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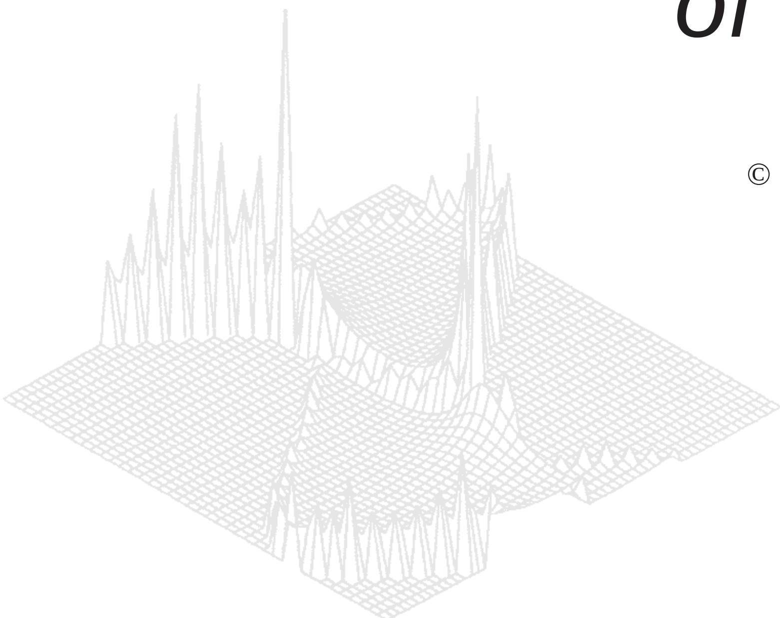

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Discretisation Errors in Landau Gauge on the Lattice

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Abstract

Lattice discretisation errors in the Landau gauge condition are examined. An improved gauge fixing algorithm in which $\mathcal{O}(a^2)$ errors are removed is presented. $\mathcal{O}(a^2)$ improvement of the gauge fixing condition improves comparison with the continuum Landau gauge in two ways: (1) through the elimination of $\mathcal{O}(a^2)$ errors and (2) through a secondary effect of reducing the size of higher-order errors. These results emphasise the importance of implementing an improved gauge fixing condition.

1. Introduction

Gauge fixing in lattice gauge theory simulations is crucial for many calculations. It is required for the study of gauge dependent quantities such as the gluon propagator in Leinweber *et al*. (1998, 1999), and is used to facilitate other techniques such as gauge-dependent fermion source smearing. However, the standard Landau gauge condition, as used by Davies *et al*. (1988), is the same as the continuum condition, $\sum_\mu \partial_\mu A_\mu = 0$, only to leading order in the lattice spacing a.

There has been some study of alternate lattice definitions of the Landau gauge condition by Giusti (1997) and Giusti *et al.* (1998). The focus of this paper is to use mean-field-improved perturbation theory (Lepage and Mackenzie 1993) to compare different lattice definitions of the Landau gauge, and quantify the sizes of the discretisation errors. In particular, we derive a new $\mathcal{O}(a^2)$ improved Landau-gauge-fixing functional which is central to estimating the discretisation errors made with the standard functionals.

In Section 2 we derive mean-field-improved expansions (in the lattice spacing and coupling constant) for three different definitions of the Landau gauge condition for the lattice. The use of an improved Landau gauge functional allows an

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estimate of the absolute error in standard lattice Landau gauge. The size of the error provides a strong argument for the use of an improved gauge fixing condition.

