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G.P. Lepage et al.

Fermi National Accelerator Laboratory
P.O. Box 500, Batavia, Illinois 60510

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Perturbative two- and three-loop coefficients from large β Monte Carlo

G. P. Lepage[a], P. B. Mackenzie[b], N. H. Shakespeare[c], and H. D. Trottier[c]

[a]Newman Laboratory of Nuclear Studies, Cornell University, Ithaca, NY, 14853

[b]Fermilab, MS 106, P.O. Box 500, Batavia, IL 60510

[c]Physics Department, Simon Fraser University, Burnaby, B.C., Canada V5A 1S6

Perturbative coefficients for Wilson loops and the static quark self-energy are extracted from Monte Carlo simulations at large β on finite volumes, where all the lattice momenta are large. The Monte Carlo results are in excellent agreement with perturbation theory through second order. New results for third order coefficients are reported. Twisted boundary conditions are used to eliminate zero modes and to suppress Z_3 tunneling.

1. INTRODUCTION

Simulations using highly improved lattice actions have become commonplace in recent years. Higher order perturbative calculations for these actions present a major challenge however, which must be overcome in order to obtain precision results for a number of observables.

A simple alternative to analytic perturbation theory, proposed in Ref. [1], is to directly measure observables in Monte Carlo simulations at very large β and to fit the coefficients of the perturbative expansion to the results. This produces coefficients with both statistical and truncation errors, so it is not a complete substitute for conventional perturbation theory. However, as we show here, it produces estimates of high order coefficients with far less effort than a conventional calculation. This method was shown to reproduce analytical results for the one-loop mass renormalization for Wilson fermions, and the one-loop additive energy for NRQCD fermions [1]. In addition, preliminary estimates of some third-order Wilson loop coefficients have been made [2]. An extension of this technique to background field calculations has also been considered [3].

In this work we make a much more extensive analysis of this method. We reproduce known second-order perturbative coefficients for Wilson loops and the static quark self-energy to high accuracy. New predictions for third-order coefficients for these observables are made, and results of extensive systematic studies are reported.

2. WILSON LOOPS

To begin with, we present results of simulations of Wilson loops for the Wilson gauge-field action on 16^4 lattices. Periodic boundary conditions were used here in order to make a direct comparison with the second order perturbative coefficients calculated by Heller and Karsch [4] on the same lattice volume. Simulations were done at nine couplings, from $\beta \approx 9$ to $\beta \approx 50$.

We analyze the logarithm of the $R \times T$ Wilson loop

$$-\frac{1}{2(R+T)} \ln W_{R,T} = \sum_n c_n \, \alpha_P^n(q^*_{R,T}),$$

scaled such that the coefficients for large loops approach those of the static self-energy. We use a renormalized coupling α_P determined from measured values of the plaquette [5,6]

$$-\ln W^{MC}_{1,1} \equiv \frac{4\pi}{3}\alpha_P(3.41/a)\,[1 - 1.185\,\alpha_P]\,.$$

This eliminates large renormalizations of the bare lattice coupling $\alpha_0 = 3/(2\pi\beta)$, as can be seen by relating α_P to α_0, using the third-order expansion of the plaquette given in Ref. [7]:

$$\alpha_P(3.41/a) \approx \alpha_0 + 4.558\,\alpha_0^2 + 28.499\,\alpha_0^3. \qquad (1)$$

The renormalized coupling is evaluated at scales $q^*_{R,T}$ determined by the procedure of Ref. [5]. It is

also possible to perform the fitting procedure using the bare coupling constant, α_0, but this leads to much larger higher order coefficients and truncation errors because of the large coefficients in Eqn. 1. These lead in turn to poorer fits with larger χ^2's.

It is very straightforward to fit the leading perturbative coefficients to the Monte Carlo data. Monte Carlo results for the 5×5 Wilson loop are presented in Fig. 1, in terms of the quantity

$$\kappa_1 \equiv -\ln W^{MC}_{R,T} \,/\, \left(2(R+T)\alpha_P(q^*_{R,T})\right) ,$$

after the known first-order contribution due to zero modes [8] is subtracted from the data. The

