Perturbative and Non-perturbative Lattice Calculations for the Study of Parton Distributions

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We discuss how lattice calculations can be a useful tool for the study of structure functions. Particular emphasis is given to the perturbative renormalization of the operators.

1. INTRODUCTION

Lattice QCD provides non-perturbative techniques for the computation of the Mellin moments of the structure functions of hadrons from first principles, without model assumptions. Many results have been obtained in the past years from the lattice, and include the calculation of the lowest moments of various structure functions of the quarks: the unpolarized structure functions, the spin-dependent structure functions $g_1$ and $g_2$, and the transversity structure function $h_1$.

Lattice perturbation theory is essential for the renormalization of the relevant operators. Perturbative calculations of renormalization factors have been carried out for the lowest three moments of all structure functions, in the case of Wilson and also of overlap fermions (which do not break chiral symmetry). For many operators these renormalization factors are also known in the improved theory. Perturbative renormalization factors have also been calculated for some higher-twist matrix elements (4-quark operators).

2. STRUCTURE FUNCTIONS

It is not possible to compute a complete structure function directly on the lattice (which is set up in Euclidean space). The reason is that the structure functions describe the physics close to the light cone, and this region of Minkowski space shrinks to a point when one goes to Euclidean space, where Monte Carlo simulations are performed. However, on a Euclidean lattice it is possible to compute the moments of the structure functions, using the operator product expansion:

$$\int_0^1 x^n F(x, Q^2) \sim C^{(n,i)} \frac{Q^2}{\mu^2} \cdot \langle h | O^{(n,i)}(\mu) | h \rangle.$$ 

The Wilson coefficients contain the short-distance physics, and can be perturbatively computed in the continuum. The matrix elements contain the long-distance physics, and can computed using numerical simulations, supplemented by a lattice renormalization of the relevant operators.

Operators of twist two (twist: dimension minus spin) dominate the expansion above. Moments of the unpolarized structure functions (which give the unpolarized distribution $q$), of the spin-dependent structure functions $g_1$ (which gives the helicity distribution $\Delta q$) and $g_2$, and of the transversity structure function $h_1$ (which gives the transversity distribution $\delta q$) are measured by towers of hadronic matrix elements:

$$\langle x^n \rangle \sim \langle h | \bar{\psi} \gamma_{(\mu} D_{\mu_1} \cdots D_{\mu_n)} \psi | h \rangle$$
$$\langle (\Delta x)^n \rangle \sim \langle h | \bar{\psi} \gamma_5 \gamma_{(\mu} D_{\mu_1} \cdots D_{\mu_n)} \psi | h \rangle$$
$$\langle x^n \rangle g_2 \sim \langle h | \bar{\psi} \gamma_{(\mu} \gamma_{(\nu} \gamma_{(\sigma} D_{\mu_1} D_{\nu_1} \cdots D_{\mu_n)} D_{\sigma_1} \psi | h \rangle$$
$$\langle (\delta x)^n \rangle \sim \langle h | \bar{\psi} \gamma_5 \sigma_{(\mu} D_{\mu_1} \cdots D_{\mu_n)} \psi | h \rangle.$$

3. OPERATOR RENORMALIZATION

To obtain physical continuum matrix elements from the lattice, the results of Monte Carlo simulations need to be renormalized from the lattice to a continuum scheme. To obtain these renormalization factors one has to compute 1-loop ma-
trix elements on the lattice as well as in the continuum. The lattice operators at tree level, for \( p \ll \pi/a \), have the same matrix elements as the original continuum operators, so that at 1 loop

\[
\langle O_{i}^{\text{lat}} \rangle = \frac{g_{0}^{2}}{16\pi^{2}} \left( -\gamma_{ij} \log a^{2}p^{2} + R_{ij}^{\text{lat}} \right) \langle O_{j}^{\text{tree}} \rangle
\]

\[
\langle O_{i}^{\text{cont}} \rangle = \frac{g_{0}^{2}}{16\pi^{2}} \left( -\gamma_{ij} \log \frac{p^{2}}{\mu^{2}} + R_{ij}^{\text{cont}} \right) \langle O_{j}^{\text{tree}} \rangle,
\]