2. Lattice Landau Gauge

Gauge fixing on the lattice is achieved by maximising a functional whose extremum implies the gauge fixing condition. The usual Landau gauge fixing functional is (Davies *et al.* 1988)

$$\mathcal{F}_1^G[\{U\}] = \sum_{\mu,x} \tfrac{1}{2}\mathrm{Tr}\left\{U_\mu^G(x) + U_\mu^G(x)^\dagger\right\}, \tag{1}$$

where

$$U_\mu^G(x) = G(x)U_\mu(x)G(x+\hat{\mu})^\dagger, \tag{2}$$

$$G(x) = \exp\left\{-i\sum_a \omega^a(x)T^a\right\}. \tag{3}$$

Taking the functional derivative of equation (1), we obtain

$$\frac{\delta\mathcal{F}_1^G}{\delta\omega^a(x)} = \tfrac{1}{2}i\sum_\mu \mathrm{Tr}\left\{\left[U_\mu^G(x-\hat{\mu}) - U_\mu^G(x) - \left(U_\mu^G(x-\hat{\mu}) - U_\mu^G(x)\right)^\dagger\right]T^a\right\}. \tag{4}$$

The gauge links are defined as

$$U_\mu(x) \equiv \mathcal{P}\exp\left\{ig\int_0^a dtA_\mu(x+\hat{\mu}t)\right\}. \tag{5}$$

Connection with the continuum is made by Taylor-expanding $A_\mu(x+\hat{\mu}t)$ about x, integrating term-by-term, and then expanding the exponential, typically to leading order in g, noting that errors are of $\mathcal{O}(g^2a^2)$. Expanding equation (4), we obtain

$$\frac{\delta\mathcal{F}_1^G}{\delta\omega^a(x)} = ga^2\sum_\mu \mathrm{Tr}\left\{\left[\partial_\mu A_\mu(x) + \tfrac{1}{12}a^2\partial_\mu^3 A_\mu(x) + \frac{a^4}{360}\partial_\mu^5 A_\mu(x) + \mathcal{O}(a^6)\right]T^a\right\} + \mathcal{O}(g^3a^4). \tag{6}$$

To lowest order in a, an extremum of equation (1) satisfies $\sum_\mu \partial_\mu A_\mu(x) = 0$, which is the continuum Landau gauge condition. What it means in practice on the lattice is that

$$\sum_\mu \partial_\mu A_\mu(x) = \sum_\mu \left\{ -\frac{a^2}{12} \partial_\mu^3 A_\mu(x) - \mathcal{H}_1 \right\}, \tag{7}$$

where $\mathcal{H}_1$ represents $\mathcal{O}(a^4)$ and higher-order terms, as shown in equation (6). Naïvely one might hope that higher-order derivatives in the brackets of (6) are small, but it will be shown that the terms on the right-hand side of equation (7) are large compared with the numerical accuracy possible in gauge fixing algorithms.

An alternative gauge-fixing functional can be constructed using two-link terms, for example

$$\mathcal{F}_2^G = \sum_{x,\mu} \tfrac{1}{2} \mathrm{Tr} \left\{ U_\mu^G(x) U_\mu^G(x+\hat{\mu}) + \mathrm{h.c.} \right\}. \tag{8}$$

Taking the functional derivative yields

$$\frac{\delta \mathcal{F}_2^G}{\delta \omega^a(x)} = \tfrac{1}{2} i \sum_\mu \mathrm{Tr} \left\{ \left[U_\mu^G(x-2\hat{\mu}) U_\mu^G(x-\hat{\mu}) - U_\mu^G(x) U_\mu^G(x+\hat{\mu}) - \mathrm{h.c.} \right] T^a \right\} \tag{9}$$

and expanding to $\mathcal{O}(a^4)$ we obtain

$$\frac{\delta \mathcal{F}_2^G}{\delta \omega^a(x)} = 4ga^2 \sum_\mu \mathrm{Tr} \Bigg\{ \Bigg[\partial_\mu A_\mu(x) + \frac{a^2}{3} \partial_\mu^3 A_\mu(x) + \tfrac{16}{360} a^4 \partial_\mu^5 A_\mu(x) + \mathcal{O}(a^6) \Bigg] T^a \Bigg\} + \mathcal{O}(g^3 a^4), \tag{10}$$

which again implies the continuum Landau-gauge-fixing condition to lowest order in a.

