Modelling the Quark Determinant in Full QCD Simulations

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The computational requirements and dynamics of Monte Carlo simulations of unquenched QCD incorporating the infrared quark eigenmodes (up to $\approx \Lambda_{QCD}$) exactly and UV modes via a loop representation are discussed. The accuracy of such a loop representation is studied for a variety of lattice volumes and quark masses. The method has been successfully applied for lattices up to 10^3x20 at a $\simeq$0.17F with improved (clover) action, and allows simulations at or near kappa critical.

1. Splitting the Quark Determinant

The essence of the truncated determinant approach [1] to unquenched QCD lies in the realization that the infrared part of the quark determinant (specifically, the determinant $\mathcal{D}(\mathcal{A})$ of the hermitian operator $H \equiv \gamma_5(D\!\!\!/(A) - m))$ can be gauge-invariantly split off, leaving an ultraviolet part which is accurately fit by a linear combination of a small number of Wilson loops. The eigenvalues λ_i of H
(1) measure quark off-shellness (for $A = 0$, $\lambda_i \rightarrow \pm\sqrt{p^2 + m^2}$),
(2) are gauge-invariant, $\lambda_i(A) = \lambda_i(A^g)$.

Thus we can write $\mathcal{D}(\mathcal{A}) = \mathcal{D}_{\mathcal{IR}}(\mathcal{A})\mathcal{D}_{\mathcal{UV}}(\mathcal{A})$, where the infrared part $\mathcal{D}_{\mathcal{IR}}(\mathcal{A})$ is defined as the product of the lowest N_λ positive and negative eigenvalues of H, with $|\lambda_i| \leq \Lambda_{QCD}$ (typically, $\simeq$ 300-400 MeV). This cutoff is chosen (a) to include as much as possible of the important low-energy chiral physics of the unquenched theory while (b) leaving the fluctuations of $\ln \mathcal{D}_{\mathcal{IR}}$ of order unity after each sweep updating all links with the pure gauge action. This ensures that the acceptance rate is sufficiently high when the infrared determinant only is used in the accept/reject stage of the procedure. The crucial point is that it is possible to achieve *both* (a) and (b) on fairly large lattices (up to physical volume $\simeq$ 20 F^4) as well as at kappa values arbitrarily close to kappa critical.

2. Efficient Computation of the IR spectrum in QCD4

The following Lanczos procedure allows us to extract the needed infrared eigenvalues of H relatively rapidly:
(1) Starting from an initial vector v_1, an orthonormal sequence $v_1, v_2, v_3, ..v_{N_L}$ is generated by the standard recursion:
$v_{k+1} = \frac{1}{\beta_k} H v_k - \frac{\beta_{k-1}}{\beta_k} v_{k-1} - \frac{\alpha_k}{\beta_k} v_k$
with the constants α_k, β_k determined from overlaps of generated vectors. In the basis of the v_i, H is tridiagonal. The corresponding real symmetric tridiagonal matrix T_{N_L} has the α_k on the diagonal and the β_k on the sub (and super) diagonal.
(2) A Cullum-Willoughby sieve [2] is used to identify and remove spurious eigenvalues.
(3) The remaining "good" eigenvalues converge most rapidly in the least dense part of the spectrum, in particular, in the needed infrared portion. This remains true even at kappa critical (in marked contrast to the *matrix inversions* needed in HMC simulations, for example), where the density of eigenvalues near zero is still small. The stability and accuracy of the converged eigenvalues has been checked extensively by gauge transforming the gauge field.
(4) The diagonalization of the T_{N_L} matrix (typically, of order 10,000 in the QCD case) can be completely parallelized using the Sturm sequence property [3] of tridiagonal matrices in

which nonoverlapping parts of the spectrum are independently extracted by a bisection procedure.

3. Fitting the UV modes- Loop representations of the Quark determinant

The effective gauge action generated by internal quark loops is a gauge-invariant functional, which can be evaluated explicitly in a hopping parameter expansion:

$$\begin{aligned}\ln\mathcal{D}(A)/V &= 288\kappa^4\sum L_1 + 2304\kappa^6\sum L_2 \\ &+ 4608\kappa^6\sum L_3 + 1536\kappa^6\sum L_4 + ..\end{aligned}$$

where V is the lattice volume, L_1 a generic plaquette, and $L_{2,3,4}$ are 6 link loops with link directions $(i,i,j,-i,-i,-j)$, $(i,j,k,-j,-i,-k)$, and $(i,j,k,-i,-j,-k)$ $(1 \leq i,j,k \leq 4)$. Unfortunately, this hopping parameter expansion is useless [4] except for extremely heavy quarks ($\kappa \to 0$), due to the contribution of large loops. Instead, large loops may be cut off by removing the IR modes $|\lambda_i| < \Lambda_{QCD}$. Now the expansion converges much more quickly, and we may write $\ln\mathcal{D}_{UV}(A) = V\sum L_i(A)$ where the sum involves only a small number of loops (as we shall see, typically less than 10) and the coefficients c_i are determined nonperturbatively. Of course, to compute $\mathcal{D}_{UV}$, we need the complete spectra for an ensemble of configurations. The computational cost for extracting a complete Dirac spectrum via Lanczos is large but manageable, as this calculation need only be done for a limited number of decorrelated configurations. For example, the complete Dirac spectrum for a 10^3x20 lattice has 240,000 eigenvalues and requires about 500,000 Lanczos sweeps, equivalent to about 1 400-Mhz-Pentium-week. The final spectrum can be checked with analytic spectral sum rules which give the sum of powers of the eigenvalues as explicit functionals of small loops.

