PROCEEDINGS OF SCIENCE

The art of smearing – can one reach $M_\pi = 140\,\mathrm{MeV}$ in quenched QCD with clover quarks ?

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Several smearing recipes (APE, stout, and a new LOG smearing) are discussed and compared, without and with the hypercubic nesting trick, which may be applied to each one of them. While the $U(1)$ projection in the APE recipe creates a challenge in defining the derivative of the smeared link with respect to the original one, the latter two recipes yield differentiable fat links. This makes them interesting for building UV-filtered fermion actions which can be simulated with a HMC algorithm. This contribution discusses the plaquette distribution and how it is affected by these recipes and their hypercubic descendents. Subsequently, the issue of how light a pion one may simulate in the quenched approximation with such low-cost nearly-chiral actions is addressed.

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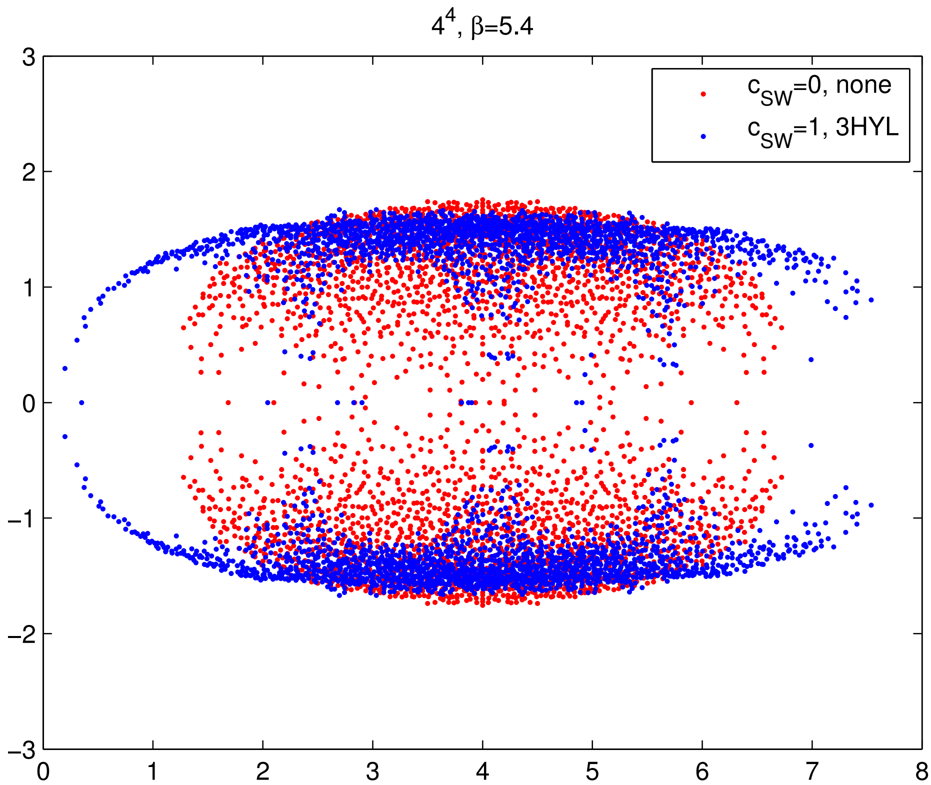

Figure 1: Dirac operator eigenvalues without smearing and improvement versus with smearing and $c_{SW} = 1$.

1. Why should one smear ?

A brief answer is: because it is *much* cheaper to calculate a physical quantity (dimensionless ratio) in the continuum limit with a pre-defined accuracy, if one uses a UV-filtered ("fat-link") fermion action. This contribution discusses the advantages and some of the caveats.

A word on history: Link-fattening has been introduced to reduce taste symmetry violations of staggered fermions. Shortly after, it was found to be equally useful to tame chiral symmetry breaking of Wilson-type fermions – see [1] for details. Fat-link perturbation theory for Wilson/clover fermions has been pioneered in the second item of [1] and specified in more detail in [2].

