Testing the stochastic LapH method in the twisted mass formulation

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We present first results using the stochastic Laplace-Heaviside (sLapH) method in the twisted mass formulation. The calculations are performed on gauge configurations provided by the European Twisted Mass (ETM) collaboration with 2+1+1 dynamical quark flavours at a single value of the lattice spacing. In particular, we compute disconnected contributions to flavour singlet pseudo-scalar mesons and compare sLapH to standard volume noise methods.

31st International Symposium on Lattice Field Theory LATTICE 2013
July 29 August 3, 2013
Mainz, Germany

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1. Introduction

Lattice QCD provides a non-perturbative method for investigating strong QCD by Markov Chain Monte-Carlo methods in Euclidean space-time. If one is interested in the hadron spectrum, lattice QCD is a very powerful tool for determining the ground states in a given channel. Higher excitations or even resonances, however, are much more intricate, because exponentially suppressed contributions must be disentangled from correlator data plagued with statistical noise.

It is well known that correlator matrices are of significant help in such a situation. With the variational approach [1, 2, 3] or factorising fit models, excited energy levels can be determined from such a matrix. Furthermore, the larger the matrix the more energy levels can be extracted with confidence.

However, building a correlator matrix from a large basis of operators is a demanding task, both in computational resources and in storage space. With these challenges in mind the Laplacian Heaviside smearing (LapH) method [4] and its stochastic version (sLapH) [5] were invented, leading to remarkable results, see for instance Refs. [6, 7, 8]. Its particular strength lies in the possibility to construct a large number of operators from a fixed (but large) number of inversions.

In this proceeding contribution we will investigate sLapH for the case of the Wilson twisted mass formulation of lattice QCD [9]. In particular, we compare sLapH with more conventional methods for the case of the η, η' mesons, which obtain significant contributions from disconnected diagrams.

2. Stochastic LapH Smearing

The LapH method is a smearing method based on the Laplace operator $\widetilde{\Delta}$ which is decomposed into its eigensystem

$$\widetilde{\Delta} = V_\Delta \Lambda_\Delta V_\Delta^\dagger. \tag{2.1}$$

The matrix V_Δ contains all eigenvectors v and Λ_Δ is a diagonal matrix containing the eigenvalues. A smearing matrix $\mathscr{S}$

$$\mathscr{S} = V_\Delta \Theta \left(\sigma_s^2 + \Lambda_\Delta \right) V_\Delta^\dagger = V_s V_s^\dagger, \tag{2.2}$$

can be defined, where $\Theta(\cdot)$ is the Heaviside function. Therefore, all eigenvalues larger than a cutoff σ_s^2 are neglected and the matrix V_s consists only of the eigenvectors belonging to the eigenvalues smaller than σ_s^2. The number of eigenvalues needed depends on the spatial volume of the lattice and the parameter σ_s^2. It was found that $\sigma_s^2 = 0.33$ is optimal [5] for excited state suppression independent of the operator. On a $48^3 \times 96$ lattice, for example, this amounts to 900 eigenvectors per timeslice. In the same reference it was shown that the shape of the source is approximately Gaussian.

A quark line $\mathscr{Q}$ can be written in terms of the smearing matrix

$$\mathscr{Q} = D^{(j)} \mathscr{S} \Omega^{-1} \mathscr{S} D^{(k)\dagger} = D^{(j)} V_s \left(V_s^\dagger \Omega^{-1} V_s \right) V_s^\dagger D^{(k)\dagger}, \tag{2.3}$$

where $D^{(j)}$ is a covariant derivative. $\mathscr{P} = V_s^\dagger \Omega^{-1} V_s$ is called perambulator, $\Omega = \gamma_4 M$, γ_4 is a Dirac matrix, and M being the lattice Dirac operator. The computation of $\Omega^{-1} v$ must be performed for each eigenvector v, which is a significant drawback of this method, in particular for large lattice volumes.

2.1 Stochastic LapH

In order to overcome this drawback the stochastic LapH method was introduced in Ref. [5]. Random noise vectors ρ which live in the time, Dirac- and Laplace eigenspace should reduce the computational cost and not change the result significantly if the following relations hold

$$E(\rho_i) = 0 \quad \text{and} \quad E(\rho_i \rho_j^*) = \delta_{ij}, \tag{2.4}$$

where $E(\cdot)$ denotes the expectation value. The propagator Ω^{-1} can then be calculated approximately by solving

$$\Omega X^r = \rho^r \tag{2.5}$$

for N_R different random vectors ρ^r. Dilution can be used to enhance the signal-to-noise ratio. The improvement factor is proportional to $\frac{1}{N_d \sqrt{N_R}}$, where N_d is the number of dilution vectors. Therefore, the signal-to-noise ratio ameliorates proportional to the number of inversions done. The dilution factorises into three subspaces, time, Dirac- and eigenspace and thus different dilution scheme can be applied in each subspace. In Ref. [5] four basic dilution schemes are discussed