The $\mathcal{O}(a^2)$ errors can be removed from the gauge fixing condition by taking a linear combination of the one-link and two-link functionals:

$$\frac{\delta \left\{ \tfrac{4}{3} \mathcal{F}_1^G - \dfrac{1}{12 u_0} \mathcal{F}_2^G \right\}}{\delta \omega^a(x)} = ga^2 \sum_\mu \mathrm{Tr} \Bigg\{ \Bigg[\partial_\mu A_\mu(x) - \tfrac{4}{360} a^4 \partial_\mu^5 A_\mu(x) + \mathcal{O}(a^6) \Bigg] T^a \Bigg\} + \mathcal{O}(g^3 a^4), \tag{11}$$

where we have introduced the mean-field (tadpole) improvement parameter u_0 to ensure that our perturbative calculation is not spoiled by large renormalisations, as explained by Lepage and Mackenzie (1993). For the tadpole-improvement parameter we employ the plaquette measure

$$u_0 = \left(\tfrac{1}{3}\mathcal{R}e\mathrm{Tr}\langle U_{\mathrm{pl}}\rangle\right)^{\frac{1}{4}} \tag{12}$$

and note that the higher order g^3a^4 terms of equations (6), (10) and (11) are to be viewed in terms of the mean-field-improved perturbation theory of Lepage and Mackenzie (1993). For future reference we shall define the improved functional, $\mathcal{F}^G_{\mathrm{imp}} \equiv \frac{4}{3}\mathcal{F}^G_1 - (1/12u_0)\mathcal{F}^G_2$.

Once a gauge-fixing functional has been defined, an algorithm must be chosen to perform the gauge fixing. We adopt a 'steepest descents' approach, like that used by Davies *et al.* (1988). Collecting terms of $\mathcal{O}(a^4)$ and higher into the $\mathcal{H}_i$, we define

$$\begin{aligned}\Delta_1(x) &\equiv \frac{1}{u_0}\sum_\mu \left[U_\mu(x-\mu) - U_\mu(x) - \text{h.c.}\right]_{\text{traceless}} \\ &= -2iga^2\sum_\mu \left\{\partial_\mu A_\mu(x) + \frac{a^2}{12}\partial^3_\mu A_\mu(x) + \mathcal{H}_1\right\}\ ,\end{aligned} \tag{13}$$

$$\begin{aligned}\Delta_2(x) &\equiv \frac{1}{4u_0^2}\sum_\mu \left[U_\mu(x-2\mu)U_\mu(x-\mu) - U_\mu(x)U_\mu(x+\mu) - \text{h.c.}\right]_{\text{traceless}} \\ &= -2iga^2\sum_\mu \left\{\partial_\mu A_\mu(x) + \frac{a^2}{3}\partial^3_\mu A_\mu(x) + \mathcal{H}_2\right\}\ ,\end{aligned} \tag{14}$$

$$\begin{aligned}\Delta_{\mathrm{imp}}(x) &\equiv \tfrac{4}{3}\Delta_1(x) - \tfrac{1}{3}\Delta_2(x) \\ &= -2iga^2\sum_\mu \left\{\partial_\mu A_\mu(x) + \mathcal{H}_{\mathrm{imp}}\right\},\end{aligned} \tag{15}$$

where the subscript 'traceless' denotes subtraction of the average of the colour-trace from each of the diagonal colour elements. The resulting gauge transformation is

$$\begin{aligned}G_i(x) &= \exp\left\{\frac{\alpha}{2}\Delta_i(x)\right\} \\ &= 1 + \frac{\alpha}{2}\Delta_i(x) + \mathcal{O}(\alpha^2),\end{aligned} \tag{16}$$

where α is a tuneable step-size parameter, and the index i is either 1, 2, or imp. At each iteration $G_i(x)$ is unitarised through an orthonormalisation procedure.