In Fig. 1 the eigenvalue spectrum of the plain Wilson operator at $am_0 = 0$ is shown on an incredibly coarse lattice – the physical branch is barely separated from the remaining four. Upon including a clover term and some link-fattening the situation changes noticeably: The physical branch becomes well-separated and moves left, i.e. the additive mass renormalization is reduced. Moreover, the physical branch gets slimmer, and this suggests that the size of $O(a^2)$ ambiguities is bound to be much smaller. Here and in subsequent plots the same type of smeared links has been used in the covariant derivative and in the clover term – see [2] for a more complete typology.

2. Four smearing recipes

The first type of smearing, known as APE smearing [3], may be written in factorized form as

$$U_\mu^{\mathrm{APE}}(x) = P_{SU(3)}\Big\{(1-\alpha)I + \frac{\alpha}{2(d-1)} \sum_{\pm\nu\neq\mu} U_\nu(x)U_\mu(x+\hat{\nu})U_\nu^\dagger(x+\hat{\mu})U_\mu^\dagger(x)\Big\}\,U_\mu(x) \tag{2.1}$$

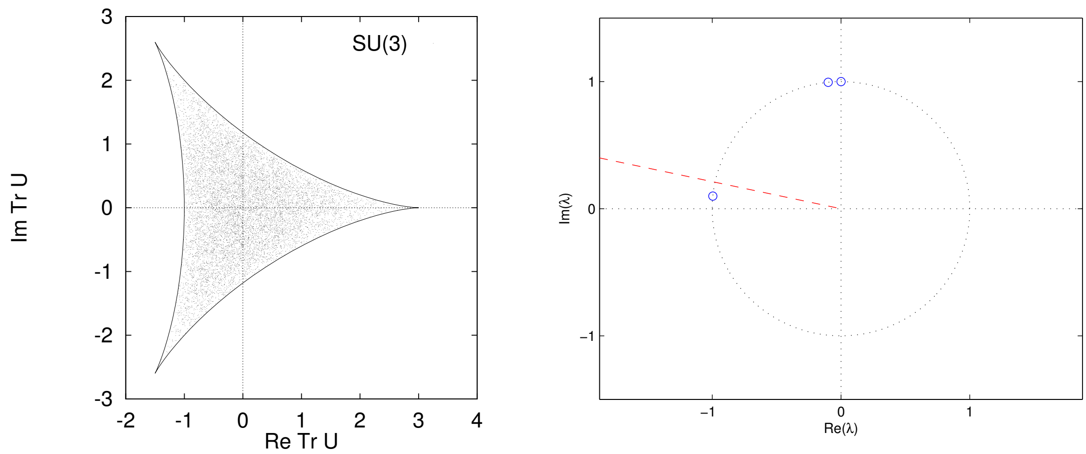

Figure 2: $\mathrm{Tr}(U)$ of $SU(3)$ matrices (stolen from Mike Creutz) and eigenvalues λ of a U with $\mathrm{Tr}\log(U) \neq 0$.

but the $U(1)$ back-projection creates a headache if one wants to use it in a HMC algorithm. Therefore, Morningstar and Peardon invented the "stout" (subsequently dubbed "EXP") smearing

$$U_\mu^{\mathrm{EXP}}(x) = \exp\Big(\frac{\alpha}{2}\sum_{\pm\nu\neq\mu}\big\{[U_\nu(x)U_\mu(x+\hat{\nu})U_\nu^\dagger(x+\hat{\mu})U_\mu^\dagger(x) - \mathrm{h.c.}] - \frac{1}{3}\mathrm{Tr}[.]\big\}\Big)\,U_\mu(x) \tag{2.2}$$

where this problem is solved. However, it turns out that stout/EXP is not very efficient in taming the UV noise. Hasenfratz, Hoffmann and Schaefer have proposed to back-project in the APE recipe to $U(3)$ only, baptizing it n-APE smearing [5]. Another option is the LOG smearing [6]

$$U_\mu^{\mathrm{LOG}}(x) = \exp\Big(\frac{\alpha}{2(d-1)}\sum_{\pm\nu\neq\mu}\log[U_\nu(x)U_\mu(x+\hat{\nu})U_\nu^\dagger(x+\hat{\mu})U_\mu^\dagger(x)]\Big)\,U_\mu(x) \tag{2.3}$$

which yields a differentiable fat link which is naturally in $SU(3)$, if the configuration is smooth.