$$
\begin{aligned}
P_{ij}^{(b)} &= \delta_{ij}, & b &= 0, & &\text{(no dilution)} \\
P_{ij}^{(b)} &= \delta_{ij}\,\delta_{bi}, & b &= 0,\ldots,N-1, & &\text{(full dilution)} \\
P_{ij}^{(b)} &= \delta_{ij}\,\delta_{b,\lfloor Ji/N \rfloor}, & b &= 0,\ldots,J-1, & &\text{(block-}J\text{)} \\
P_{ij}^{(b)} &= \delta_{ij}\,\delta_{b,i \bmod J}, & b &= 0,\ldots,J-1, & &\text{(interlace-}J\text{)},
\end{aligned}
$$

where N is the size of the subspace (time, Dirac- and eigenspace) and N/J is an integer. N_d is 1 for no dilution, N for full dilution and J for interlace or block dilution. Another possibility for a dilution scheme would be to combine the interlace and the block dilution schemes.

Using random noise vectors and a dilution scheme, one arrives at a similar expression for the stochastic quark lines as in eq. 2.3

$$\mathscr{Q} = \sum_b E\left(D^{(j)}\mathscr{S}\Omega^{-1}V_s P^{(b)}\rho\,(D^{(k)}V_s P^{(b)}\rho)^\dagger\right). \tag{2.6}$$

Here, the first part, $\phi = D^{(j)}\mathscr{S}\Omega^{-1}V_s P^{(b)}\rho$, acts as a quark sink and the second part, $\eta = D^{(k)}V_s P^{(b)}\rho$ as a quark source. A stochastic perambulator $\mathscr{P}_s$ can be defined

$$\mathscr{P}_s = V_s \Omega^{-1} V_s P^{(b)}\rho. \tag{2.7}$$

Its computation is the computationally most expensive part of this method. However, the number of inversions which need to be performed only depends on the number of random vectors and the dilution scheme. The volume dependence of the non-stochastic LapH method has almost disappeared and appears only very mildly in certain dilution schemes if at all. This might be useful for larger lattices with many eigenvectors.

To illustrate the problem of computational cost and storage, the number on inversions and the storage space needed for a $48^3 \times 96$ lattice is calculated. 900 eigenvectors per timeslice are needed and hence the matrix V_s would need roughly 427 GB of storage space. To calculate the full perambulator $\mathscr{P}$, $900 \cdot 96 \cdot 4 = 345600$ inversions would have to be performed and the final

perambulator would need approximately 1780 GB. The computational cost of the inversions and the storage requirements make it unfeasible to use this method for larger lattices at the moment.

Using the stochastic ansatz reduces the computational cost significantly. With full dilution in time and in Diracspace and an interlace-8 dilution in eigenspace (TF,DF,LI8), the number of inversions would reduced to 3072, while the storage space would reduce to 15.8 GB. Usually, it is not necessary to use full dilution in time, the computational cost could be reduced further. Using an interlace-16 scheme in time (TI16,DF,LI8) would result in 512 inversions and a storage size of only 2.6 GB. The latter scheme is entirely independent of the lattice size.

3. Numerical Experiments

3.1 Simulation parameters

Our simulations were performed on the $A60.24$ ensemble with $N_f = 2 + 1 + 1$ dynamical Wilson twisted mass fermions as produced by the European Twisted Mass collaboration [10, 11, 12]. The volume of this lattice is $V = 24^3 \cdot 48$ with a lattice spacing of $a = 0.086$ fm, and a pion mass of about 390 MeV. In total, 314 gauge configurations were used. For strange and charm quarks the so-called Osterwalder-Seiler mixed action [13] with $a\mu_s = 0.02322$ and $a\mu_c = 0.27678$ (c. f. [14]) was used. More details on this approach can be found in a contribution to this conference [14]. The inversions and the computation of the eigenvectors were performed with the tmLQCD software suite [15].

