The Numerical Estimation of the Error Induced by the Valence Approximation

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We describe a systematic expansion for full QCD. The leading term in the expansion gives the valence approximation. The expansion reproduces full QCD if an infinite number of higher terms are included.

1. INTRODUCTION

The observation that recent valence approximation predictions are quite close to experiment strongly suggests that, at least for some observables, the systematic error arising from this approximation is quite small. It then seems natural to ask whether an independent quantitative estimate can be made of the systematic error of the valence approximation. In this article, we describe an expansion for full QCD \cite{1} which has the valence approximation as its leading term, reproduces full QCD exactly if an infinite number of higher terms are included, allows the numerical calculation of lattice QCD quantities for any finite truncation of the expansion, and allows the estimation of the error induced by any such finite truncation.

The basic idea behind the scheme we suggest is to develop an effective action to approximate the log of the determinant of the fermion hopping matrix. The valence approximation replaces this term by a quantity proportional to the pure gauge action. Improved approximations can be generated by replacing the log of the determinant by a more complicated function of the links. A useful set of such functions is generated by sums of traces of products of links about closed paths.

2. DEFINITIONS

We will work with Wilson’s formulation of lattice QCD. If $M(\kappa)$ is Wilson’s hopping matrix for a single flavor fermion with hopping parameter $\kappa$, then our aim is to find an approximation for $\det M (= \sqrt{\det M^\dagger M})$. Numerical simulations of QCD work on finite lattices, with $\kappa$ not too big. For almost all configurations on such lattices $M^\dagger M$ is positive definite and has finite, strictly positive minimum $\lambda_{\text{min}}$ and maximum $\lambda_{\text{max}}$ eigenvalues. Also, it is simple to see (for example by considering a hopping parameter expansion) that $\det (M^\dagger M)$ can be expressed as a finite linear combination of sums of traces of products of links about closed paths. These two observations allow us to define $\log (\det (M^\dagger M))$ as an infinite series, convergent with respect to a suitably defined norm \cite{4}:

$$\log \det (M^\dagger M) = \text{Tr} \log M^\dagger M = \sum_{i=0}^{\infty} a_i S_i(U) \quad (1)$$

where the $S_i(U)$ are a maximal linearly independent set of functions which involve sums of traces of products of links about closed paths.

Crucial to obtaining a useful truncation of the expansion in Eq. (1) is the ordering assigned to the lattice, and our approximation scheme involves expanding the determinant of the hopping matrix as a linear combination of these functions.
the sequence of $S_i(U)$. We choose to partially order these functions by the length of the closed paths involved. For what follows we need explicit forms only for the constant (path length 0) term
\[ S_0(U) = 1 \] (2)
and the path length 4 term
\[ S_1(U) = \frac{1}{3} \sum_{\square} \text{Re} \text{Tr} U_{\square} \] (3)
involving a sum over all plaquettes of the real part of the trace of the product $U_{\square}$ of links about a plaquette.

3. APPROXIMATION SCHEME

The series expansion for $\text{Tr} \log M^\dagger M$ defined in \[\text{(1)}\] allows us to develop a series of approximations for full QCD expectation values of observables $F$. If we include two equal mass flavors of fermions, (the case most simply treated with exact algorithms), we have
\[
\langle F \rangle = Z^{-1} \int d\mu \ F \ \exp (\beta S_1 + \text{Tr} \log M^\dagger M)
\]
\[
= Z^{-1} \int d\mu \ F \ \exp (\beta S_1 + \sum a_i S_i) \tag{4}
\]
We approximate these expectation values by truncating the series for $\text{Tr} \log M^\dagger M$.

If $L_n = \sum_{i=0}^{n} a_i S_i$ is such a truncated series, and if $R_n = \text{Tr} \log M^\dagger M - L_n$ is the remainder after truncation, then we define our approximate expectation $\langle F \rangle_n$ after this truncation by
\[
\langle F \rangle_n = Z^{-1} \int d\mu \ F \ \exp (\beta S_1 + L_n) \tag{5}
\]
The systematic error induced by the truncation is $\langle F \rangle - \langle F \rangle_n$, and if the correlations of $F$ and $R_n$ are small, then an estimate of this error is
\[
\langle F \rangle - \langle F \rangle_n \approx \langle (F - \langle F \rangle_n) (R_n - \langle R_n \rangle_n) \rangle_n \tag{6}
\]

Still to be determined at this stage are values for the coefficients $a_i$. The norm implicit in Eq. \[\text{(1)}\] yields
\[
\lim_{n \to \infty} \left\langle \left( \text{Tr} \log M^\dagger M - \sum_{i=0}^{n} a_i S_i \right)^2 \right\rangle = 0. \tag{7}
\]
We can find approximate values for the coefficients at any given truncation by minimizing
\[
\langle R_n^2 \rangle_n = \langle (\text{Tr} \log M^\dagger M - L_n)^2 \rangle_n \tag{8}
\]
as a function of $a_0 \ldots a_n$. In the limit $n \to \infty$ the coefficients $a_i$ will approach their exact values determined by \[\text{(1)}\] or equivalently \[\text{(2)}.\]