where for the continuum one chooses the \( \overline{\text{MS}} \) scheme, since the Wilson coefficients are known in this scheme. In general \( R_{ij}^{\text{lat}} \neq R_{ij}^{\text{cont}} \), and the 1-loop renormalization factors on the lattice and in the continuum are different. The anomalous dimensions are equal, and thus for \( \mu = 1/a \) only a finite renormalization connects the two schemes. The matching between Monte Carlo numbers and the renormalized physical results is then

\[
\langle O_{i}^{\text{cont}} \rangle = \left( \delta_{ij} - \frac{g_{0}^{2}}{16\pi^{2}} \left( R_{ij}^{\text{lat}} - R_{ij}^{\text{cont}} \right) \right) \langle O_{j}^{\text{lat}} \rangle.
\]

Since Lorentz symmetry is broken on the lattice (which is invariant under the hypercubic group), and for Wilson fermions also chiral symmetry, the mixing of operators under renormalization is more complicated than in the continuum theory. Operators multiplicatively renormalizable in the continuum may mix with other operators when they are put on the lattice. Sometimes these mixing coefficients are even power divergent, that is they behave like \( 1/a^{n} \). In general then the matching factors \( R_{ij}^{\text{lat}} - R_{ij}^{\text{cont}} \) are not square matrices.

4. WILSON FERMIONS

Most calculations are done using the discretization of the (Euclidean) QCD action proposed by Wilson. Wilson fermions however break chiral symmetry, and this causes an additive mass renormalization even for a zero bare mass, and a heavy pion (\( m_{\pi} \sim 500 \) MeV). Extrapolations to the chiral limit are then needed, and this source of systematic errors has to be controlled.

Lattice perturbation theory is quite cumbersome: there are more vertices and more diagrams than in the continuum, the expressions contain a huge number of terms, and the integrals are more complicated. The Wilson quark propagator is

\[
\delta^{ab} \frac{-i}{\pi} \frac{1}{6\pi^{2}} \left( \frac{\gamma_{\mu} \sin \alpha k_{\mu} + \alpha f \left[ \sum_{\mu} \sin^{2} \frac{\alpha k_{\mu}}{2} \right] }{\left[ 2 \sum_{\mu} \sin^{2} \frac{\alpha k_{\mu}}{2} + \alpha f \right]^{2}} \right),
\]

which in the continuum limit gives

\[
\delta^{ab} \frac{-i}{\pi} \frac{1}{6\pi^{2}} \left( \frac{\gamma_{\mu} \sin \alpha k_{\mu} + \alpha f \left[ \sum_{\mu} \sin^{2} \frac{\alpha k_{\mu}}{2} \right] }{\left[ 2 \sum_{\mu} \sin^{2} \frac{\alpha k_{\mu}}{2} + \alpha f \right]^{2}} \right),
\]

and the gluon propagator (in covariant gauge) is

\[
\frac{\delta^{ab}}{a^{2}} \left( \frac{\sin \frac{\alpha k_{\mu}}{2}}{\sum_{\mu} \sin^{2} \frac{\alpha k_{\mu}}{2}} \right) \left( \frac{\sin \frac{\alpha k_{\nu}}{2}}{\sum_{\mu} \sin^{2} \frac{\alpha k_{\mu}}{2}} \right).
\]

The lattice theory has exact gauge invariance at any finite \( a \). This causes the presence in the action of the group elements \( U_{\mu} = \exp(iq_{0}A_{\mu}) \) instead of the algebra elements \( A_{\mu} \). One has then to expand the \( U_{\mu} \)'s in terms of the \( A_{\mu} \)'s, and this generates an infinite number of vertices, of which only a finite number is needed at any given order in \( g_{0} \). The quark-quark-gluon vertex is

\[
-i g_{0} (t^{a})^{bc} \left( \frac{\sin \alpha s_{0}}{2} + r \frac{\cos \alpha s_{0}}{2} \right),
\]

(1)

where \( s = p_{1} + p_{2} \), the momenta of the quarks, which for \( a \rightarrow 0 \) gives \(-g_{0} (t^{a})^{bc} i \gamma_{\mu} \), while the quark-quark-gluon-gluon vertex is

\[
-\frac{1}{2} a_{g}^{2} \delta_{\mu \nu} \{ t^{a}, t^{b} \}^{cd} \left( i \gamma_{\mu} \sin \frac{\alpha s_{0}}{2} + r \cos \frac{\alpha s_{0}}{2} \right). \]

(2)

This is an irrelevant vertex (is zero in the continuum limit), but still gives non-vanishing contributions to Feynman diagrams in divergent loops.

