Systematic errors of Lüscher’s fermion method and its extensions

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Abstract

We study the systematic errors of Lüscher’s formulation of dynamical Wilson quarks and some of its variants, in the weak and strong coupling limits, and on a sample of small configurations at finite $\beta$. We confirm the existence of an optimal window in the cutoff parameter $\varepsilon$, and the exponential decrease of the error with the number of boson families. A non-hermitian variant improves the approximation further and allows for an odd number of flavors. A simple and economical Metropolis test is proposed, which makes the algorithm exact.

1 Introduction

Hybrid Monte Carlo (HMC) is now the standard method to simulate fermionic field theories [1]. It is exact, relatively simple to implement, and its cost grows just a little faster than the volume $V$ of the system [2]. This should not stop us from searching for better algorithms.

Fermionic interactions give rise, after integration of the fermionic fields, to a non-local determinant. HMC addresses the problem of the non-locality of this determinant by linearizing the action in a succession of molecular dynamics steps. The calculation of the force at each step is obtained via the iterative solution of a sparse linear system. But this linearization implies infinitesimal steps, which in turn make narrow, very high energy barriers nearly impassable. Thus very long autocorrelation times have been observed, eg. for the topological charge [3], and ergodicity may be questionable when the vanishing of the fermion determinant divides phase space into disconnected regions [4]. A finite step-size algorithm is highly desirable.

All such algorithms have been abandoned, because of their high cost proportional to $V^2$ [5]. Recently however, Lüscher proposed a finite-step bosonic formulation where one can control, through the number of auxiliary bosonic fields, the trade-off between accuracy and computer cost [6]. Surprisingly, no systematic investigation of this trade-off has appeared in the literature, except in full-blown studies of the complete QCD theory [7, 8]. It is our purpose to fill this gap here, by studying the weak and strong coupling limits, and the interacting theory on a sample of HMC configurations. In Section 2, we recall Lüscher’s formulation of the QCD determinant, and explain our methodology. In Section 3, we present our results for the systematic error of the method. In Section 4, we investigate the effect of the usual ‘even-odd splitting’ of the Dirac operator. In Section 5, we propose a non-hermitian variant, with improved convergence, suited also for an odd number of quark flavors. Section 6 describes a simple Metropolis test which makes the algorithm exact. Conclusions follow.
2 Lüscher’s method

In cases where the fermionic determinant can be written as a square \( \det Q^2 \), Lüscher has proposed a general method to approximate it by a local bosonic action. The essential steps are:

- find a real polynomial \( P(x) \) of even degree \( n \), approaching \( 1/x \) as \( n \to \infty \) over the spectrum of \( Q^2 \), which must be real.
- decompose \( P(x) \) into a product of monomials

\[
P(x) \equiv c_n x^n + \ldots + c_1 x + c_0 = c_n \prod_{k=1}^{n} (x - z_k)
\]

such that

\[
\det P(Q^2) = c_n^N \prod_{k=1}^{n} \det (Q - \sqrt{z_k}) \det (Q - \sqrt{z_k})
\]

where \( N \) is the rank of \( Q^2 \).
- express each factor above as a Gaussian integral over bosonic fields, so that finally

\[
\det Q^2 \approx \frac{1}{\det P(Q^2)} = \frac{1}{c_n^N (2\pi)^n} \int \prod_{k=1}^{n} [d\phi_k^+] [d\phi_k] e^{-\phi_k^+(Q - \sqrt{z_k})^1(Q - \sqrt{z_k}) \phi_k}
\]

Thus one trades the initial non-local determinant for a bosonic action which is a sum of \( n \) local terms. This bosonic action can be viewed as a discrete path integral; it converges to the exact determinant as the discretization step \( \sim 1/n \) tends to zero. Note that the normalization factor \( c_n \) of the polynomial drops out of any expectation value.