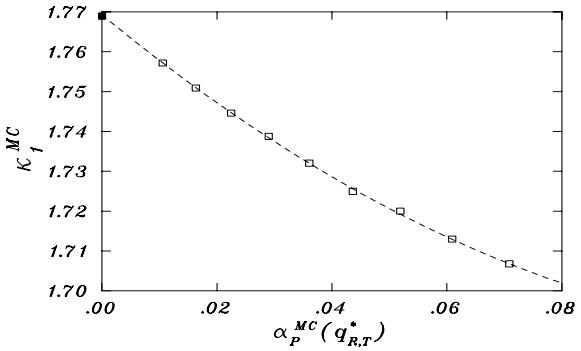

Figure 1. Monte Carlo results for κ_1 for the 5×5 Wilson loop, with best fit.

dashed line in Fig. 1 is the result of a fit to $\kappa_1 \approx c_1 + c_2\alpha_P + c_3\alpha_P^2$; the filled square shows the analytical value of c_1, while the curvature in the results for κ_1 demonstrates a signal for c_3.

The measured values of $c_{1,2}$ for various small loops are shown in Table 1. They are in excellent agreement with perturbation theory.

We also make new predictions for the third-order coefficients c_3. To improve the accuracy of these results, it is helpful to subtract the analytically known first- and second-order perturbative contributions from the data. Monte Carlo results for the residual

$$\kappa_3 \equiv \frac{1}{\alpha_P^3}\left[-\frac{1}{2(R+T)}\ln W^{MC}_{R,T} - c_1\alpha_P - c_2\alpha_P^2\right]$$

are shown in Fig. 2 for the 5×5 loop, with the results of a fit to $\kappa_3 \approx c_3 + c_4\alpha_P$.

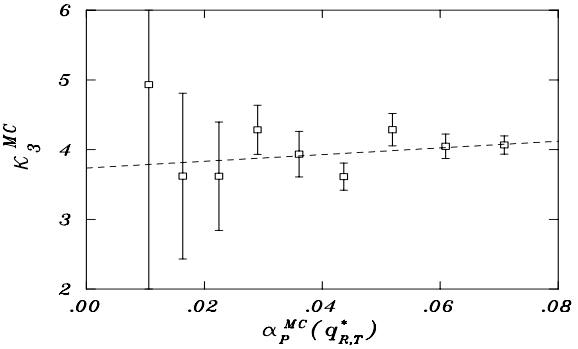

Figure 2. Monte Carlo results for κ_3 for the 5×5 Wilson loop, with best fit.

The data are not accurate enough to resolve c_4, although the best fit errors indicate that c_4 is of the same order as c_3 for these Wilson loops. To obtain errors on the c_3 that take into account the effects of truncation in α_s, we include the c_4 term in our fits. In the results for c_3 given in Table 2, the quoted errors come from the fit including c_4, which effectively includes an uncertainty due to the possible values of c_4 allowed by the data.

We used periodic boundary conditions in these tests on small Wilson loops in order to be able to compare directly with Ref. [4]. The known leading effects of the resulting zero modes were subtracted by hand. We have not corrected for the contribution from zero modes beyond first order; these effects should be very small for small Wilson loops. In fact there is no visible effect of zero modes beyond first order, within statistical errors. (This would show up in singular behavior in κ_3 at small α_P).

3. STATIC QUARK SELF-ENERGY

To calculate quantities more complicated than Wilson loops, we need to solve some additional problems. In general, the effects of zero modes are

Table 1
Perturbative coefficients $c_{1,2}$ of Wilson loops from Monte Carlo simulations and perturbation theory.

Loop	c_1^{MC}	$c_1^{PT}(q^*_{R,T})$	c_2^{MC}	$c_2^{PT}(q^*_{R,T})$	$q^*_{R,T}$
1×2	1.2037(1)	1.2039	-1.248(08)	-1.257	3.07
1×3	1.2586(2)	1.2589	-1.186(09)	-1.195	3.01
2×2	1.4336(2)	1.4338	-1.314(08)	-1.320	2.65
3×3	1.6088(3)	1.6089	-1.205(12)	-1.204	2.46
4×4	1.7065(4)	1.7066	-1.202(16)	-1.198	2.30
5×5	1.7692(6)	1.7690	-1.191(36)	-1.166	2.23

Table 2
Monte Carlo results for third order coefficients c_3 of Wilson loops.