3. LOG smearing sub-varieties

On a thermalized background there may be some plaquettes for which $\mathrm{Tr}\log(U_{\mu\nu}(x)) = \pm 2\pi\mathrm{i}$. There are several options how to specify (2.3) completely (in all cases, see [6] for details):

0. Take the principal log in (2.3); the result will be a smeared link in $U(3)$, just as in [5].
1. Replace $\log[.] \;\rightarrow\; \log[.] - \frac{1}{3}\mathrm{Tr}\log[.]$ in (2.3).
2. Include weights $c_{\pm\nu}$ in the sum in (2.3) which are zero in the case where $\mathrm{Tr}\log(U_{\mu\nu}(x)) \neq 0$.
3. Choose the non-principal ("trace-free") matrix logarithm where the cut is smoothly deformed such as to maintain $\mathrm{Tr}\log(U_{\mu\nu}(x)) = 0$ (see Fig. 2 for an illustration).
4. Add a constraint to the gauge action which prevents plaquettes with $\mathrm{Re}\,\mathrm{Tr}(U_{\mu\nu}(x)) \leq -1$.

4. Hypercubic nesting trick

Clearly, upon iterating the smearing the benefits may be enhanced, but the delocalizing effect gets enhanced, too. A neat strategy is the hypercubic nesting trick [7] where three iterations are

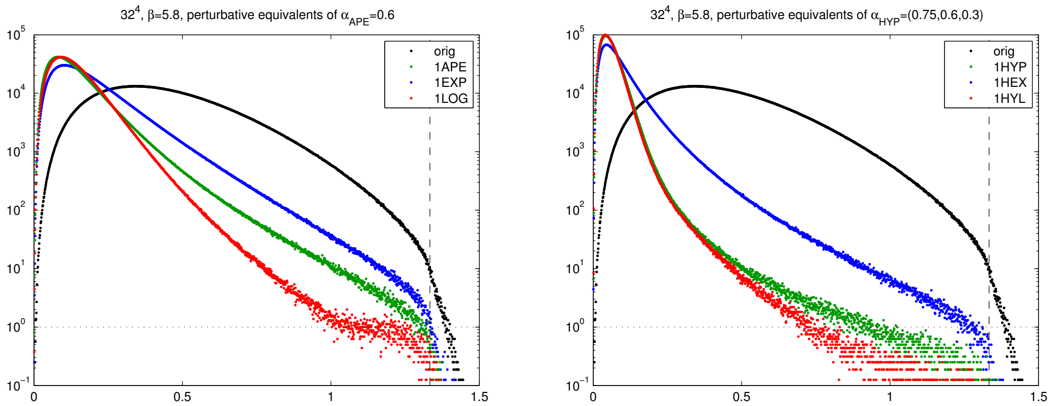

Figure 3: Histogram of $1-\mathrm{Re\,Tr}\log(U_{\mu\nu})/3$ without smearing (black) and after 1 APE/EXP/LOG smearing (left) or their hypercubically nested descendents (right). Equivalent parameters have been used (see text).

nested in such a way that the final link depends only on the thin links in the adjacent hypercube. Originally, it was formulated for the APE core recipe, and it has been generalized to the EXP and LOG recipes in [2] and [6], respectively. The result will be called HEX and HYL smearing.