The gauge fixing algorithm proceeds by calculating the relevant Δ_i in terms of the mean-field-improved links, and then applying the associated gauge transformation, equation (16), to the gauge field. The algorithm is implemented in parallel, updating all links simultaneously, and is iterated until the lattice Landau gauge condition is satisfied, to within some numerical accuracy.

3. Discretisation Errors in the Gauge Fixing Condition

The approach to Landau gauge is usually measured by a quantity such as

$$\theta_i = \frac{1}{VN_c} \sum_x \mathrm{Tr}\left\{\Delta_i(x)\Delta_i(x)^\dagger\right\} , \tag{17}$$

which should tend to zero as the configuration becomes gauge fixed. Here N_c is the number of colours, i.e. 3.

A configuration fixed using $\Delta_1(x)$ will satisfy equation (7). Substituting (7) into equation (14) yields

$$\begin{aligned}\Delta_2(x) = & -2iga^2 \sum_\mu \left\{ -\frac{a^2}{12}\partial_\mu^3 A_\mu(x) + \frac{a^2}{3}\partial_\mu^3 A_\mu(x) - \mathcal{H}_1 + \mathcal{H}_2 \right\} \\ = & -2iga^2 \sum_\mu \left\{ \frac{a^2}{4}\partial_\mu^3 A_\mu(x) - \mathcal{H}_1 + \mathcal{H}_2 \right\}\end{aligned} \tag{18}$$

and similarly,

$$\Delta_{\mathrm{imp}}(x) = -2iga^2 \sum_\mu \left\{ -\frac{a^2}{12}\partial_\mu^3 A_\mu(x) - \mathcal{H}_1 + \mathcal{H}_{\mathrm{imp}} \right\} . \tag{19}$$

Since the improved measure has no $\mathcal{O}(a^2)$ error of its own, equation (19) provides an estimate of the absolute size of these discretisation errors.

4. Calculations on the Lattice

(4a) The Gauge Action

The $\mathcal{O}(a^2)$ tadpole-improved action is defined as

$$S_G = \frac{5\beta}{3} \sum_{\mathrm{pl}} \mathcal{R}e\mathrm{Tr}(1 - U_{\mathrm{pl}}(x)) - \frac{\beta}{12u_0^2} \sum_{\mathrm{rect}} \mathcal{R}e\mathrm{Tr}(1 - U_{\mathrm{rect}}(x)) , \tag{20}$$

where the operators $U_{\mathrm{pl}}(x)$ and $U_{\mathrm{rect}}(x)$ are defined as

$$U_{\mathrm{pl}}(x) = U_\mu(x)U_\nu(x+\hat{\mu})U_\mu^\dagger(x+\hat{\nu})U_\nu^\dagger(x) , \tag{21}$$

$$U_{\rm rect}(x) = U_\mu(x)U_\nu(x+\hat\mu)U_\nu(x+\hat\nu+\hat\mu)U_\mu^\dagger(x+2\hat\nu)U_\nu^\dagger(x+\hat\nu)U_\nu^\dagger(x)$$
$$+U_\mu(x)U_\mu(x+\hat\mu)U_\nu(x+2\hat\mu)U_\mu^\dagger(x+\hat\mu+\hat\nu)U_\mu^\dagger(x+\hat\nu)U_\nu^\dagger(x)\,. \quad (22)$$

The link product $U_{\rm rect}(x)$ denotes the rectangular 1×2 and 2×1 plaquettes. Equation (20) reproduces the continuum action as $a\to 0$, provided that β takes the standard value of $6/g^2$. The $\mathcal{O}(g^2a^2)$ corrections to this action are estimated to be of the order of two to three percent by Alford *et al.* (1995). Note that our $\beta = 6/g^2$ differs from that used in Alford *et al.* (1995), Lee and Leinweber (1999) and Fiebig and Woloshyn (1996). Multiplication of our β in equation (20) by a factor of $\frac{5}{3}$ reproduces their definition.