Here we study this approach when applied to dynamical Wilson fermions. Let us denote the Dirac matrix by

\[
D = (1 - \kappa M)
\]

where \( M \) is the lattice Wilson hopping operator and \( \kappa \) the hopping parameter. Lüscher chooses for \( Q \) the hermitian operator

\[
Q = c_0 \tilde{Q} ; \quad \tilde{Q} = \gamma_5 D
\]

where \( c_0 = (1 + 8\kappa)^{-1} \) is introduced to guarantee that the norm of \( Q \) is bounded by one, and his method to approximate \( \det Q^2 \) applies to 2 degenerate quark flavors.

The particular polynomial adopted by Lüscher is built from Chebyshev polynomials \( T_n(x) \), with the definitions

\[
T_0(x) = 1
\]
\[
T_1(x) = x = \cos \theta
\]
\[
T_n(x) = \cos(n \theta)
\]

The approximation polynomial is then defined by

\[
P(x) = \frac{1 - R(x)}{x} = c_n \prod_{k=1}^{n} (x - z_k)
\]

where \( R(x) \) is the scaled and translated Chebyshev polynomial such that \( R(0) = 1 \),

\[
R(x) = \frac{T_{n+1}(\frac{2x}{1+\varepsilon} - \frac{1+\varepsilon}{1+\varepsilon})}{T_{n+1}(\frac{1+\varepsilon}{1-\varepsilon})}
\]

with \( \varepsilon \) an adjustable parameter \( \in (0, 1) \). By straightforward algebra, one verifies that the zeroes of \( P(x), z_k, k = 1, \ldots, n \) are given by
\[ z_k = \frac{1 + \varepsilon}{2} (1 - \cos \frac{2\pi k}{n+1}) - i\sqrt{\varepsilon} \sin \frac{2\pi k}{n+1} \] (11)

A very important advantage of using Chebyshev polynomials is that the error of the approximation can be bounded, and the bound converges exponentially with \( n \):

\[ |R(x)| = |1 - xP(x)| \leq 2 \left( \frac{1 - \sqrt{\varepsilon}}{1 + \sqrt{\varepsilon}} \right)^{n+1}, \forall x \in [\varepsilon, 1] \] (12)

The proof is given in section 5.

Our methodology to assess the error of this method and to compare it with other variants, is the following: we compute the quantity

\[ y \equiv \det Q^2P(Q^2) \] (13)

by calculating the eigenvalues of \( Q^2, \lambda_i, i = 1, \ldots, N \), so that

\[ y = \prod_{i=1}^{N} \lambda_i P(\lambda_i) \] (14)

To properly cover the full range of gauge couplings, we study the variations of \( y \) in 3 different cases.

i) For free fermions the spectrum of \( Q \) is known analytically; we estimate the error by monitoring \(|y^{1/N} - 1|\).

ii) In the strong coupling limit we generate a sample of quenched 4\(^4\) configurations, and measure the fluctuation of \( y \) by monitoring

\[ \Delta \equiv \frac{1}{\langle y \rangle} \sqrt{\langle y^2 \rangle - \langle y \rangle^2} \] (15)

The reason for the normalization factor \( 1/\langle y \rangle \) is to remove the dependence of the error on the arbitrary constant \( c_n \) (eq.(9)).

iii) At intermediate coupling, we perform the same analysis for a set of matrices \( Q^2 \) generated by hybrid Monte Carlo at \( \beta = 6 \) and \( \kappa = 0.14 \) on a 4\(^4\) lattice.

3 Systematic errors of Lüscher’s method

In the case of free fermions, our definition \(|y^{1/N} - 1|\) of the error depends on the normalization coefficient \( c_n \). A simple way to compute \( c_n \) relies on the observation that \( R(\frac{1+\varepsilon}{2}) = 0 \), so that

\[ c_n^{-1} = \frac{1 + \varepsilon}{2} \prod_{i=1}^{n} \left( \frac{1 + \varepsilon}{2} - z_k \right) \] (16)

We then show in Fig.1a the error as a function of the parameter \( \varepsilon \), for 20, 54, 90 and 148 boson fields (\( \kappa = 0.11 \), on an 8\(^4\) lattice). As expected, there is an optimal value for \( \varepsilon \): if \( \varepsilon \) is too large, the polynomial approximation degrades over the lower part of the spectrum of \( Q^2 \); if \( \varepsilon \) is too small, the approximation becomes poor over the whole spectrum, because \((1 - \sqrt{\varepsilon})/(1 + \sqrt{\varepsilon})\) approaches 1 (see eq.(12)). Not surprisingly, the optimal value of \( \varepsilon \) is slightly larger than the smallest eigenvalue of \( Q^2 \), and approaches it as the number of bosonic fields increases.