The results of a fit of $\ln\mathcal{D}_{UV}$ to a linear combination of Wilson loops on an ensemble of 10^3x20 lattices at beta=5.7 (with clover improvement) and κ=0.1425 is shown in Fig.1 The configurations were generated including the truncated determinant $\ln\mathcal{D}_{IR}$ and therefore already contain the exact low-energy chiral physics. The fit is very good once 4, 6 and 3 figure-8 8-link operators are included in the fit . These results suggest that the full determinant can be accurately modelled by computing the low eigenvalues exactly and including the remaining high modes via an approximate loop action. In any event, we expect that the UV fluctuations affect primarily the scale of the theory, while for the low energy spectrum, quark off-shellness is limited to about Λ_{QCD} and dimensionless mass ratios should therefore be largely insensitive to $\mathcal{D}_{UV}$.

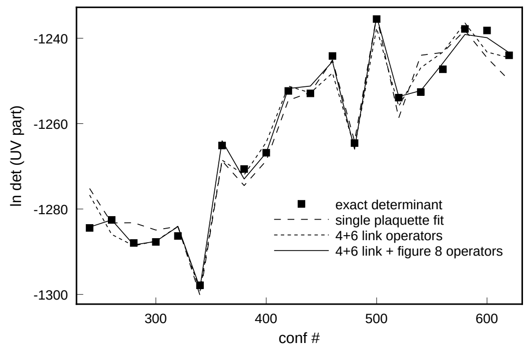

Figure 1. Fit of UV Determinant to Loop Action, κ=0.1425

4. MonteCarlo Dynamics for QCD4 Simulations with the Truncated Determinant

In the truncated determinant approach to QCD4 [1], unquenched configurations are generated by the following algorithm:

1. Update the gauge configuration with the pure gauge action, using a procedure compliant with detailed balance. We have used Metropolis link updates applied to a randomly chosen block of noninterfering links to ensure detailed balance while maintaining parallelizability of the computation.

2. Apply a metropolis accept/reject criterion based on the the effective quark action

$$S_{\text{quark}} = N_F \ln\det\mathcal{D}_{IR}(A) \quad (N_F = 2) \qquad (1)$$

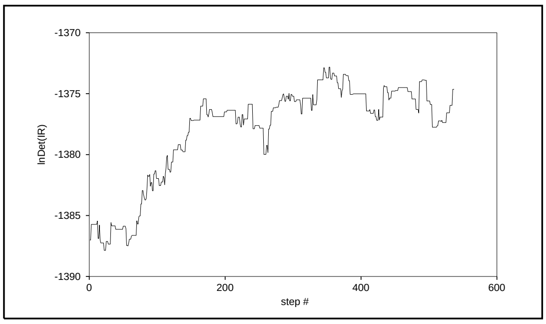

Figure 2. Determinant relaxation, κ=0.1440

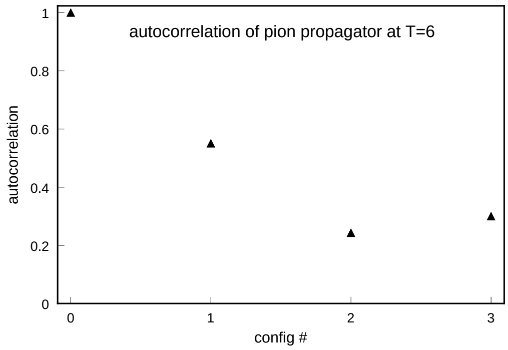

Figure 3. Decorrelation of pion propagator, κ=0.1425

Typically, we use an IR cutoff for the truncated determinant corresponding to a gauge-invariant eigenvalue of 300-400 MeV. This procedure leads to tolerable acceptance rates on lattices of fairly large physical volume - we have explored systems up to 20 F^4, while controllable finite size errors in electromagnetic fine structure lattice studies [5] with a long range massless U(1) field require lattice volumes $\geq$6 F^4. The simulations in progress are on three different lattice sizes:
(1) 10^3x20 lattices at β=5.7 (clover improved) at κ=0.1415, 0.1425, 0.1436 and 0.1440 (the last value being very close to kappa critical). This corresponds to a physical volume of roughly $(1.7\mathrm{F})^3$x3.4F.
(2) 6^4 lattices at an effective β of 4.5, but using the O(a^2) improved gauge action of Alford et al,[6], at kappa critical.
(3) 8^4 lattices at an effective β=4.5 (O(a^2) improved), again at kappa critical.

For the 10^3x20 lattices we have checked that the truncated determinant simulations succeed in equilibrating the configurations, and that they decorrelate reasonably rapidly subsequent to equilibration. The equilibration can be studied by looking at the relaxation of S_{quark} from the quenched value corresponding to the starting configuration. Even at $\kappa = \kappa_c$, the 10^3x20 lattices equilibrate after a few hundred sweeps (see Fig. 2).

To measure decorrelation we have calculated the autocorrelation of the pion propagator at various time separations, keeping configurations separated by 20 steps of the basic algorithm. A typical example, from the 10^3x20 runs with κ=0.1425, is shown in Fig.3, where the pion correlator at time slice 6 is seen to be effectively decorrelated after about 30 steps of the algorithm.

Cases (2,3) represent physically large lattices (33 F^4 and 105 F^4 resp.) at kappa critical and display critical slowing down (several thousand sweeps are needed to equilibrate the configurations). However the lattice sizes are small: new configurations can be generated and the truncated determinant computed quite rapidly ($\simeq$ 20 minutes for the 6^4 lattices, two hours for the 8^4 lattices, on a Pentium 400 Mhz processor). These lattices will allow a detailed study of string-breaking and other unquenched dynamical effects (see talk of Eichten, this conference).

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