(4b) Numerical Simulations

Gauge configurations are generated using the pseudoheat-bath algorithm of Cabbibo and Marinari (1982) with three diagonal $SU(2)$ subgroups. The mean link, u_0, is averaged every 10 sweeps and updated during thermalisation.

For the exploration of gauge fixing errors we consider 6^4 lattices at a variety of β for both standard Wilson and improved actions. For the standard Wilson action we consider $\beta = 5\cdot 7$, $6\cdot 0$ and $6\cdot 2$, corresponding to lattice spacings of $0\cdot 18$, $0\cdot 10$ and $0\cdot 07$ fm respectively. For the improved action we consider $\beta = 3\cdot 92$, $4\cdot 38$ and $5\cdot 00$, corresponding to lattice spacings of approximately $0\cdot 3$, $0\cdot 2$ and $0\cdot 1$ fm respectively.

The configurations were gauge fixed, using conjugate gradient Fourier acceleration (suggested by Cucchieri and Mendes 1998), until $\theta_1 < 10^{-12}$. Then $\theta_{\rm imp}$ and θ_2 were measured to see the size of the residual higher order terms. The evolution of the gauge fixing measures is shown for one of the lattices in Fig. 1. This procedure was then repeated, fixing with each of the other two functionals, and the results are shown in Table 1. The same procedure was performed with three $\mathcal{O}(a^2)$-improved lattices, and the results are shown in Table 2.

Comparing equation (7) with (19), we can see that if we fix a configuration to Landau gauge by using the basic, one-link functional, the improved measure will consist entirely of the discretisation errors. Looking at Table 1, we see that at $\beta = 6\cdot 0$, $\theta_{\rm imp} = 0\cdot 058$, i.e.

$$\frac{1}{VN_c}\sum_x {\rm Tr}\left\{\sum_\mu \partial_\mu A_\mu(x)\left(\sum_\nu \partial_\nu A_\nu(x)\right)^\dagger\right\} = 0\cdot 058\,, \quad (23)$$

a substantial deviation from the continuum Landau gauge when compared with $\theta_1 < 10^{-12}$.

As a check of our simulations, we note that the definition for $\Delta_{\rm imp}$, equation (15), provides a constraint on the measures when gauge fixed. For example, we have

$$\frac{\theta_{\rm imp}}{\theta_2} = \frac{(-\frac{1}{12})^2}{(-\frac{1}{12}+\frac{1}{3})^2} = \tfrac{1}{9} \simeq 0\cdot 111\,. \quad (24)$$

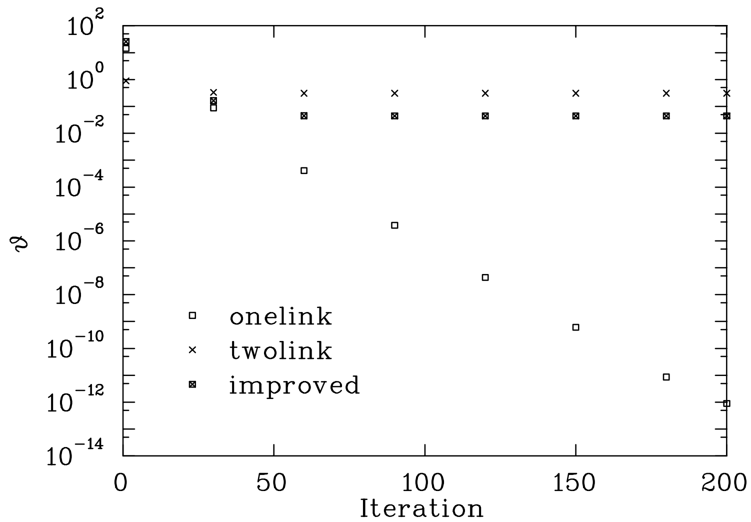

Fig. 1. Gauge fixing measures for a 6^4 lattice with Wilson action at $\beta = 6{\cdot}0$. This lattice was gauge fixed with Δ_1, so θ_1 drops steadily whilst θ_2 and θ_{imp} plateau at much higher values.