At finite \( \beta \), fluctuations of \( \lambda_{\text{min}}(Q^2) \) complicate the matter: configurations with small \( \lambda_{\text{min}}(Q^2) \) contribute larger errors, so that \( \varepsilon \) must be tuned slightly below \(<\lambda_{\text{min}}(Q^2)>\) in order to minimize
the average error, when this error is small. This behaviour is shown in the (quenched) strong coupling in Fig.1b for \( \kappa = 0.2 \). It remains unchanged at intermediate couplings \( \beta = 6 \) in Fig.1c, where we also illustrate a typical spectrum of the matrix \( D \) in Fig.2a.

From these figures, it appears that the optimal ratio \( \varepsilon / \lambda_{\text{min}}(Q^2) \) is relatively insensitive to \( \beta \). This should simplify the task of tuning \( \varepsilon \).

Rescaling the matrix

As mentioned in [7], rescaling the matrix \( Q \) (see eq. (5)) to \( Q/c_M \) can be useful. This is equivalent to rescaling the roots of the polynomial \( z_k \rightarrow c_M^2 z_k \). In [8] one assumes \( c_M \geq 1 \) to guarantee that the spectrum is bounded by one. Nonetheless, one may let \( c_M \) be less than one, if one monitors the largest eigenvalue of \( Q^2 \). Under rescaling, this largest eigenvalue approaches 1, making use of the full interval \( [\varepsilon, 1] \) of validity of the approximation (3). Simultaneously the smallest eigenvalue of \( Q^2 \) increases, with corresponding gains in convergence. One readily sees from equation (12) that the number \( n \) of boson fields can be multiplied by \( \approx c_M \).

The benefits of tuning \( c_M \) vanish in the weak coupling limit, since the largest eigenvalue of \( Q^2 \) then tends to 1. Even in the strong coupling, the advantage remains small, \( O(10 - 20)\% \). But the normalization of \( Q \) must be considered carefully when one uses even-odd splitting of the lattice sites.

4 Even-odd splitting

Lüscher’s method is based on a polynomial approximation of the inverse, just like iterative methods to find the quark propagator, with the difference that the polynomial is predetermined in Lüscher’s case, whereas it is built recursively and adaptively by an iterative linear solver. The similarity of the two approaches should encourage us to try here what works well there. In this section we test the simplest such idea, that of partitioning the lattice sites into ‘even’ and ‘odd’, and of factorizing \( detQ^2 \) into equal, even and odd factors.

To justify such a factorization, we simplify the derivation used in [1] for staggered fermions. Define a diagonal operator \( \Sigma \) with entries 1 on even sites and \(-1\) on odd sites. This operator anticommutes with the hopping matrix \( M \), since \( M \) connects even and odd sites. Noting that \( \Sigma^2 = 1 \), one gets

\[
\text{det} D = \text{det}(1 - \kappa M) = \text{det}\Sigma(1 + \kappa M)\Sigma = \text{det}(1 + \kappa M) \tag{17}
\]

Now \( D^\dagger = \gamma_5 D \gamma_5 \), and \( \gamma_5 = 1 \), so that

\[
\text{ det} Q^2 = (\text{det} D)^2 = \text{det}(1 - \kappa^2 M^2) \tag{18}
\]