Also in the pure gauge part there is an infinite number of vertices. The 3-gluon vertex is

\[
-i g_{0} f^{abc} \left\{ \delta_{\mu \nu} \frac{\sin \alpha (k - p)_{\mu}}{2} \cos \frac{ak_{\nu}}{2} \right. + \delta_{\nu \rho} \frac{\sin \alpha (p - q)_{\nu}}{2} \cos \frac{ak_{\rho}}{2} \left. + \delta_{\rho \mu} \frac{\sin \alpha (q - k)_{\rho}}{2} \cos \frac{ak_{\mu}}{2} \right\},
\]

which in the continuum limit becomes

\[
i g_{0} f^{abc} \left\{ \delta_{\mu \nu} (k - p)_{\rho} + \delta_{\nu \rho} (p - q)_{\mu} + \delta_{\rho \mu} (q - k)_{\nu} \right\}.
\]
The 4-gluon vertex is too complicated to be reported here. Furthermore, the gauge measure at order $g_0^2$ gives a $1/a^2$ mass counterterm. Finally, using a Faddeev-Popov procedure one can obtain the Feynman rules for the ghost propagator and the ghost interactions. The effective ghost-gauge field interaction is not linear in the gauge potential $A_\mu$, and thus also in this sector new vertices appear that have no continuum analog, like the ghost-ghost-gluon-gluon vertex.

5. OVERLAP FERMIONS

A Dirac operator $D = \gamma_\mu D_\mu$ which satisfies the Ginsparg-Wilson relation $\gamma_5 D + D \gamma_5 = a/\rho D \gamma_5 D$ defines fermions with maintain an exact chiral symmetry also for non-zero lattice spacing and also keep all other fundamental properties.

One of the possible solutions of the Ginsparg-Wilson relation is given by overlap fermions. In the massless case the overlap-Dirac operator is

$$D_N = \frac{1}{a} \rho \left[ 1 + \frac{X}{\sqrt{X^\dagger X}} \right], \quad X = D_W - \frac{1}{a} \rho,$$

where $D_W$ is the Wilson-Dirac operator. For $0 < \rho < 2r$ one has the right spectrum of massless fermions. Additive mass renormalization is then forbidden, and one avoids a source of systematic errors always present using Wilson fermions.

The massless quark propagator in the overlap is more complicated than in Wilson, and is

\[
\delta_{ab} \left( \frac{-i \sum_\mu \gamma_\mu \sin ak_\mu}{2 \rho (\omega(k) + b(k))} + \frac{a}{2} \right),
\]

where $b(k) = 1/a \left( 2r \sum_\mu \sin^2 ak_\mu / 2 - \rho \right)$,

$$\omega(k) = \sqrt{X^\dagger(k)X_0(k)},$$

and

$$X_0(k) = \frac{1}{a} \left( i \sum_\mu \gamma_\mu \sin ak_\mu + 2r \sum_\mu \sin^2 \frac{ak_\mu}{2} - \rho \right).$$

The overlap vertices can be expressed in terms of the vertices of the QED Wilson action $W_{1\mu}$ and $W_{2\mu}$, which are the vertices (4) and (5) without the color matrices, and of the quantity $X_0$. For example, the quark-quark-gluon-gluon vertex is

\[
-\frac{1}{\omega(p_1) \omega(p_2)} X_0(p_2) W_{1\mu}^\dagger(p_1, p_2) X_0(p_1).
\]

The quark-quark-gluon-gluon vertex is very long and will not be given here (see for example (1)).

6. IMPROVEMENT

It is very expensive to decrease the errors due to the granularity of the lattice just by reducing the lattice spacing $a$, because the cost would grow like $a^{-5}$ in the quenched theory, and in full QCD it would grow even faster. Halving the discretization errors in this way would then be at least 30 times more expensive. A more effective way is to improve actions and operators.

