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Proton Spin Structure from Monte Carlo Global Qcd Analyses

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Proton Spin Structure from Monte Carlo Global QCD Analyses

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APPROVAL PAGE

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the requirements for the degree of

Doctor of Philosophy

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ABSTRACT

Although significant progress has been made in recent years in understanding the composition of the proton’s spin from its quark and gluon constituents, a complete picture has yet to emerge. Such information is encoded in spin-dependent parton distribution functions (PDFs) that, as a consequence of being inherently nonperturbative, must be extracted through global QCD analyses of polarized lepton-nucleon and proton-proton collisions. Experiments that measure a final state hadron from these reactions are particularly useful for separating the individual quark and anti-quark polarizations, but require knowledge of parton-to-hadron fragmentation functions (FFs) to describe theoretically.

In this thesis, we present a new approach to global QCD analyses, that were performed recently by the Jefferson Lab Angular Momentum (JAM) Collaboration to determine the spin PDFs and FFs from deep inelastic scattering (DIS), semi-inclusive DIS, and single inclusive electron-positron annihilation observables. While previous global QCD studies typically used a single $\chi^2$ minimization procedure, the JAM Collaboration applies a robust Monte Carlo fitting methodology to extract the central values and uncertainties of the relevant distributions. The results from these JAM global QCD analyses, which include a first ever simultaneous fit of the spin PDFs and FFs, resolve a long-standing puzzle regarding the strange quark polarization and provide new information about the proton spin structure.
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PROTON SPIN STRUCTURE FROM MONTE CARLO GLOBAL QCD ANALYSES
CHAPTER 1

Introduction

The discovery of the nucleus by Rutherford in the early 20th century was a crucial turning point in our understanding of atomic structure. The collection of positively charged protons in the nucleus contradicted what was understood about the electromagnetic force: that particles of like charge repel one another. Clearly there existed an additional force, one that acted more strongly over smaller distance scales, that bound the protons and neutrons in the nucleus together. The following decades of particle scattering experiments revealed that these protons and neutrons, or nucleons, were not fundamental particles, but instead constructed of point-like constituents known as quarks. A picture of the nucleon as a dynamical system of these quarks, which carry a quantum property called color, and their interactions via gluons, the particle mediating the strong force, quickly emerged as the leading explanation for the formation of nucleons and nuclei. Thus, quantum chromodynamics (QCD) was born as the theory that describes the interactions of quarks and gluons, the constituents of all atomic nuclei.
1.1 Perturbative QCD and Factorization

Before discussing further about the structure of the nucleon, it is important to understand two defining features of QCD, namely confinement and asymptotic freedom. Both can be understood by considering the strength of the quark-gluon interactions \( g_s \), or more commonly the QCD strong coupling \( \alpha_s = g_s^2/(4\pi) \), a function that depends on the number of active quark flavors \( N_f \) and a renormalization scale \( \mu_R \) that arises from regulating ultraviolet divergences. In energy regions where the number of quark flavors is constant, the approximate analytical solution for \( \alpha_s \) at lowest order is

\[
\alpha_s(\mu_R) \simeq \frac{12\pi}{(11C_A - 4N_fT_R)\ln(\mu_R^2/\Lambda^2)} \tag{1.1}
\]

where \( C_A \) and \( T_R \) are SU(3) color factors [1]. The additional scale \( \Lambda \) is a QCD constant of integration, and indicates the region in which \( \alpha_s \) becomes divergent (\( \mu_R \sim \Lambda \)). By setting the renormalization scale to the momentum transfer of a particle scattering process, \( \mu_R = Q \), it becomes clear that there are two distinct regions for the strength of the coupling.