Furthermore we observe that \( M^2 \) commutes with \( \Sigma \); then if \( \vec{x} \) is an eigenvector of \( M^2 \), so is \( \Sigma\vec{x} \), or \( (1 \pm \Sigma)\vec{x} \), which is non-zero on even or odd sites respectively. Therefore all eigenvalues are two-fold degenerate, and one has

\[
\text{det}(1 - \kappa^2 M^2)_{\text{even}} = \text{det}(1 - \kappa^2 M^2)_{\text{odd}} \tag{19}
\]

So we can finally write

\[
\text{det} Q^2 = \text{det}(1 - \kappa^2 M^2)_{\text{even}}^2 \tag{20}
\]

This way we can work with bosonic fields defined on even sites only, saving a factor 2 in memory. The bosonic action however is now less local, so that a bosonic update requires about as many operations as before. Nonetheless, further gain may come through a reduction in the number of bosonic families required for a given accuracy.
The reason for this potential gain becomes clear when one looks at the spectrum of a typical configuration: the spectrum of Fig. 2a shrinks to that of Fig. 2b after even-odd preconditioning. One can now readjust \( \varepsilon \) and vary the number \( n \) of bosonic families, with and without even-odd splitting. In both cases, the error decreases exponentially with \( n \), as predicted by eq. (12); but it does so much faster in the even-odd splitting formulation, as illustrated in Figs. 3a and 3b for \( \beta = 0 \) and \( \beta = 6 \) respectively. In both figures the gain is a factor 2 to 3 in \( n \).

This large gain can be understood by considering the spectral radius of \( \kappa M \), say \( \rho \equiv 1 - \gamma \); the smallest eigenvalue of entering the determinant eq. (17) is \( \gamma \ll 1 \), but that in eq. (20) is \( \sim 2 \gamma \). Thus the optimal value of \( \sqrt{\varepsilon} \) should also increase by a factor 2, which according to eq. (12) allows a reduction of \( n \) by the same factor. In addition, one can achieve important gains by tuning the rescaling constant \( c_M \) to bring the largest eigenvalue of \( Q^2 \) close to 1, as explained in the previous section. The normalization constant which guarantees that the norm of \( \gamma_5 (1 - \kappa^2 M^2)_{\text{even}} \) is bounded by one is now \( c_0 = (1 + 64 \kappa^2)^{-1} \). But with this normalization, the largest eigenvalue of \( Q^2 \) becomes rather small away from \( \beta = \infty \). Thus in Figs. 3a and 3b both, we tuned \( c_M \) to 0.6 instead of its default value of 1.

5 Non-hermitian variant

5.1 Formulation

Another lesson can be learned from iterative solvers [10]: the method of biconjugate gradients (BiCG) [11] requires less work than that of conjugate gradients (CG) [12]. BiCG applies Lanczos polynomials on the matrices \( D \) and \( D^\dagger \) to construct the solution, whereas CG applies the Lanczos polynomial on the matrix \( Q^2 \). This observation motivated us to look for an approximation to \( 1/D \) itself, instead of \( 1/Q^2 \). This should be possible as long as \( \det D \) is positive. But a negative determinant can only be caused by negative real eigenvalues; this situation can only occur for very small quark masses as studied in the quenched case by [13], beyond those reachable by present-day simulations of full QCD. The benefits of the approach proposed below are two-fold: convergence of the approximation is improved; and the simulation of an odd number of quark flavors (or of any number of non-degenerate flavors) becomes possible.

Let \( P(z) \) be a polynomial of even degree \( n \), with real coefficients, defined in the complex plane (since the spectrum of \( D \) is complex), with complex conjugate roots \( z_k, \text{Im} z_k \neq 0, k = 1, ..., n \). Assume that this polynomial satisfies \( P(z) \to 1/z \) for \( n \to \infty, \forall z \in S \), where \( S \) is a domain in the complex plane containing the spectrum of \( D \). Then one can write

\[
det P(D) = c_n^n \prod_{k=1}^{n/2} \det(D - \bar{z}_k) \det(D - z_k)
\]

Using the fact that \( D = \gamma_5 D^\dagger \gamma_5 \) and \( \gamma_5^2 = 1 \) one gets

\[
det(D - \bar{z}_k) = det(D^\dagger - \bar{z}_k)
\]