$O(a)$ improvement removes the contributions of order $a$ to the systematic error arising from the finiteness of the lattice spacing by adding a counterterm to the fermion action, so that

$$\langle p | \hat{O}_L | p' \rangle_{\text{MC}} = a^d \left[ \langle p | \hat{O} | p' \rangle_{\text{ph}} + O(a^2) \right].$$

For Wilson fermions, this is achieved in on-shell matrix elements adding a counterterm whose coefficient $c_{\text{sw}}$ has to be exactly tuned. Only for its appropriate value, for a given $g_0$, the $O(a)$ effects are canceled and one gets a faster convergence to the continuum limit. Due to this action counterterm one has to add to the Wilson vertex (6) the improved quark-quark-gluon interaction vertex

\[
-(c_{\text{sw}} + g_0) r D^b c \cdot \cos \frac{aq_\mu}{2} \sum_\lambda \sigma_{\mu\lambda} a q_\lambda,
\]

where $q$ is the difference between the incoming and outgoing momenta of the quarks. In addition to this, one also has to improve the various operators, that is one must add a basis of higher dimensional (irrelevant) operators with the same quantum numbers, with $\dim(\hat{O}_i) = \dim(O) + 1$:

$$O \rightarrow O^{\text{imp}} = (1 + b_0 a m) O + a \sum_i c_i \hat{O}_i.$$

The $O(a)$ improvement for overlap fermions is much simpler. The action is already improved,\footnote{The fermion propagator and the vertices with an even number of gluons are instead not modified by the improvement. Neither is the gluon propagator: the first corrections to the pure gauge action are already of order $a^2$.}
and thus there is no need of new interactions. The improved operators are given, to all orders, by

\[ O^{\text{imp}} = \bar{\psi} \left( 1 - \frac{1}{2\rho} a D_N \right) \tilde{O} \left( 1 - \frac{1}{2\rho} a D_N \right) \psi \]

(while for Wilson fermions the improvement construction is different for each operator). One thus gets full \( O(a) \) improvement without tuning any coefficients, and to all orders of perturbation theory. For Wilson fermions, instead, one has to determine the coefficients of the operator counterterms order by order in perturbation theory.\footnote{This appears to be a difficult task, and even for the first moment of unpolarized distributions all lowest-order improvement coefficients have not yet been determined.}

7. FORM CODES

Due to the complexity of the calculations, to the possible great number of diagrams, and above all to the huge amount of terms in each diagram, computer codes have to be used. To evaluate the Feynman diagrams and obtain the algebraic expressions for the renormalization factors, we have thus developed sets of computer codes written in the symbolic manipulation language FORM. These codes take as input the Feynman rules for the particular combination of operators, propagators (Wilson or overlap) and vertices (Wilson, improved, or overlap) appearing in each diagram, expand them in the lattice spacing \( a \), evaluate the gamma algebra on the lattice, and then work out everything until the final expressions are obtained. The main difficulty in developing such codes is that the (Euclidean) Lorentz group \( O(4) \) breaks down to the hypercubic group \( W_4 \). A representation which is irreducible under the (Euclidean) Lorentz group is thus in general reducible under the symmetry group of the lattice. This gives rise to a whole new class of problems, of which the most serious concerns the Einstein summation convention.

The FORM language has been developed having in mind the usual continuum calculations. There are therefore many useful built-in features which are sometimes somewhat of an hindrance when one tries to perform lattice perturbative calculations. A blind use of them would give, for example,

\[ \sum_{\lambda} \gamma_{\lambda p} \sin k_{\lambda} \rightarrow \gamma' \sin k_{\lambda}. \]

One thus needs to develop special routines to cope with the gamma algebra on the lattice.

Integrals are done over the first Brillouin zone

\[ \int_{-\frac{\pi}{a}}^{\frac{\pi}{a}} \frac{d^4k}{(2\pi)^4} f(ak, ap) \rightarrow \int_{-\pi}^{\pi} \frac{d^4k'}{(2\pi)^4} a^{-4} f(k', ap) \]

with the rescaling \( k' = ak \), and in general an expansion in \( ap \) is needed. FORM codes become then necessary also because of the huge number of terms arising from the Taylor expansions of the Fourier transforms of operators, propagators, vertices and covariant derivatives. The \( n \)-th moment of a parton distribution behaves like

\[ \langle \bar{\psi} \Gamma D_{\mu_1} \cdots D_{\mu_n} \psi \rangle \sim \frac{1}{a^n}, \]