At sufficiently high energies (\( \Lambda \ll Q \)), or very small distance scales, the coupling becomes small and the quarks can be treated essentially as free particles in the nucleon. This is known as asymptotic freedom, and is the basis of perturbative QCD (pQCD). Within the pQCD framework, experimental observables can be formulated as a series expansion in \( \alpha_s \). Such predictive power is lost, however, if the scale of the reaction becomes small (\( Q \sim \Lambda \)). This is the region of confinement, and, as the name suggests, is the reason why free quarks and gluons have not been observed directly. The nonperturbative region of QCD has yet to be fully understood, especially the process in which the quarks and gluons become hadrons, and remains an important challenge for QCD studies such as this work.
The structure of the nucleon in terms of its constituent quarks and gluons, or more generally partons, can be determined from high energy particle collisions where the reactions can be described from pQCD. However, even in pQCD calculations of observables, one finds large logarithms that spoil the convergence of the perturbative series (i.e. logarithms that depend on a scale that is of the order $\Lambda$ in the definition of the strong coupling). This is supported by the fact that experiments can only measure bound state hadrons, and therefore observables must have dependence on the long-distance energy scales related to the hadronization process.

This issue is resolved by factorizing the perturbative and nonperturbative regions in calculations of high energy scattering observables [2]. Consider, for example, deep inelastic scattering (DIS) where a lepton scatters from a proton target. In the limit of large momentum transfer $Q$, the leading contribution to the cross section can be approximated as a convolution of the hard scattering cross section, $d\hat{\sigma}_f$, with a soft nonperturbative function, $f$,

$$d\sigma(x, Q^2) \simeq \sum_f \int_x^1 \frac{d\xi}{\xi} f\left(\frac{x}{\xi}, Q^2\right) d\hat{\sigma}_f(\xi, Q^2),$$

(1.2)

where higher order $1/Q$ corrections can be safely neglected. At leading order (LO) in $\alpha_s$, the cross section has a probabilistic interpretation in that $d\hat{\sigma}_f$ is the probability for an electron to scatter from a quark of flavor $f$ and $f(x)$ is the parton distribution function (PDF) that describes the probability for the struck quark to carry momentum fraction $x$ of the total proton momentum. The differential cross section for the electron-proton scattering as a function of $x$ and $Q^2$ is then the sum over all possible quark flavors in the proton.

Factorization is a powerful tool that allows us to determine the partonic momentum structure of hadrons through PDFs. Because these objects are nonperturbative, they
cannot be directly computed in pQCD but are determined in analyses of high energy experimental data instead. Significant progress has been made over the past several decades to constrain PDFs through global QCD analyses [3–6]. In addition to momentum distributions, experiments which polarize the scattering particles can provide information about the spin structure of the proton as well. This is encoded in spin-dependent PDFs, the determination of which will be the focus of this thesis.

1.2 History of Proton Spin Structure

The first measurement of the proton spin structure from polarized DIS by the European Muon Collaboration (EMC) revealed a rather surprising result [7]. While one might expect the quarks to carry all of the nucleon spin from a naïve quark model picture, a more careful prediction from Ellis and Jaffe [8] suggested the quark contribution to the proton spin at the EMC scale, assuming zero strange quark polarization, is $\Delta \Sigma(Q_{EMC}^2) \sim 0.6$, roughly 60% of the total spin [9]. However, the EMC analysis determined $\Delta \Sigma(Q_{EMC}^2) \sim 0.1$, a factor of six difference! The discovery that the quarks carry such a small fraction of the proton spin became famously known as the “proton spin crisis.”

Consequently, various attempts to explain the proton spin puzzle quickly emerged. One such effort proposed a large cancellation of the quark contribution through a gluonic term in $\Delta \Sigma$ generated by the axial anomaly [10]. This prompted intense interest in measuring the gluon polarization in the proton, $\Delta G$. While subsequent DIS experiments struggled to find any indication of a nonzero gluon spin contribution, recent measurements from proton-proton collisions at the Relativistic Heavy Ion Collider (RHIC) provided evidence for a small $\Delta G$ [11, 12]. Unfortunately, the extracted value from RHIC data was significantly smaller than what was needed to account for the EMC result [13]. Subsequent experiments also failed to validate explanations that suggested a large negative sea
polarization in the proton.