Table 1. Values of the gauge-fixing measures obtained using the Wilson gluon action on 6^4 lattices at three values of the lattice spacing, fixed to Landau gauge with the one-link, two-link and improved functionals respectively

β	u_0	Functional	θ_{imp}	θ_2	$(\theta_{\text{imp}}/\theta_2)$
5·7	0·865	1	0·0679	0·611	0·111
6·0	0·877	1	0·0578	0·520	0·111
6·2	0·886	1	0·0522	0·469	0·111
β	u_0	Functional	θ_{imp}	θ_1	$(\theta_1/\theta_{\text{imp}})$
5·7	0·865	2	59·0	33·2	0·563
6·0	0·877	2	65·1	36·6	0·563
6·2	0·886	2	61·7	34·7	0·563
β	u_0	Functional	θ_1	θ_2	(θ_1/θ_2)
5·7	0·865	imp	0·0427	0·684	0·0625
6·0	0·877	imp	0·0367	0·588	0·0625
6·2	0·886	imp	0·0332	0·531	0·0625

Similarly, by fixing with $\Delta_2(x)$ we expect

$$\frac{\theta_1}{\theta_{\text{imp}}} = \frac{(-\frac{1}{3}+\frac{1}{12})^2}{(-\frac{1}{3})^2} = \tfrac{9}{16} \simeq 0{\cdot}563\,, \tag{25}$$

and fixing with $\Delta_{\text{imp}}(x)$ leads to

$$\frac{\theta_1}{\theta_2} = \tfrac{1}{16} = 0{\cdot}0625\,. \tag{26}$$

Table 2. Values of the gauge-fixing measures obtained using the improved gluon action on 6^4 lattices at three values of the lattice spacing, fixed to Landau gauge with the one-link, two-link and improved functionals respectively

β	u_0	Functional	$\theta_{\rm imp}$	θ_2	$(\theta_{\rm imp}/\theta_2)$
3·92	0·837	1	0·102	0·921	0·111
4·38	0·880	1	0·0585	0·526	0·111
5·00	0·904	1	0·0410	0·369	0·111
β	u_0	Functional	$\theta_{\rm imp}$	θ_1	$(\theta_1/\theta_{\rm imp})$
3·92	0·837	2	57·5	32·3	0·563
4·38	0·880	2	53·4	30·0	0·563
5·00	0·904	2	52·2	29·4	0·563
β	u_0	Functional	θ_1	θ_2	(θ_1/θ_2)
3·92	0·837	imp	0·0638	1·02	0·0625
4·38	0·880	imp	0·0366	0·586	0·0625
5·00	0·904	imp	0·0261	0·417	0·0625

These ratios are reproduced by the data of Tables 1 and 2.

A three-link functional can also be constructed, e.g.

$$\mathcal{F}_3^G[\{U\}] = \sum_{\mu,x} \tfrac{1}{2}\mathrm{Tr}\left\{U_\mu^G(x-\mu)U_\mu^G(x)U_\mu^G(x+\mu) + \mathrm{h.c.}\right\}\,, \tag{27}$$

the functional derivative of which

$$\frac{\delta\mathcal{F}_3^G}{\delta\omega^a(x)} = \tfrac{1}{2}i\sum_\mu \mathrm{Tr}\{[U_\mu^G(x-3\mu)U_\mu^G(x-2\mu)U_\mu^G(x-\mu) - U_\mu^G(x)U_\mu^G(x+\mu)U_\mu^G(x+2\mu) - \mathrm{h.c.}]T^a\} \tag{28}$$

leads to

$$\Delta_3(x) = -2iga^2\sum_\mu \{\partial_\mu A_\mu(x) + \tfrac{3}{4}a^2\partial_\mu^3 A_\mu(x) + \tfrac{9}{40}a^4\partial_\mu^5 A_\mu(x) + \mathcal{O}(a^6)\} + \mathcal{O}(g^3a^4)\,. \tag{29}$$

If leading order errors dominate, then we should be able to make ratios like those above, but involving θ_3. However, we find that the values taken from our simulations are very different from ratios based solely on leading, $\mathcal{O}(a^2)$ errors. This indicates that the sum of higher-order errors is also significant.