The Euclidean correlation functions for the η, η' system is given by

$$\mathscr{C}(t)_{qq'} = \langle \mathscr{O}_q(t'+t) \mathscr{O}_{q'}(t') \rangle, \quad q, q' \in \ell, s, c, \tag{3.1}$$

where the operators $\mathscr{O}_\ell = (\bar{u}i\gamma_5 u + \bar{d}i\gamma_5 d)/\sqrt{2}$, $\mathscr{O}_s = \bar{s}i\gamma_5 s$ and $\mathscr{O}_c = \bar{c}i\gamma_5 c$ were used. For this operator basis the resulting matrix $\mathscr{C}$ is a 3×3 matrix which is diagonalised by solving the Generalised Eigenvalue Problem. The effective masses

$$aM^{(n)} = -\log(\lambda^{(n)}(t, t_0)/(\lambda^{(n)}(t+1, t_0)) \tag{3.2}$$

are computed from the eigenvalues $\lambda^{(n)}(t, t_0)$. In this ansatz the η meson corresponds to the ground state ($n = 0$) and the η' meson to the first excited state ($n = 1$). The second excited state ($n = 2$) corresponds to the η_c meson but cannot be resolved due to the small correlation matrix. In addition, we investigate the disconnected contribution to the neutral pion, corresponding to the operator $\mathscr{O}_{\pi^0} = (\bar{u}i\gamma_5 u - \bar{d}i\gamma_5 d)/\sqrt{2}$.

For the calculation of the eigenspace of the Laplace operator, two iterations of 3D HEX [16] smearing with parameters $(0.76, 0.95)$ were applied to the spatial gauge fields. On each timeslice we calculated 120 eigenvectors and we used the previously introduced dilution scheme (TF, SF, LI8).

The sLapH method is tested against a standard approach of computing correlation functions. In this standard approach, connected diagrams were computed by using stochastic timeslice sources and the so called "one-end-trick" [17]. Disconnected diagrams which need an all-to-all approach were sampled using 24 stochastic volume sources with complex Gaussian noise. Two different methods were used to improve the signal-to-noise ratio. The first one is a hopping parameter
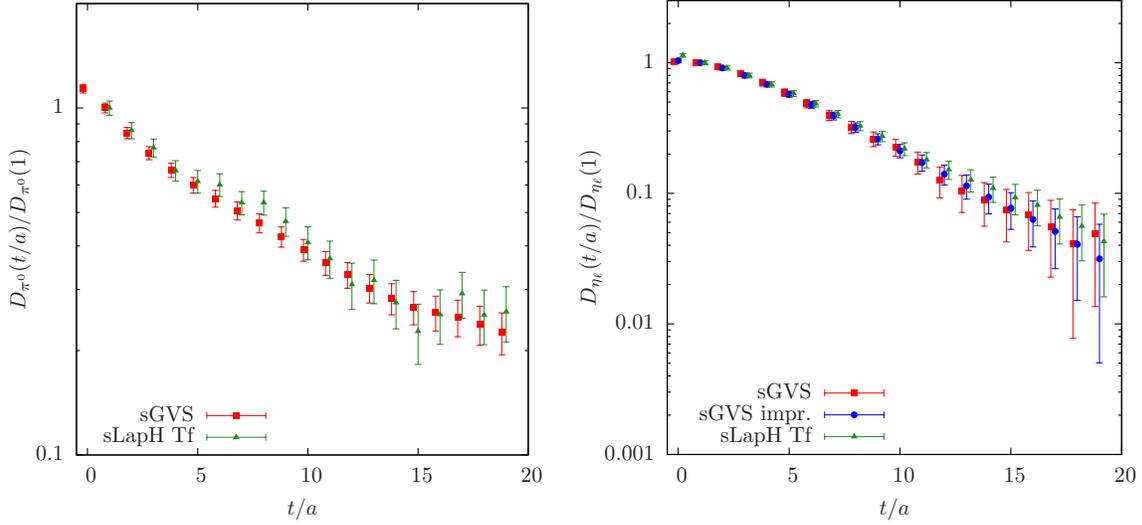
Figure 1: Disconnected contribution to the π^0 (left) and the η_ℓ (right) correlation functions are shown. Both are normalised to $t/a = 1$. The points are slightly displaced for better legibility.

variance reduction scheme, see Ref. [17], which will be denoted with sGVS. The second one is only available for the η, η' system in the twisted mass formulation and it relies on the identity [18]

$$D_u^{-1} - D_d^{-1} = -2i\mu_l D_d^{-1}\gamma_5 D_u^{-1} \,, \tag{3.3}$$

where $D_{u,d}$ are the up and down lattice Dirac operators and μ_l is the twisted mass parameter corresponding to the light quarks. It can be applied for strange and charm quarks as well by introducing a doublet of strange (charm) quarks, see Ref. [14] for details. This noise reduction will be denoted by improved sGVS.

The efficiency of sLapH as a smearing method to suppress excited state contribution can be tested by comparing the effective mass plateaus computed from sLapH, sGVS and improved sGVS. In the latter two methods only local operators were used and the size of the correlation matrix was 3x3. Hence, a direct comparison was possible and a notable reduction of excited state contributions in case of sLapH should be observable.

