Prospects of ‘Topologically Unquenched QCD’ from a study of the analogous importance sampling method in the massive Schwinger model

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I give a quick summary of my proposal for simulating an improvement on quenched QCD with dynamical fermions which interact with the gluon configuration only via the topological index of the latter. It amounts to include only the topological part of the functional determinant into the measure, thereby absorbing a correction factor into the observable. I discuss the prospects of this concept from a study in the massive \( N_f \)-flavour Schwinger model, where the correction factor is indeed found to be of order \( O(1) \).

Simulations of lattice QCD have, to date, used the quenched and the partially quenched approximations, where internal fermion loops are omitted or heavily suppressed by giving the dynamical quarks a mass heavier than that of the propagating current quarks. Such an approximation turns out to be necessary, since presently available update algorithms with dynamical fermions tend to slow down rather dramatically if the fermion mass is taken light. From a physical point of view this critical slowing down does not come as a surprise, since it reflects the very nonlocal nature of the fermion determinant. The problem with the quenched and, to a milder extent, the partially quenched approximations, however, is that they introduce unphysical degrees of freedom which persist in low energy observables and render the whole theory sick, if the chiral limit is taken \([1,2]\).

An alternative path towards full QCD is “Topologically unquenched QCD” \([3]\). The aim is to simulate full QCD, but in an unconventional way: The functional determinant is split into a “topological factor”, which is included into the measure and a “correction factor” which is absorbed in the observable. The “topological factor” is defined as the determinant of a suitably chosen “standard configuration” which shares with the actual configuration nothing but the overall topological charge. This means that the importance sampling pays attention only to the first (“topological”) factor in the decomposition

\[
\det(D + m) = \det(D_{\text{std}} + m) \frac{\det(D + m)}{\det(D_{\text{std}} + m)}. \quad (1)
\]

In the language of full QCD this amounts to a statistical guess of the determinant of a configuration on the basis of its topological index. The last factor (i.e. the ratio of the true determinant of the configuration to the guess on the basis of which it has gotten accepted in the “topologically unquenched” Metropolis test) is calculated only when a measurement is done (into which it is included). Hence, the number of determinant ratios to be calculated is reduced quite drastically – at the price of computing for a configuration, whenever possible (see below), its topological index.

From this outline it is clear that for the concept to work two conditions have to hold true. First, there must be a correlation between the logarithm of the determinant evaluated on a certain configuration and the topological index of the latter. Second, the costs (in terms of CPU time) for determining the topological index must be smaller than the savings on determinant evaluation.

The idea of “topologically unquenched QCD” has been launched \([3]\) with a strong focus on theoretical aspects, merely arguing that a correlation between the functional determinant and the topological index (in the continuum theory) is to be expected from the Instanton Liquid Model \([4]\). At this time is seems appropriate to do the next step and to put it to the (numerical) test. A toy theory where the principal issue of “topological
unquenching” can be studied without having to worry about many technical aspects of the implementation (which do indeed matter in QCD) is the multi-flavour Schwinger model (MSM), i.e. QED(2) with \( N_f \geq 2 \) light degenerate fermions. The physics of this theory resembles in many aspects QCD(4) slightly above the phase transition (see refs. \[5\] and references cited in the second of them). Technically, however, there is a difference: Even though the gauge fields in the MSM (in the continuum-version on the torus) fall into topologically distinct classes, there is no precise analog of the instanton, i.e. no topologically non-trivial object which is simultaneously a minimum of the classical action and localized in space-time. As a consequence, the “standard configuration” in each topological sector cannot be constructed artificially but must be chosen as the “most typical” configuration in that sector (i.e. the one which is in its classical/effective action closest to the sectoral average) — cf. strategy (ii) in \[3\].

In order to test the “topological unquenching” idea, I have chosen to implement the Schwinger model with 2 dynamical staggered fermions both full and “topologically unquenched”, as well as the quenched approximation, always using the unimproved gauge action \( S_{\text{class}} = \beta \sum (1-\cos(\theta_{\Box})) \). The three theories are compared to each other using each time \( \sim 1500 \) independent indexed (see below) configurations on a lattice of common size \( V = 14 \times 6 \) with periodic/thermal boundary conditions. The common coupling is \( \beta = 1/g^2 = 3.0 \) and the fermion mass is \( m = 0.1 \). These values are chosen such that the “pion” (pseudo-scalar isosinglet) has a mass \( M_{\pi} \simeq 2.066 \ g^{1/3} \ m^{2/3} \approx 0.3706 \) a configuration is as-signed an index and used for measurements only if the geometric and the naive definition, after rounding to the nearest integer, agree (which, at \( \beta = 3.0 \), holds true for \( \sim 93\% \) of them). The first thing to look at is whether there is a correlation between the effective action or its components \((S_{\text{class}}, -\log(\det(D+m)))\) of a configuration and its topological index. The result which merely extends work initiated in the liter-

\[2\]In practice, it proves useful to relax this condition somewhat and to construct the “standard determinant” as the geometric average of a few determinants of configurations which have an action close to the sectoral average.

Figure 1. Histograms of \( S_{\text{class}}, -\log(\det(\mathcal{D}+m)) \) [for 2 continuum flavours, after an overall-shift] and \( S_{\text{tot}} \) in the full theory with a pair of staggered fermions \((\beta=3.0, m=0.1)\) — each for \( |\nu| = 0, 1, 2 \).
Figure 2. Static quark-antiquark potential and distribution of $\nu_{\text{nai}}$ in the full, quenched and “topologically unquenched” (without the correction factor) theories, as well as after the correction factor (RHS: distribution of its log) has been included. LHS: error bars $\approx 2$ size of the symbols.

Figure 3. Potential in the full theory, if only configurations with $\nu = 0$ or $\nu = \pm 1$ are evaluated.

importance sampling. In terms of CPU time, however, there is a big difference: In the present example, the standard approach turned out to be more expensive by two orders of magnitude.

The physical reason why “topologically unquenched” importance sampling turns out to be useful is elucidated by considering the hypothetical potentials in the full theory, if only configurations in a certain topological sector are taken into account. As one can see from fig. 3, these “sectoral potentials” agree with the correct potential at short distances, but they deviate at larger separations. Given the fact that the correct potential is, loosely speaking, a weighted average of these sectoral potentials, it is clear that it is desirable to preserve the relative weight of the different topological sectors in the full theory — even if importance sampling is done w.r.t. to a different measure. Needless to say that this is exactly what the “topological unquenching” proposal is aiming at.

Issues which need more extensive coverage (e.g. potential sensitivity on accidental misidentification of $\nu$, typical correction factors in larger volumes, physical reason for the effect seen in fig. 3) are hoped to be presented elsewhere.

REFERENCES
5. A. Smilga, J. Verbaarschot, Phys. Rev. D54,