Loop	$c_3^{MC}(q^*_{R,T})$	$q^*_{R,T}$
1×2	0.40(08)	3.07
1×3	0.63(10)	3.01
1×4	0.82(10)	2.97
1×5	0.92(10)	2.95
2×2	1.38(09)	2.65
2×3	1.89(11)	2.56
2×4	2.26(11)	2.49
2×5	2.51(11)	2.46
3×3	2.49(12)	2.46
3×4	2.94(11)	2.38
3×5	3.23(13)	2.35
4×4	3.35(14)	2.30
4×5	3.67(19)	2.27
5×5	3.74(33)	2.23

unknown and not small, so we must remove them from the first. Further, most quantities are highly sensitive to the effects of tunneling between the various Z_3 vacua of $SU(3)$, so we must suppress this, too. We test our ability to do this by calculating the static quark self-energy E_0.

Zero modes can be eliminated by using twisted boundary conditions [9], and remaining finite size effects can be removed by extrapolating results from several lattice volumes.

We measured the gauge-invariant Polykaov line on lattices of various volumes $L^3\times(T=L)$

$$P_4(L)\equiv\frac{1}{3L^3}\sum_{\vec{x}}\mathrm{ReTr}\prod_{x_4=1}^{L}U_4(x).$$

Defining $E_0(L)\equiv-\ln P_4(L)/L$, we have $E_0\equiv E_0(L\to\infty)$. The two-loop expression for E_0 can be obtained from perturbative results for P_4 [4,10]

$$E_0=2.1173\,\alpha_P(1.68/a)-1.124\,\alpha_P^2+O(\alpha_P^3).$$

The Polyakov line is an order parameter for the Z_3 degenerate vacua of the gauge theory, and has different values in different Z_3 phases. To make its vacuum expectation value well defined and nonzero in a Monte Carlo simulation, one can add an external field to the action to pin the simulation into one of the Z_3 states and take the limit of the external field going to zero as the volume goes to infinity.

In order to minimize these nonperturbative effects, we start the simulation with all links initialized to $U_\mu=I$; tunneling and domain formation are suppressed by working at sufficiently large lattice volumes and couplings β. We found that with periodic boundary conditions, tunnelings were quite frequent, even at the surprisingly large β's of $50-100$. On the other hand, we find that twisted boundary conditions lead to a dramatic suppression of these effects. Twisting in two directions strongly suppresses tunneling and twisting in three directions virtually eliminates it, even on runs of hundreds of thousands of sweeps and relatively low β. Thus, so far, adopting the pinning method has been unnecessary.

Finite-size effects are consistent with perturbative expectations. We estimate E_0 by fitting

$E_0(L)$ to the perturbative form of the interaction between the static quark and its images in the box walls:

$$E_0(L) = E_0 - (a_1 + a_2 \ln(L))/L.$$

Simulations were done with twisted boundary conditions on 9 volumes, $L = [3, 11]$. Measurements were made at 9 couplings on each volume, from $\beta \approx 9$ to $\beta \approx 60$. Results for $E_0(L)$ at $\beta = 9.5$ are shown in Fig. 3; in all cases, the fits yield $a_1 = O(\alpha_P)$ and $a_2 = O(\alpha_P^2)$, as expected.

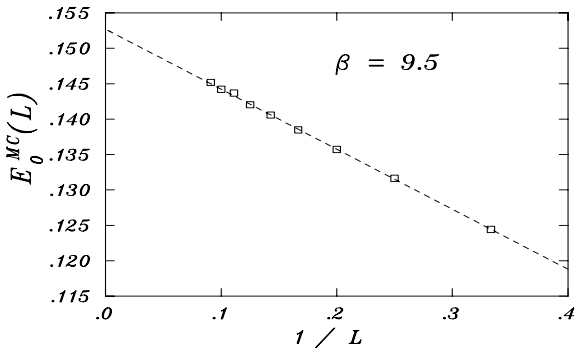

Figure 3. Infinite volume extrapolation of the static quark self-energy $E_0(L)$.

Results for $\kappa_1 \equiv E_0/\alpha_P(q^* = 1.68)$ are shown in Fig. 4. Best fits to $\kappa_1 \approx c_1 + c_2\alpha_P + c_3\alpha_P^2$ yield $c_1^{MC} = 2.117(3)$ and $c_2^{MC} = -1.18(18)$, in good agreement with perturbation theory. We also obtain a new prediction for the third order term; using the analytical values for c_1 and c_2, the best fit yields

$$c_3^{MC} = 5.6(1.8). \qquad (2)$$

As for the loops, we include a fourth order term in the fit. This guards against the presence of an anomalously large c_4, and enlarges the error bar.