5. Impact on plaquette distribution

One way to obtain detailed information about the efficiency of a given smearing recipe is to monitor how it affects the plaquette distribution $\rho(1-\mathrm{Re\,Tr}(U)/3)$. Without smearing the distribution bears some similarity with the black body radiation: $\rho(s)$ is essentially a power-law at low s and close to an exponential fall-off at large s (for low β the constraint $s\leq 1.5$ is perceptible).

With smearing the distribution is essentially shifted to the left, towards “colder temperature” (though there is no equivalent of the Wien law, as the distribution is not specified by a single parameter). In Fig. 3 the change is shown after one step of APE/EXP/LOG smearing. Clearly, EXP is less efficient than APE. On the other hand, LOG is better or equally efficient as APE, depending on whether one looks at large or extremal plaquettes. From the right-hand panel a similar conclusion is drawn if each one of these recipes is used in a hypercubically nested arrangement. In these graphs the equivalent of $\alpha_\mathrm{APE}=0.6$ and $\alpha_\mathrm{HYP}=(0.75,0.6,0.3)$ has been used.

6. Impact on residual mass

One way (the simplest, not necessarily the best one) to quantify the amount of chiral symmetry breaking is to measure the *residual mass*, here defined as the PCAC mass at $am_0=0$.

The main result of [2] is convincing evidence that the two well-known tricks to reduce the amount of chiral symmetry breaking – link-fattening and clover improvement – would amplify when applied together. Put in a populist manner: When $c_\mathrm{SW}=1$ would reduce am_res by a factor 2 and a certain type of smearing would reduce it by a factor 7, then the two effects would enhance each other, so 2×7 could be as much as 26. An obvious need is thus to determine how the new LOG/HYL smearing fares in this respect and to compare it to the established recipes.

At this point it seems appropriate to give action and algorithm details. The investigation has been carried out with Wilson glue and quenched tree-level clover fermions, i.e. $c_\mathrm{SW}=1$. Point

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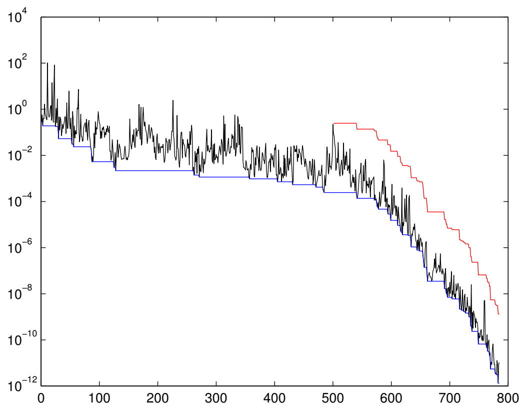

Figure 4: Typical residual norm history in the EO preconditioned BCGγ_5-algorithm. See text for details.

sources and sinks were used, and the inversions aimed at $||r|| < 10^{-12}$. I have implemented three algorithms: conjugate gradient on normal equations (CGNE), conjugate gradient on the hermitean Dirac operator (CGH), bi-conjugate gradient on an operator with γ_5-symmetry (BCGγ_5). Since EO-preconditioning leads to a reduced operator $D_\mathrm{red} = \frac{1}{2}(D_\mathrm{oo} - D_\mathrm{oe}D_\mathrm{ee}^{-1}D_\mathrm{eo})$ which is γ_5-symmetric, the same algorithms may be used again. It is well known that the fastest algorithm out of these, BCGγ_5, suffers from instabilities, due to round-off errors, which often prevent proper convergence. I find that I can make this algorithm perform satisfactorily, upon applying three tricks:

1. Do the summation in indefinite scalar products in quadruple precision (everything else in double precision).
2. Recompute the true residual much more frequently than one would do in an algorithm with standard scalar products.
3. Keep track of the vector which lead to the smallest residual, and restart from it if certain conditions are met (e.g. $||r|| > 10^3||r_\mathrm{best}||$ and last restart dates back at least 500 steps).

A typical convergence history (in a case without restart) is shown in Fig. 4. The high precision seems essential to enter the regime with superlinear convergence.