It follows that

\[
det P(D) = c_n \prod_{k=1}^{n/2} \det(D - z_k)^\dagger \det(D - z_k)
\]

and, in analogy with eq. (3)

\[
det D \approx \frac{1}{det P(D)} = \frac{1}{c_n^n \cdot (2\pi i)^{n/2}} \int \prod_{k=1}^{n/2} [d\phi_k][d\phi_k^\dagger] e^{-\phi_k^\dagger (D - z_k) \phi_k} e^{-\phi_k^\dagger (D - z_k) \phi_k^\dagger}
\]

The approximation polynomial can be defined as before by
\[ P(z) = \frac{1 - R(z)}{z} = c_n \prod_{k=1}^{n} (z - z_k) \]  

(25)

where \( R(z) \) is a polynomial of degree \( n + 1 \) such that \( R(0) = 1 \). \(|R(z)| \) should be small in the domain \( S \) of the approximation. The spectrum of \( D \) has a more or less elliptical shape, as can be seen from Fig.2a. It is then natural to choose for the boundary \( \partial S \) an ellipse. In that case (provided the origin is not inside the ellipse), it turns out that the polynomial which minimizes \( \max_S |R(z)| \) is again a Chebyshev polynomial \([14]\).

The same definitions eqs.(6-8) remain valid for \( T_n(w) \), where now \( w = x + iy \) and \( \theta = \theta_1 + i \theta_2 \), that is

\[ w = \cos \theta = \cos \theta_1 \cosh \theta_2 - i \sin \theta_1 \sinh \theta_2 \]  

(26)

where \( \theta_1 \in [-\pi, \pi] \) and, for instance, \( \theta_2 \in [0, +\infty[ \). Note that, for \( \theta_2 \) fixed, \( w(\theta_1) \) describes an ellipse in the complex plane, with foci \( \pm 1 \) and semi-axes \( \cosh \theta_2 \) and \( \sinh \theta_2 \).

From these definitions we can now specify the form of \( R(z) \). Choose for \( \partial S \) the ellipse centered at \((d, 0)\), with large semi-axis \( a < d \), and focal distance \( c \leq a \). Then the scaled and translated Chebyshev polynomial \( R(z) \) is defined by

\[ R(z) = \frac{T_n+1(z-d)}{T_n+1(-\frac{d}{c})} \]  

(27)

From this definition one can show, in analogy with the hermitian case, that the roots of \( P(z) \), \( z_k, k = 1, \ldots, n \) are

\[ z_k = d(1 - \cos \frac{2\pi k}{n+1}) - i \sqrt{d^2 - c^2} \sin \frac{2\pi k}{n+1} \]  

(28)

so that the \( z_k \)'s lie on the ellipse of same center and foci as \( \partial S \), which goes through the origin.

We can now derive an error bound for the above polynomial approximation in the complex plane. It states that

\[ |R(z)| = |1 - zP(z)| \leq 2 \left( \frac{a + \sqrt{a^2 - c^2}}{d + \sqrt{d^2 - c^2}} \right)^{n+1}, \forall z \in S \]  

(29)

Proof. By definition

\[ R(z) = \frac{\cos(n+1)\theta}{\cos(n+1)\theta_0} \]  

(30)

where

\[ \cos \theta = \frac{z - d}{c}, \quad \cos \theta_0 = -\frac{d}{c} \]  

(31)

From eq.(26), one sees that \( \theta_0 = \pi + i\alpha \), where \( \alpha \equiv \cosh^{-1}d/c \). Writing \( \theta = \theta_1 + i \theta_2 \), one gets

\[ R(z) = \frac{-1}{\cosh(n+1)\alpha}(\cos(n+1)\theta_1 \cosh(n+1)\theta_2 - i \sin(n+1)\theta_1 \sinh(n+1)\theta_2) \]  

(32)

so that

\[ |R(z)| \leq \frac{\cosh(n+1)\theta_2}{\cosh(n+1)\alpha} \]  