A result for the third order term in the expansion of E_0 in the bare lattice coupling has also been reported in this conference, using coupled Langevin equations [11]. Large coefficients in the

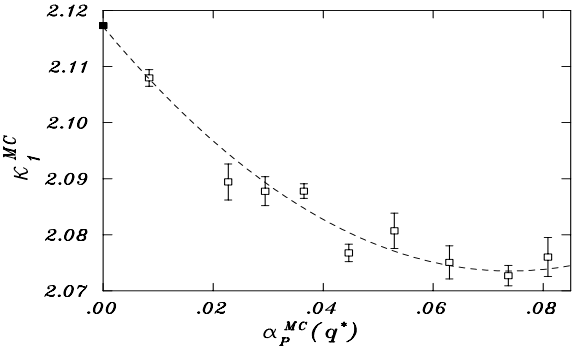

Figure 4. Monte Carlo results for κ_1 for the static quark self-energy, with best fit.

expansion in terms of α_0 reflect the need to renormalize the coupling; for example, combining our result for c_3^{MC} with Eqn. (1), we find

$$E_0 \approx 2.1173\,\alpha_0 + 11.152\,\alpha_0^2 + 81(2)\,\alpha_0^3. \qquad (3)$$

The absolute errors in Eqns. 2 and 3 are the same. The relative error in Eqn. 3 seems surprisingly small because the size of the coefficient itself has been increased by analytic terms from Eqn. 1.

4. ALGORITHMIC INVESTIGATIONS

These calculations have been done using standard pseudo-heat bath algorithms to create the gauge fields. The calculation of E_0 took a little over a month running on about 20 PC's. Clearly finding the best simulation algorithms is an essential element of the method. In this section, we report some preliminary investigations into algorithms specifically appropriate to perturbative simulations.

In principle, microcanonical based methods [12] have the potential to outperform ordinary heat bath methods since they have a critical scaling dimension of 1 instead of 2. In practice, for QCD they don't achieve this. Correlations between nearly degenerate modes last a long time, and nonperturbative effects cause averages over uncorrelated configurations to add up statistically, as $1/\sqrt{n}$. If we examine the perturbative

case carefully, however, we see that this need not be the case.

A single harmonic oscillator evolving under a microcanonical algorithm approaches its average as $1/n$:

$$\langle\phi\rangle = \frac{1}{n}\sum_{m=0}^{n}\exp(im\delta) = \frac{1}{n}\frac{1-\exp(in\delta)}{1-\exp(i\delta)}. \qquad (4)$$

Therefore, free field theory, which is just a collection of independent oscillators, does the same. However, the usual microcanonical evolution equations,

$$H \equiv T + S, \qquad T \equiv \frac{1}{2}\sum_i p_i^2, \qquad S \equiv S(\phi_i) \qquad (5)$$

$\rightarrow$

$$\frac{dp_i}{d\tau} = -\frac{\partial S(\phi)}{\partial \phi_i}, \qquad \frac{d\phi_i}{d\tau} = p_i, \qquad (6)$$

do not make a good simulation algorithm for free field theory. Many sets of momentum modes, e.g., $(1,0,0,0)$ and $(0,1,0,0)$, have same the frequencies and never decorrelate, so that configuration space never gets completely covered.

Since the "momenta" in microcanonical updating of quantum field theories are fictitious, this problem and be removed by introducing a "nondegenerate microcanonical method" using randomized fictitious masses m_i:

$$H \equiv T + S, \qquad T \equiv \frac{1}{2}\sum_i \frac{p_i^2}{m_i}, \qquad S \equiv S(\phi_i), \qquad (7)$$

$\rightarrow$

$$\frac{dp_i}{d\tau} = -\frac{\partial S(\phi)}{\partial \phi_i}, \qquad \frac{d\phi_i}{d\tau} = \frac{p_i}{m_i}, \qquad (8)$$

$a_1 < m_i \leq a_2$, where a_1 and a_2 are of order 1, say 0.8 and 1.2. Mathematical classical mechanics often starts from periodic system system with nondegenerate frequencies. Such systems have more tractable mathematics, for example no zeros in perturbation theory denominators. With these equations, the frequencies of free field theory are nondegenerate and configuration space is covered densely. The KAM theorem then tells us that for small perturbations of nondegenerate unperturbed system, dense tori covered by system's evolution through phase space deformed only slightly. Therefore we expect the covering of configuration space to remain dense in weakly coupled systems, and the convergence to the average to continue to go as $1/n$. It is easy to test that for scalar field theory, things work out in more or less this way.