3.2 Correlation functions

The disconnected parts of the correlation functions for the π^0 and the η_ℓ are shown in Figure 1. They are normalised to $D(1)$ due to an unknown normalisation factor in sLapH. The η_ℓ contains only the light quark contributions to the η and η' mesons. Within errors, the results obtained from different methods for these observables do agree quite well. While the errors for the disconnected part of the π^0 are compatible in between sLapH and sGVS, sLapH and improved sGVS turn out to outperform sGVS for the disconnected part of the η_ℓ. sLapH and improved sGVS give roughly equal error estimates with a slight advantage for sLapH. However, the computation cost is a factor 24/512 in favour of improved sGVS.
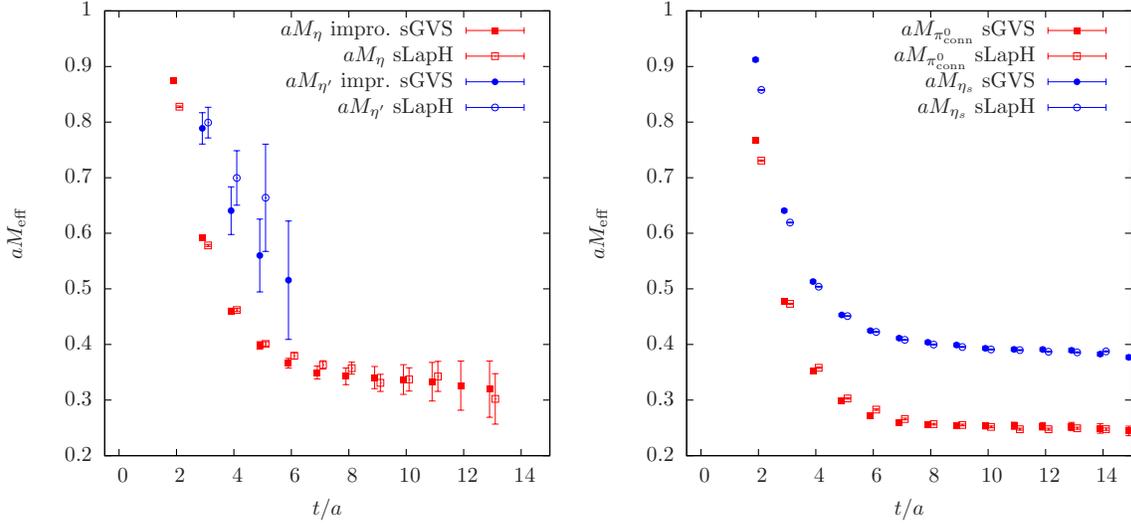
Figure 2: (left) Effective mass plot of the η (squares) and η' (circles) using the sGVS method (full symbols) and the sLapH method (empty symbols). (right) The same as (left), but with connected contributions only. The points are slightly displaced for better legibility.

3.3 Effective Masses

In the left panel of Figure 2 the effective masses of the η (filled symbols) and the η' (open symbols) are shown for the sGVS and sLapH method. General agreement within errors can be observed. However, the number of gauge configurations and the size of the correlation matrix are too small to obtain a good signal for the η' state.

Unfortunately, sLapH seems not to suppress excited states very much, only at $t/a = 2, 3$ a small effect can be observed. This can be seen even better by looking at the connected correlators only, corresponding to a connected neutral pion and the so called η_s state, a pion made out of strange quarks. The effective masses of these states are shown in the right panel of figure 2. The poor suppression of excited state contributions might be due to poorly chosen parameters for the link smearing used in the Laplace operator. The eigenvalues of the Laplace operator are squeezed quite strongly for our choice of smearing parameters compared to unsmeared gauge links. This results in a more shallow increase of the eigenvalues. In conclusion, much more eigenvectors would be needed to achieve a good reduction of excited state contributions. Well chosen link smearing parameters should have the very opposite effect and stretch the spectrum of the Laplace operator. Hence, less vectors would be needed to gain a good reduction.

4. Summary

In this article we presented a first test of the sLapH method in comparison to standard stochastic methods in the twisted mass formulation for the η, η' mesons. The results for the meson masses extracted from the different methods do agree within errors but with the sLapH method being roughly 20 times more expensive. However, the higher expense, which comes mainly from the increased number of inversions, can be put into perspective by noting that the inversions, which

can be easily stored in form of perambulators on a hard drive, can be reused for other observables. In addition, the contractions to build correlation functions are cheaper for the sLapH method compared to standard methods which would become more relevant for a larger operator basis.

As a surprise we did not observe that sLapH suppresses excited states efficiently. In fact, in a comparison to a local-local correlator matrix we see only marginal improvements. This is most probably due to a bad tuning of link smearing in the Laplace operator. The explicit impact of the link smearing and the impact of the lattice spacing on the efficiency of sLapH are under investigation at the moment.

Other physical channels will be studied as well. sLapH clearly still has the advantage of providing the possibility to compute many operators for a fixed number of inversions.

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