(33)

The coordinates of any point \( z \) in \( S \) can be expressed as \((\theta_1, \theta_2)\). Successive \( \theta_2 \)'s define nested ellipses, all of center \( d \) and focal distance \( c \): the innermost one, for \( \theta_2 = 0 \), is the real segment \([d - c, d + c]\); the outermost one, for \( \theta_2 = \theta_{\text{max}} \equiv \cosh^{-1}a/c \), is \( \partial S \). Along each such ellipse \(|R(z)|\)
is bounded by \( \frac{\cosh(n+1)\theta_{\max}}{\cosh(n+1)\alpha} \), and reaches this bound when \( z \) is real. The bound increases with \( \theta_2 \), so that over \( S \), \( |R(z)| \) is bounded by

\[
\frac{\cosh(n+1)\theta_{\max}}{\cosh(n+1)\alpha} = e^{(n+1)(\theta_{\max} - \alpha)} \frac{1 + e^{-2(n+1)\theta_{\max}}}{1 + e^{-2(n+1)\alpha}}
\]

(34)

The second factor is bounded by 2. Substituting \( \theta_{\max} \) and \( \alpha \) by their definitions in terms of \( a, c, d \), one recovers eq.(29).

This derivation makes it clear that the error \( |R(z)| \) is maximum on the real points of \( \partial S \), but decreases exponentially inside \( S \). This is in sharp contrast with the hermitian approximation of Lüscher.

5.2 Optimization and comparison with the hermitian case

Two limiting cases for \( \partial S \) are of special interest: the circle \((c = 0)\), which corresponds to the spectrum of \( D \) in the (quenched) strong coupling; and the real line segment \([d - a, d + a] \) \((c = a)\), which corresponds to the spectrum of \( Q^2 \) originally considered by Lüscher. For these 2 cases the error bound eq.(29) becomes \( 2(\frac{a}{d + \sqrt{d^2 - a^2}})^{n+1} \) and \( 2(\frac{a}{d + \sqrt{d^2 - a^2}})^{n+1} \) respectively. To make contact with the hermitian error bound eq.(13), we just express \( a = \frac{1 - \varepsilon}{2} \) and \( d = \frac{1 + \varepsilon}{2} \). We recover then eq.(13) over the real segment \([\varepsilon, 1]\); over the circle we get:

\[
|R(z)| \leq 2 \left( \frac{1 - \varepsilon}{1 + \varepsilon} \right)^{n+1}
\]

(35)

We are now in a position to compare the hermitian and non-hermitian approximations, in the strong coupling limit. Call \( \eta \sim m_{\text{quark}} \) the smallest eigenvalue of \( D \). Then the smallest eigenvalue of \( Q^2 \) will be \( \eta^2 \), and the hermitian and non-hermitian bounds eqs.(12) and (35) are identical\(^1\). It is true that only \( n/2 \) bosonic fields are necessary to generate \( \det(D) \) in the non-hermitian case; but for \( 2 \) degenerate quark flavors, one needs another \( n/2 \) fields to finally approximate \( \det(D)^2 \), for the same total of \( n \) fields as in the hermitian case.

When \( \beta \) increases, the error bound for the non-hermitian case improves. The spectrum of \( D \) can then be contained in a more elongated ellipse whose aspect ratio tends to \( 2 \) in the free field limit. It is straightforward to verify from eq.(29) that the convergence rate is multiplied by 2, allowing a reduction of \( n \) by the same factor.

As importantly, the error in the non-hermitian approximation decreases exponentially inside \( S \). To exhibit this difference with the hermitian approximation, we show in Fig.4 the magnitude of the error along the real axis, for \( \eta = 0.1 \) and \( n = 20 \). That is, the range of the approximation in the hermitian case is \([0.01, 1]\), whereas in the non-hermitian case it is \([0.1, 1]\). In the hermitian case, the error oscillates with constant amplitude \( \mathcal{O}(10^{-2}) \) over the interval \([\eta^2, 1]\). In the non-hermitian case, when \( \partial S \) is a circle the error at \( x = \eta \) and \( x = 1 \) is also \( \mathcal{O}(10^{-2}) \); when \( \partial S \) is an ellipse of aspect ratio 2, the error at \( x = \eta \) and \( x = 1 \) is about squared. Either way, the error falls off exponentially inside the approximation range, until it becomes uniformly oscillating in the segment \([d - c, d + c]\). So the accuracy on interior eigenvalues of \( D \) is much improved.