4. CALCULATING $\text{Tr} \log M^\dagger M$

In order to evaluate the coefficients $a_i$ (by minimizing \[\text{(8)}\]), or to estimate the systematic error by equation \[\text{(8)}\], we must be able to evaluate the expectation value of $\text{Tr} \log M^\dagger M$ over a set of link configurations. We use two different ideas to evaluate these expectations. Firstly, we estimate $\text{Tr} \log M^\dagger M$ as
\[
\text{Tr} \log M^\dagger M = \frac{1}{N_\phi} \sum_{a=1}^{N_\phi} \phi_a^\dagger \log M^\dagger M \cdot \phi_a \tag{9}
\]
were $\phi_a$ are $N_\phi$ pseudofermion vectors each with independent random Gaussian components. Secondly, to calculate $\log M^\dagger M \cdot \phi$ we use a Chebyshev polynomial iterative scheme
\[
\log M^\dagger M = \sum_{i=0}^{N} b_i T_i^* \left( \frac{1 - M^\dagger M / \lambda_{\max}}{1 - \lambda_{\min} / \lambda_{\max}} \right) + \delta \log M^\dagger M \tag{10}
\]
where the $T_i^*$ are Chebyshev polynomials, the $b_i$ are constants which can be calculated using standard methods for orthogonal polynomials \[\text{(8)}.\], and $\delta$ is bounded by
\[
\delta < 2 \exp \left( -2N \sqrt{\lambda_{\min} / \lambda_{\max}} \right) \tag{11}
\]
Convergence of this series is determined by $\delta$, and since $\log M^\dagger M \cdot \phi$ must be calculated a number of times in order to evaluate the trace we have found that the most efficient implementation of these ideas is first to calculate $\lambda_{\min}$ and $\lambda_{\max}$ for each configuration being analyzed using a Lanczos algorithm \[\text{(8)}.\], then to evaluate $\phi^\dagger \log M^\dagger M \cdot \phi$ with a Chebyshev polynomial approximation whose order $N$ is defined to keep $N \sqrt{\lambda_{\min} / \lambda_{\max}}$ on each configuration constant. We have also found that it helps to precondition
the log $M^\dagger M$ calculation by premultiplying $M$ by the inverse of a free hopping matrix $M_0(\kappa_0)$ which has hopping parameter $\kappa_0$, and has all links set to the identity. This preconditioner has no effect on the physics since, if $N = M_0^{-1}(\kappa_0)M$, we have $\text{Det} M_0^\dagger N = \text{const} \times \text{Det} M^\dagger M$. However, simple tuning of $\kappa_0$ reduced the work to calculate the determinant in our example calculation by almost a factor of two. Details of our exact implementation of these ideas can be found in [1].

5. EXAMPLE APPLICATION

As a first demonstration of these ideas, we have studied a $6^4$ QCD simulation at $\beta = 5.7$ with two equal mass Wilson fermions of hopping parameter $\kappa = 0.16$. We considered only the first two terms in our expansion

$$\text{Tr} \log N^\dagger N \to L_1 = a_0 + a_1 S_1(U).$$

(12)

Observable expectations in this approximation have the form

$$\langle F \rangle_1 = Z^{-1} \int d\mu \ F \ \exp ((\beta + a_1)S_1(U) + a_0).$$

(13)

This expectation value is a valence approximation calculation but we now obtain an explicit number for the shift in $\beta$ compensating for omission of the fermion determinant. The coupling at which we simulate becomes $\beta_{\text{sim}} = \beta + \delta \beta$, where $\delta \beta = a_1$ is the effective shift in the coupling due to the fermion determinant. To calculate $\delta \beta$ we generated 160 independent configurations using the Cabbibo-Marinari-Okawa algorithm with $\beta_{\text{sim}} = 5.7$. On these configurations, we calculated $\text{Tr} \log N^\dagger N$ using 140 independent $\phi$'s per configuration.

The major result of all our analysis is a prediction for the constant $\delta \beta$ which is generated by minimizing $\langle \delta \beta \rangle$. We found $\delta \beta = -0.261 \pm 0.014$. We interpret this result to mean that a valence calculation at $\beta = 5.7$ is approximately equivalent to a full QCD calculation at $\beta = 5.439$ (5.700–0.261) for two equal mass flavors of Wilson fermions with hopping parameter $\kappa = 0.16$. The agreement is approximate because we have truncated the expansion of $\text{Tr} \log N^\dagger N$ at two terms.

To confirm the approximate equivalence, we have also calculated the expectation values of the plaquette operator $P = 1 - \frac{1}{4} \text{Re} \text{Tr} U^\dagger$ in a variety of different ways. A pure gauge calculation at $\beta = 5.439$ gives $\langle P \rangle_0 = 0.5190 \pm 0.0004$. A full QCD hybrid Monte Carlo calculation at $\beta = 5.439$ with two flavors of Wilson fermions gives $\langle P \rangle = 0.4451 \pm 0.0004$. Our approximation using the $\beta = 5.7$ valence calculation gives $\langle P \rangle_1 = 0.4499 \pm 0.0004$ with a systematic error of $0.0000 \pm 0.0025$. The fact that our estimate of the systematic error has a central value of 0.0 is simply a consequence of our algorithm for finding $\delta \beta$ since we have chosen $\delta \beta$ explicitly to make this central value equal to 0.0. Other observables will have non-zero systematic shifts which can be calculated in exactly the same manner.

6. COMMENT

The major question which we have not answered yet is whether our scheme is more efficient computationally than simulating with an exact full QCD algorithm. In our simple test the extra work required to evaluate $\text{Tr} \log M^\dagger M$ turned out to be about equivalent to the time required to generate a single decorrelated configuration with the Cabbibo-Marinari algorithm. How this might change as the size of the lattice increases, and as the gauge coupling and quark hopping parameters become more physical is still to be determined.

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