The results for am_res at $m_0 = 0$ for $\beta = 5.6, 5.8, 6.0, 6.2$ and with one step of APE/EXP/LOG or HYP/HEX/HYL smearing with the equivalent of $\alpha_\mathrm{APE} = 0.6$ and $\alpha_\mathrm{HYP} = (0.75, 0.6, 0.3)$ are tabulated in [6]. They are shown in graphical form in the two panels of Fig. 5. It turns out that the 1-loop perturbative prediction for am_res of UV-filtered clover fermions in [2] applies to the LOG/HYL smearing, too. Hence, it seems natural to fit the data with the ansatz

$$am_\mathrm{res} = \left\{ \begin{matrix} 4.90876 \\ 1.98381 \end{matrix} \right\} \frac{g_0^2}{12\pi^2} \, \frac{1 + c_1 g_0^2}{1 + c_2 g_0^2} \tag{6.1}$$

and such fits are included in Fig. 5, together with the respective linear asymptotic slope and the asymptotic counterparts for unfiltered Wilson/clover fermions. The bottom line is that LOG/HYL fares at least as good as APE/HYP, and these are considerably better than EXP/HEX.

7. How light can one go ?

An obvious questions is “how light can one go with fat-link clover fermions at $a \sim 0.1\,\mathrm{fm}$ or $a \sim 0.05\,\mathrm{fm}$?” and, along with it, “what is the (possibly hidden) price to pay ?”.

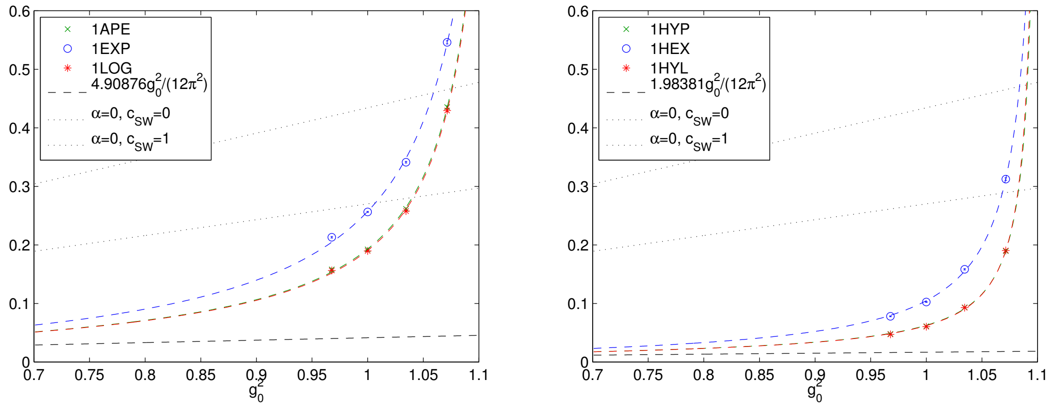

Figure 5: $am_{\rm res}$ versus g_0^2 after 1 APE/EXP/LOG smearing (left) or their hypercubically nested descendents (right). The non-perturbative values are fitted to the ansatz (6.1) which obeys the respective 1-loop perturbative asymptotic constraint (dashed slope at the bottom). The non-perturbative data for $\beta \geq 6.0$ (left) or $\beta \geq 5.8$ (right) lie beneath the 1-loop predictions for $c_{\rm SW} = 0$ and $c_{\rm SW} = 1$ thin-link Wilson/clover fermions.