We make numerical tests of this non-hermitian approximation for HMC and strong coupling configurations. We apply the same methodology as before, but in the non-hermitian case we measure the fluctuations of the quantity

\[
y = \prod_{i=1}^{N} (\lambda_i P(\lambda_i))^2
\]

(36)

\(^1\) We greatly simplify here a subtle issue: if the smallest singular value of \( D \) is \( \eta \), then the smallest eigenvalue of \( Q^2 \) is \( \eta^2 \), but the relationship between eigenvalues of \( D \) and of \( Q^2 \) could be quite different, especially in the chirally broken phase. In particular one easily proves that \( \sigma_{\min}(D) \leq |\lambda|_{\min}(D) \), so the comparison we make here is a worst case scenario: the non-hermitian variant will always be at least as accurate as the hermitian one.
where now \( \lambda_i, i = 1, \ldots, N \) are eigenvalues of the quark matrix \( D \). With this definition of \( y \) we can compare the results directly to the hermitian case. In Figs.5 we show that the errors of the non-hermitian approximation are reduced faster than in the hermitian approximation. From Fig.5a we can see that in the quenched strong coupling, the gain is a factor 4 to 5, increasing as the quark mass is reduced. This large gain is caused by the high density of interior eigenvalues. In Fig.5b at \( \beta = 6 \), the gain is a factor \( \sim 1.5 \), coming mostly from the elliptical shape of \( \partial S \). Note that simulating one flavor to the same accuracy would require half as many fields.

6 Metropolis test

Lüscher’s original proposal includes the monitoring of the error, and the possibility of obtaining exact results by re-weighting the Monte Carlo measurements of each observable. The natural way to calculate the error eq.\((13)\) is to express it in an eigenbasis of \( Q^2 \), obtained by the Lanczos algorithm. However two obstacles appear: the Lanczos algorithm is affected by roundoff errors, which can be controlled only if eigenvalue multiplicities are known \( [15] \) and its cost grows like the square of the volume \( V \) of the lattice, so that it becomes overwhelmingly expensive on large lattices. Nevertheless attempts at using the Lanczos method in a Metropolis test show that most if not all of the error can be removed \( [13] [3] \).

In fact, it is sufficient to construct an unbiased estimator of the ratio of errors between the new and the old configurations. One can then use the noisy Monte Carlo method of \( [17] \), which was successfully applied to fermionic simulations before the advent of Hybrid Monte Carlo \( [4] [8] \).

The ratio to estimate is \( \frac{\text{det}(D'P(D'))^2}{\text{det}(DP(D))^2} \), calling \( D' \) and \( D \) the Dirac operators for the new and old configurations respectively. Taking the denominator as a partition function, this ratio can be rewritten

\[
< e^{-\eta^T(W^TW-1)\eta} > \tag{37}
\]

where the average \( <> \) is taken over all Gaussian vectors \( \eta \), and \( W = [D'P(D')]^{-1}DP(D) \). It is sufficient to estimate this ratio by taking one Gaussian \( \eta \) only. This requires the solution of a linear system, which will take just a few iterations since the matrix \( D'P(D') \) is almost the identity. The cost of this additional step is therefore similar to that of an update of the \( \phi_k \)'s. As the volume \( V \) of the lattice grows, one should keep constant the acceptance of this Metropolis test. This is achieved if the error per eigenvalue scales like \( V^{-1} \). Because the approximation is exponential in \( n \), this can be accomplished by a modest increase \( \propto \log V \) in \( n \), and a CPU cost scaling like \( V(\log V)^2 \). Under this rescaling of \( V \), the number of iterations necessary to solve the linear system above remains constant, so that the overhead of the Metropolis test, measured in update sweeps, does not change. Similarly, when the quark mass is decreased but the acceptance is kept constant, the overhead of the Metropolis step, measured in update sweeps, will not change.