In QCD, however, gauge symmetry creates a new complication. The random mass method may be adapted to gauge theories in two ways It is straightforward to implement gauge covariant random masses that break most but not all mode degeneracy:

$$T \equiv \frac{1}{2}\sum_i \frac{TrH_i^2}{m_i}, \qquad S \equiv S(U) \qquad (9)$$

$\rightarrow$

$$i\frac{dH_i}{d\tau} = -\frac{\partial S(U)}{\partial U_i}, \qquad \frac{dU_i}{d\tau} = \frac{1}{m_i}iHU, \qquad (10)$$

$H_i = \sum_a \lambda_a h_i^a$.

Mode degeneracy may be broken completely by color breaking random masses:

$$T \equiv \sum_{a\,i}\frac{{h_i^a}^2}{m_i^a}, \qquad S \equiv S(U) \qquad (11)$$

$\rightarrow$

$$i\frac{dH_i}{d\tau} = -\frac{\partial S(U)}{\partial U_i}, \qquad \frac{dU_i}{d\tau} = i\sum_a \frac{h_i^a\lambda^a}{m_i^a}U. \qquad (12)$$

However, they also break gauge invariance. This necessitates gauge fixing, which is more work and may introduce extra correlations.

We have investigated the first of these methods. New complications are present in gauge theories. Free field behavior can only be approached as $\beta \rightarrow \infty$, $U_P \rightarrow 1$. But at very high β, round off becomes important, which destroys the anticorrelations leading to $1/n$ behavior. At small β, Z_3 tunneling occurs. Nonperturbative effects can (and do) destroy the anticorrelations, restoring $1/\sqrt{n}$ statistical behavior. Hence, twisted periodic boundary conditions are required. At moderate β, we find at least partial success with the plaquette. Fig. 5 shows the error obtained on the plaquette using standard binning procedures from the heat bath algorithm

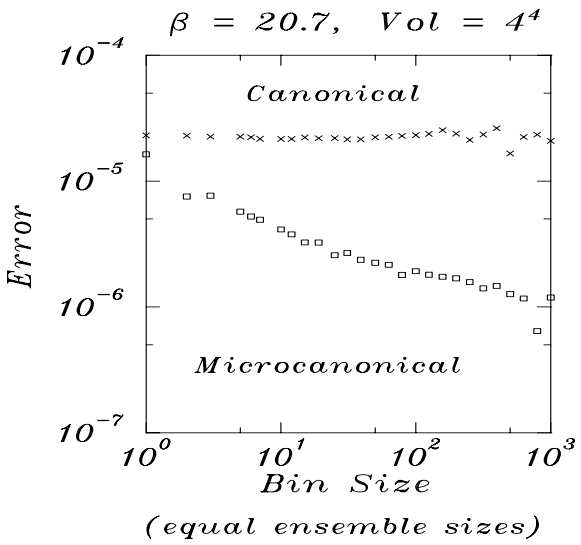

Figure 5. Statistical error on the plaquette obtained with standard binning procedure from the heat bath algorithm (canonical) and the nondegenerate microcanonical algorithm (microcanonical).

(labeled canonical) and the nondegenerate microcanonical algorithm (labeled microcanonical). When anticorrelations as in Eqn. 4 are present, standard formulae, which assume $1/\sqrt{n}$ behavior, should produce errors that drop as $1/\sqrt{n}$ in bin size, as observed. The results obtained are $W_{1,1} = 0.900346(1)$ with the microcanonical method and 0.900271(23) with the canonical method for equal ensemble sizes. We have not extrapolated to infinite volume, which we believe accounts for the small discrepancy.

The plaquette is speeded up beautifully, achieving the full $1/n$ approach to its average even with gauge covariant random masses. However, the plaquette turns out to be a special case, presumably because it is also the action of the theory. For other loops, the great speed up is not observed, which is disappointing but not entirely unexpected in view of the remaining correlations. Full breaking of mode degeneracy appears necessary for most quantities. We are encouraged by the results with the plaquette, but more work is necessary to make this a general method.

5. SUMMARY

In summary, results presented here demonstrate that second order perturbative coefficients are readily accessible in Monte Carlo simulations at large β. Reasonable estimates of third-order terms can also be made, especially when analytic results for lower order terms are available. We are currently working on gauge-fixed quark propagators, in order to measure second order mass renormalizations for NRQCD and Fermilab fermions.

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