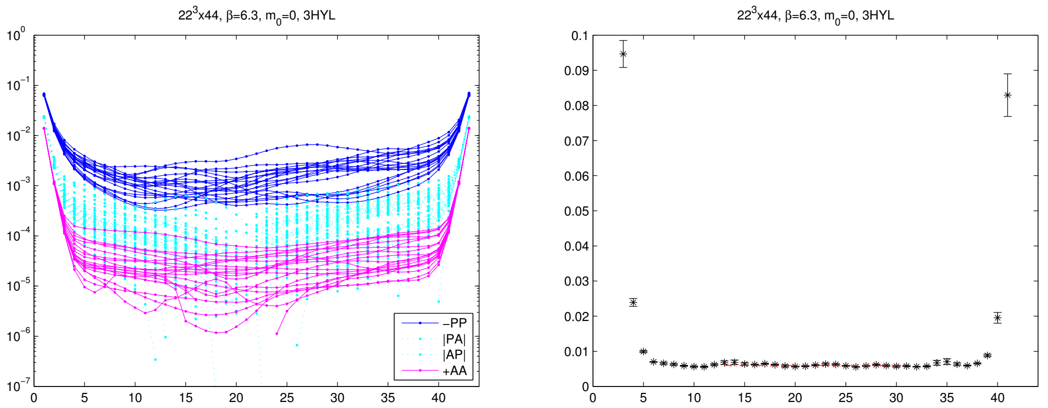

Figure 6: Pion correlators at $am_0 = 0$ and $\beta = 6.3$ with 3 HYL steps and resulting PCAC mass plateau.

Upon adding "... without dialing a negative bare mass" the first question can be answered without difficulties. With $am_0 = 0$ one finds $am_{\rm res} = 0.0110(7)$ at $\beta = 6.0$ and $am_{\rm res} = 0.0068(3)$ at $\beta = 6.2$, if 3 steps of HYL smearing with the standard parameter $\alpha_{\rm HYL} = (0.75, 0.6, 0.3)$ are used. Fig. 6 shows (for 3 HYL steps and an even higher β) the correlators and the PCAC mass. While the former become quite fuzzy at such a small quark mass, the latter stays remarkably quiet. Upon converting these values into physical units ($m^{\rm PCAC} = 0.0110 \times 2.12\,\mathrm{GeV} = 23\,\mathrm{MeV}$ and $m^{\rm PCAC} = 0.0068 \times 2.91\,\mathrm{GeV} = 20\,\mathrm{MeV}$), one feels tempted to speculate that $M_\pi \simeq 320\,\mathrm{MeV}$ is a natural limit for 3 HYL actions with $am_0 = 0$. Note that no attempt has been made to quantify the systematics.

8. How much smearing is "optimal" ?

With these figures at hand, it is natural to ask whether some additional smearing would allow to reach the physical pion mass, while still keeping $am_0 = 0$. Indeed, exploratory runs with 7 HYL steps suggest that such actions yield $M_\pi \simeq 160\,\mathrm{MeV}$ at $am_0 = 0$. While in principle any fixed type of smearing yields a legal action (see e.g. the discussion in [2]), it is clear that very high smearing levels may again lead to an action with suboptimal scaling properties. In the absence of a detailed study, choosing a modest amount of smearing (e.g. 1 step of HYL) is certainly a reasonable strategy. In any case it is clear that this is an engineering issue and not a fundamental one.

9. Summary

1. Smearing is medicine against UV-noise; one should try to avoid both under- and overdosing. What exactly is the "optimum" amount of smearing (to compute a given observable with a predefined error in the continuum limit with a minimal amount of CPU time) could only be determined through a multi-action scaling study, but it is definitely not zero.
2. Criteria one may ask for, when selecting the core recipe, include: (*i*) whether it smears efficiently (satisfied by APE, n-APE, LOG), (*ii*) whether the link is differentiable (EXP, n-APE, LOG), (*iii*) whether the link is in $SU(3)$ (APE, EXP, LOG). The last point is mostly esthetic, albeit it might facilitate agreement with perturbation theory. Whenever possible, one should use hypercubic nesting.
3. Comparison of different smearing recipes and/or parameters may proceed via the plaquette distribution or via the signal-to-noise ratio of a physical correlation function.
4. Clover improvement and HYL-smearing together yield Wilson fermions with much reduced chiral symmetry breaking (mutatis mutandis with staggered fermions: Naik term and taste breaking). The main conclusion is that the new LOG/HYL smearing provides powerful means to build UV-filtered actions suitable to simulate full QCD with a HMC algorithm.

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