7 Conclusion

We have studied the systematic errors of Lüscher’s method to simulate dynamical quarks, in the full range of strong to weak coupling. Two parameters define the approximation, \( \varepsilon \) and \( n \): \( \varepsilon \) is the lower cutoff of the polynomial approximation, \( n \) is the number of auxiliary bosonic families. We confirm the importance of tuning \( \varepsilon \) near the minimum eigenvalue of \( Q^2 \); the optimal ratio \( \varepsilon / < \lambda_{\text{min}}(Q^2) > \) approaches 1 from above as \( n \) increases, in a manner almost independent of \( \beta \); it actually becomes slightly less than 1 for large \( n \), because configurations with small \( \lambda_{\text{min}}(Q^2) \) give larger errors. For \( \varepsilon \) fixed, we confirm the exponential convergence of the approximation with \( n \).

In addition, we have studied the improvement of even-odd preconditioning: it allows a reduction of \( n \) by a factor 2 to 3. A full reduction however can only be achieved by tuning to less than 1 the normalization parameter \( c_M \) of the matrix \( Q \).

We have introduced a non-hermitian variant, which allows the simulation of an odd number of quark flavors. The number of bosonic families is proportional to that of flavors. For 2 flavors,
the non-hermitian formulation allows a reduction of $n$ by a factor 1.5 to 5. Full Monte Carlo tests of this variant are in progress. They will shed some light on the critical dynamics of the bosonic fields $\phi_k$, which depend on the singular values of $(D - z_k)$, and might be different from the original hermitian version.

Even-odd preconditioning and non-hermitian formulation are most advantageous for large quark masses and small $\beta$ respectively. These two improvements can be combined when appropriate.

Finally we have proposed a Metropolis test which removes any approximation. The overhead of this Metropolis test is modest and independent of the lattice volume and the quark mass.

The error we have considered is that on the fermionic determinant itself. The error measured on a given observable during a Monte Carlo simulation of the Lüscher action will depend on the overlap of that observable with the various eigenmodes of the determinant, and may be smaller than we measured here.

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Figures:

- Figure 1: the magnitude of the error on the determinant as a function of $\varepsilon$, for $n = 20, 54, 90, 148$, in the case of free field (Fig.1a), (quenched) strong coupling (Fig.1b), and at $\beta = 6$ (Fig.1c). $\kappa = 0.11, 0.2, 0.14$ respectively. Arrows mark the minimum and the average of $\lambda_{\min}(Q^2)$ over the ensemble of configurations.

- Figure 2: a typical spectrum of the Dirac matrix $D$, eq.(4), in the complex plane ($4^4$ lattice, $\beta = 6, \kappa = 0.14$). In Fig.2b the spectrum is shown after even-odd preconditioning.

- Figure 3: the magnitude of the error on the determinant as a function of $n$, in the original formulation (dotted line) and after even-odd preconditioning (solid line). Fig.3a corresponds to $\beta = 0, \kappa = 0.2$, Fig.3b to $\beta = 6, \kappa = 0.14$.

- Figure 4: the magnitude of the error of the polynomial approximation $P(x)$ as $x$ varies from 0 to 1. The three approximations shown are the original hermitian approximation of Lüscher, the non-hermitian approximation inside a circle as appropriate for $\beta = 0$, and the non-hermitian approximation inside an ellipse of aspect ratio 2, as appropriate for $\beta = \infty$. All cases correspond to the same quark mass.

- Figure 5: the magnitude of the error on the determinant as a function of $n$, in the original formulation (dotted line) and in the non-hermitian variant (solid line). Fig.5a corresponds to $\beta = 0$, Fig.5b to $\beta = 6$. 
