 1986.

[9] Steven Gottlieb, W. Liu, D. Toussaint, R. L. Renken, and R. L. Sugar. Empirical study of the hybrid-molecular-dynamics approach to the simulation of QCD. *Phys. Rev.*, D36(12):3797–3803, December 1987.

[10] H. C. Andersen. *J. Chem. Phys*, 72:2384, 1980.

[11] David J. E. Callaway and Aneesur Rahman. Microcanonical ensemble formulation of lattice gauge theory. *Phys. Rev. Lett.*, 49(9):613–616, 1982.

[12] Arunabha Guha and S.-C. Lee. Stochastic quantization of matrix and lattice gauge models. *Phys. Rev.*, D27(10):2412–2422, May 1983.

[13] J. Polonyi and H. W. Wyld. Microcanonical simulation of fermionic systems. *Phys. Rev. Lett.*, 51:2257, 1983. Erratum: ibid. 52:401, 1984.

[14] J. Polonyi and H. W. Wyld. A microcanonical method for fermionic systems. *Nucl. Phys.*, A418:491C–498C, 1984.

[15] Simon Duane, A. D. Kennedy, Brian J. Pendleton, and Duncan Roweth. Hybrid Monte Carlo. *Phys. Lett.*, 195B(2), 1987.

[16] A. D. Kennedy. Hybrid Monte Carlo. In A. Billoire, R. Lacaze, A. Morel, O. Napoly, and J. Zinn-Justin, editors, *Field Theory on the Lattice*, pages 576–579, 1988. 1987 International Conference on Field Theory on a Lattice, Seillac, France.

[17] A. D. Kennedy and Pietro Rossi. *Classical Mechanics on Group Manifolds.* Technical Report FSU–SCRI–89–69, UCSD 89/03, SCRI, May 1989. To appear in Nucl. Phys. B.

[18] Ian T. Drummond, Simon Duane, and Ron R. Horgan. The stochastic method for numerical simulations: higher order corrections. *Nucl. Phys.*, B220 [FS8]:119–136, 1983.

[19] Simon Duane, Richard D. Kenway, Brian J. Pendleton, and Duncan Roweth. Acceleration of gauge field dynamics. *Phys. Lett.*, B176:143, 1986.

[20] Steven Gottlieb, W. Liu, D. Toussaint, R. L. Renken, and R. L. Sugar. Hybrid-molecular-dynamics algorithms for the numerical simulation of Quantum Chromodynamics. *Phys. Rev.*, D35(8):2531–2542, April 1987.

[21] P. J. Rossky, J. D. Doll, and H. L. Friedman. Brownian dynamics as smart Monte Carlo simulation. *J. Chem. Phys.*, 69(10):4628–4633, November 1978.

[22] Steven Gottlieb, W. Liu, D. Toussaint, and R. L. Sugar. Testing an exact algorithm for simulation of fermionic QCD. *Phys. Rev.*, D35:2611, 1987.

[23] O. Klein. *Arkiv Mat. Astr. Fys.*, 16(5), 1922.

[24] G. G. Batrouni, G. R. Katz, A. S. Kronfeld, G. P. Lepage, B. Svetitsky, and K. G. Wilson. Langevin simulations of lattice field theories. *Phys. Rev.*, D32:2736, 1985.

[25] A. Ukawa and M. Fukugita. Langevin simulation including dynamical quark loops. *Phys. Rev. Lett.*, 55:1854, 1985.

[26] Alan Horowitz. *Phys. Lett.*, 156B:89, 1985.

[27] Alan Horowitz. The second order Langevin equation and numerical simulations. *Nucl. Phys.*, B280[FS18](3):510–522, March 1987.

[28] R. V. Gavai, J. Potvin, and S. Sanielevici. Numerical tests of Langevin lattice QCD. *Phys. Rev.*, D27(6):1912–1921, September 1987.

[29] Rajan Gupta, Gregory W. Kilcup, and Stephen R. Sharpe. Tuning the hybrid Monte Carlo algorithm. *Phys. Rev.*, D38(4):1278–1287, August 1988.

[30] Akira Ukawa. Hybrid Monte Carlo algorithm as applied to dynamical Wilson fermion. In Andreas S. Kronfeld and Paul B. Mackenzie, editors, *Lattice 88*, pages 463–468, 1989. Proceedings of the 1988 Symposium on Lattice Field Theory, Fermilab.

[31] Paul B. Mackenzie. *An Improved Hybrid Monte Carlo Method.* Technical Report FERMILAB–89/100–T, Fermilab, March 1989.

[32] Michael Creutz. Algorithmic alternatives. In A. Billoire, R. Lacaze, A. Morel, O. Napoly, and J. Zinn-Justin, editors, *Field Theory on the Lattice*, pages 547–556, 1988. 1987 International Conference on Field Theory on a Lattice, Seillac, France.

[33] Michael Creutz. Global Monte Carlo algorithms for many fermion systems. *Phys. Rev.*, D38(4):1228–1238, August 1988.

[34] A. D. Kennedy. Higher-order Hybrid Monte Carlo. In Andreas S. Kronfeld and Paul B. Mackenzie, editors, *Lattice 88*, pages 457–462, 1989. Proceedings of the 1988 Symposium on Lattice Field Theory, Fermilab.

[35] Massimo Campostrini and Paolo Rossi. *A Comparison of Numerical Algorithms for Dynamical Fermions.* Technical Report IFUP–TH 12/89, Università di Pisa, April 1989.

[36] Michael Creutz and Andreas Gocksch. *Higher Order Hybrid Monte Carlo Algorithms.* Technical Report, Brookhaven, March 1989.

[37] A. D. Kennedy and B. J. Pendleton. *Some Exact Results for Hybrid Monte Carlo.* Technical Report, SCRI, 1989. In preparation.

[38] H. Gausterer and M. Salmhofer. Remarks on global Monte Carlo algorithms. *Phys. Rev.*, D40(8):2723–2726, October 1989.