because \( D \sim 1/a \), and thus one has to perform an expansion in \( a \) to order \( n \) for every quantity. For example, the Wilson quark propagator to \( O(a) \) is

\[ \delta^{ab} D^{-1}(k) \left\{ \left( -i \sum_{\mu} \gamma_{\mu} \sin k_{\mu} + 2r \sum_{\mu} \sin^2 \frac{k_{\mu}}{2} \right) \right. \]

\[ + a \cdot \left( -i \sum_{\mu} \gamma_{\mu} q_{\mu} \cos k_{\mu} + r \sum_{\mu} q_{\mu} \sin k_{\mu} + m_f \right) \]

\[ - D^{-1}(k) \left( -i \sum_{\rho} \gamma_{\rho} \sin k_{\rho} + 2r \sum_{\rho} \sin^2 \frac{k_{\rho}}{2} \right) \]

\[ \times \left( 2 \sum_{\mu} q_{\mu} \sin k_{\mu} \cos k_{\mu} \right) \]

\[ + \left. 4r \sum_{\mu} \sin^2 \frac{k_{\mu}}{2} \left( r \sum_{\nu} q_{\nu} \sin k_{\nu} + m_f \right) \right\}, \]

where the denominator is

\[ D(k) = \sum_{\mu} \sin^2 k_{\mu} + \left( 2r \sum_{\mu} \sin^2 \frac{k_{\mu}}{2} \right)^2. \]

As a consequence, a huge number of terms appear (at least in the initial stages of the manipulations), and also the gamma algebra becomes quite cumbersome to do by hand. All this also implies a limitation on the number of moments of structure functions that one can compute.\footnote{This comes on top of the limitation coming from operator...}
8. RESULTS

We have calculated the renormalization in the MS scheme of several operators measuring the lowest moments of structure functions [3, 4]. In some cases for a given moment we have computed two operators, labeled (a) and (b), which belong to two different representations of the discrete Euclidean Lorentz group (see Table 1). Operator mixing for overlap fermions is simpler than for Wilson fermions: chiral symmetry is not broken and thus it prohibits any mixing with operators of different chirality. Mixing coefficients which are power-divergent like $a^{-n}$ in the continuum limit can be eliminated from the start from overlap calculations if the corresponding operators belong to multiplets with the wrong chirality. In the Wilson case, indeed, the operators measuring the moments of the $g_2$ structure function present additional mixings with wrong-chirality operators with power-divergent coefficients. Furthermore, the $Z'$s of the $n$-th moments of $q$ and $\Delta q$ are not constrained to be equal anymore.

For reasons of computing power, structure functions have been studied mostly in the quenched approximation, and only recently computations in full QCD have become feasible. On the lattice the Grassmann variables have to be analytically integrated, and the partition function

$$ Z = \int DUD\bar{\psi}e^{-S_{q}[U]+\bar{\psi}(\mathcal{D}[U]+m_f)\psi} $$

becomes in the simulations

$$ Z = \int D\mathcal{D} det(\mathcal{D}[U]+m_f)e^{-S_{q}[U]} , $$

which is equivalent to use an effective action

$$ S_{eff}[U] = S_q[U] - \ln det(\mathcal{D}[U]+m_f) . $$

Quenching amounts to doing simulations with $det(\mathcal{D}[U]+m_f) = 1$. This means that there are no sea quarks: all internal quark loops are neglected. Although it looks quite drastic, it is not a bad approximation for many physical quantities, and apparently (as it has been understood recently) also for structure functions.

Table 1
Renormalization constants of multiplicatively renormalized structure function operators, for $a = 0.1 \text{ fm}$, in the MS scheme.