Whilst one could proceed to combine Δ_1, Δ_2 and $\Delta_{\rm imp}$ to eliminate both $\mathcal{O}(a^2)$ and $\mathcal{O}(a^4)$, it is likely that $\mathcal{O}(g^2a^2)$ errors are of similar size to the $\mathcal{O}(a^4)$ errors. We will defer such an investigation to future work.

A configuration fixed using $\Delta_{\rm imp}(x)$ will satisfy

$$\sum_\mu \partial_\mu A_\mu(x) = \sum_\mu \{-\mathcal{H}_{\rm imp}\}\,. \tag{30}$$

Substituting this into equation (13) yields

$$\Delta_1(x) = -2iga^2 \sum_\mu \left\{ \frac{a^2}{12} \partial_\mu^3 A_\mu(x) + \mathcal{H}_1 - \mathcal{H}_{\text{imp}} \right\} . \tag{31}$$

A comparison of this equation with (19) reveals that the coefficients of the terms in curly brackets, expressing the discretisation errors in these two cases, differ only by an overall sign, which is lost in the calculation of the corresponding θ_i. If the three different methods presented all fixed in exactly the same way, then the θ_{imp} of a configuration fixed with Δ_1, would be equal to θ_1 when the configuration is fixed with Δ_{imp}. It is clear from the tables that they are not, signaling the higher-order derivative terms $\partial_\mu^n A_\mu(x)$ take different values depending on the gauge fixing functional used.

Examining the values in Tables 1 and 2 reveals that in every case θ_1 is smaller when we have fixed with the improved functional than θ_{imp} under the one-link functional. This suggests that the additional long range information used by the improved functional is producing a gauge fixed configuration with smaller, higher-order derivatives; a secondary effect of improvement.

Equally, one can compare the value of θ_2 when fixed using the one-link functional, and θ_1 when fixed using the two-link functional. In this case, their differences are rather large and are once again attributed to differences in the size of higher-order derivatives of the gauge field. The two-link functional is coarser, knows little about short range fluctuations, and fails to constrain higher-order derivatives. Similar conclusions are drawn from a comparision of θ_2 fixed with the improved functional and θ_{imp} fixed with the two-link functional.

It is also interesting to note that in terms of the absolute errors, the Wilson action at $\beta = 6{\cdot}0$ is comparable to the improved lattice at $\beta = 4{\cdot}38$, where the lattice spacing is three times larger.

5. Conclusions

We have fixed gluon field configurations to Landau gauge by three different functionals: one-link and two-link functionals, both with $\mathcal{O}(a^2)$ errors, and an improved functional, with $\mathcal{O}(a^4)$ errors. Using these functionals we have devised a method for estimating the discretisation errors involved. Our results indicate that order $\mathcal{O}(a^2)$ improvement of the gauge fixing condition will improve comparison with the continuum Landau gauge in two ways: (1) through the elimination of $\mathcal{O}(a^2)$ errors and (2) through a secondary effect of reducing the size of higher-order errors. These conclusions are robust with respect to lattice spacing and we have also verified the stability of our conclusions by considering additional configurations to that presented here. We plan to investigate improved gauge fixing on larger volume lattices to see if these effects of improvement persist. Lattice Landau gauge, in its standard implementation, is substantially different from its continuum counterpart, despite fixing the Lattice gauge condition to one part in 10^{12}.

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