| moment | overlap Wilson |
|--------|----------------|
| $\rho = 1.0$ | $\rho = 1.9$ |
| $\langle x \rangle_q$ | 1.41213 | 1.21841 | 0.98920 |
| $\langle x \rangle_{\Delta q}$ | 1.41213 | 1.21841 | 0.99709 |
| $\langle x \rangle_{\Delta q}$ | 1.40847 | 1.21309 | 0.97837 |
| $\langle x \rangle_{\delta q}$ | 1.51968 | 1.32436 | 1.09763 |
| $\langle x^2 \rangle_{\Delta q}$ | 1.51968 | 1.32436 | 1.10231 |
| $\langle x^3 \rangle_{\Delta q}$ | 1.61872 | 1.42279 | 1.19722 |
| $\langle x^3 \rangle_{\Delta q}$ | 1.61872 | 1.42279 | 1.20040 |
| $\langle x^3 \rangle_{\Delta q}$ | 1.63737 | 1.44159 | 1.21534 |
| $\langle x^3 \rangle_{\Delta q}$ | 1.63737 | 1.44159 | 1.21944 |
| $\langle x \rangle_{g_2}$ | 1.34794 | 1.18456 | mixing |
| $\langle x^2 \rangle_{g_2}$ | 1.47816 | 1.30997 | mixing |
| $\langle x^3 \rangle_{g_2}$ | 1.58943 | 1.41900 | mixing |
| $\langle 1 \rangle_{\delta q}$ | 1.27252 | 1.08648 | 0.85631 |
| $\langle x \rangle_{\delta q}$ | 1.41153 | 1.21851 | 0.99559 |
| $\langle x^2 \rangle_{\delta q}$ | 1.51865 | 1.32355 | 1.10021 |
The disconnected diagrams are however flavor independent, and do not contribute to the difference between $u$ and $d$ structure functions (for $SU(2)$ degeneracy). This means that quantities like $g_A = \Delta u - \Delta d$ and $\langle x^n \rangle_{u-d}$ do not receive contributions from disconnected diagrams. Their lattice results seem also to be closer to the experimental numbers.

The chiral extrapolations of the lattice data linear in $m_q \sim m_\pi^2$ could also be responsible for the discrepancies with experiment. It has been recently suggested that extrapolations using chiral perturbation theory could solve these discrepancies (see [6] and references therein). In fact, the pion cloud of the nucleon is not adequately described by current lattices. Extrapolation formulae which use chiral perturbation theory look like

$$\langle x^n \rangle_{u-d} = A_n \left[ 1 - \frac{(3g_A^2 + 1)}{4\pi f_\pi} m_\pi^2 \ln \left( \frac{m_\pi^2}{m_\pi^2 + \Lambda^2} \right) \right]$$

$$+ B_n (m_\pi r_0)^2 + C_n (a/r_0)^2,$$

where $\Lambda$ is a phenomenological cutoff related to the size of the source generating the pion cloud.

These extrapolation formulae seem able to resolve the discrepancy with experiment. However, results can be reproduced only with $\Lambda$’s with a range so wide to have no predictive power, and the currently available lattice data do not even discriminate between linear and chiral perturbation theory fits. The problem is that the available pions are not sufficiently light. A smaller pion mass ($m_\pi < 250 \text{ MeV}$) is needed before the parameters of the chiral expansions can be well determined on the lattice. Such calculations require about 8 Teraflops for one year. The next generation of computers, coming in a couple of years, will be able to perform these calculations.

There is no doubt that the pion cloud of the proton is very important. For it to be adequately included in the lattice box and properly measured in Monte Carlo simulations, the pion correlation length should be much smaller than the lattice size. This points to the use of larger lattices.

Higher-twist corrections have also been studied [5]. The lattice results for the twist four $(1/Q^2)$ corrections are (in a few particular cases) quite small. The renormalization factors of four-quark operators like $\sum_{a} \bar{\psi} \gamma_\mu \gamma_5 t^a \psi \cdot \bar{\psi} \gamma_\nu \gamma_5 t^a \psi$ have been calculated in perturbation theory, and the twist-4 results for the first moment of the unpolarized pion and proton structure functions turn out to be much smaller than the corresponding twist-2 matrix elements computed on the lattice, and also smaller than the phenomenological numbers. These are not however complete and systematic studies, like the ones concerning leading-twist operators. Only particular flavor and isospin combinations could be considered, to avoid mixing with lower-dimensional operators.

9. CONCLUSIONS

The lattice provides invaluable techniques for investigating moments of structure functions non-perturbatively from first-principles. The matching to the MS scheme is done by computing renormalization factors in perturbation theory (Wilson and overlap). Simulations with Wilson fermions are now also performed in full QCD, but many discrepancies between lattice and experiment remain. More control on the systematic errors is required.

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