The unaccounted spin is yet to be identified, however, the attention is now focused on orbital angular motion of the quarks and gluons [9, 14]. Such information can be accessed from transverse momentum dependent (TMD) distributions or generalized parton distributions (GPDs) which are functions of quark transverse momentum $k_T$ and transverse spatial distance $b$, respectively, in addition to the quark longitudinal momentum fraction.

The focus of this work, however, is on the collinear helicity distributions, $\Delta f = f^\uparrow - f^\downarrow$, defined here as the difference between parton distributions with spin aligned ($\uparrow$) and anti-aligned ($\downarrow$) with the proton spin. Much of the information about quark spin PDFs has come from global analyses of polarized DIS experiments. Tremendous improvement in both experimental and theoretical precision has led to well determined distributions for the valence quarks [15–20]. In more recent years, additional information has come from polarized semi-inclusive deep inelastic scattering (SIDIS) and single spin asymmetries in $W^\pm$ boson production, which are more sensitive to the sea quark polarizations.

The total strange and anti-strange helicity distribution $\Delta s^+ = \Delta s + \Delta \bar{s}$, in particular, has been of interest in the last decade. Since polarized DIS observables are weakly dependent on the strange polarization, global analyses typically use SU(3) flavor symmetric (SU(3)$_f$) constraints from weak baryon decays to extract such information. However, this requires the integral of $\Delta s^+$ over all parton momentum fraction $x$ to have a value of $\sim -0.1$ at $Q^2 \sim 1$ GeV$^2$, an overall negative contribution to the spin of the proton. Furthermore, fit parameters that control the shape of the strange polarization in the region of large $x$ are often fixed such that $\Delta s^+(x)$ contains a negative peak at $x \sim 0.1$.

While an entirely negative $\Delta s^+$ has been determined from inclusive DIS data, global fits that incorporated polarized SIDIS measurements showed a dramatic shift in the shape of the strange PDF, changing sign and becoming positive in the intermediate-$x$ region instead [20, 21]. Various questions soon emerged about the cause of this discrepancy, which
became known as the “strange polarization puzzle” [21]. If polarized SIDIS observables prefer a positive strange helicity at $x \sim 0.1$, why does this not appear as a possible distribution obtained in analyses of DIS only? Is there a tension between DIS and SIDIS data? Such questions can be answered through rigorous Monte Carlo based QCD analyses. By analyzing experimental data with robust statistical procedures, we can obtain a better understanding of the spin structure of the proton.

1.3 Outline

Much of the work presented here has already been published and can be found in Refs. [15, 22–25]. We will begin with a review of the theoretical formalism for polarized DIS, SIDIS, and unpolarized single-inclusive $e^+e^-$ annihilation (SIA) processes in Chapter 2. The pQCD expressions for DIS and SIDIS are not only written as a series expansion in the strong coupling $\alpha_s$, but also contain higher order $1/Q$ corrections from higher twist operators in the operator product expansion (OPE). Furthermore, experiments often perform DIS and SIDIS with nuclear targets such as deuterium and $^3$He, which require careful treatment to extract quark spin structure information [22, 23]. Both higher twist and nuclear corrections are discussed in detail in Chapter 3.

An essential part of any global QCD analysis is the methodology one uses to fit the experimental data. We will discuss various aspects of fitting, including both Hessian and Monte Carlo based fitting techniques, in Chapter 4. Function parameterizations and features of experimental data included in the global fits will also be discussed in this chapter. Following details on PDF extraction methods, we will present results from three different global analyses in Chapter 5. The first studies the impact of Jefferson Lab DIS data and higher twist corrections on the parton spin dependent distributions [15]. The second is the first Monte Carlo analysis of $e^+e^-$ annihilation to extract fragmentation
functions (FFs) [24], which play a significant role in spin PDF extractions from SIDIS observables and will be introduced in Chapter 2.

Lastly, we will present results from an analysis that, for the first time, fit simultaneously the quark helicity distributions and FFs in a combined QCD analysis of DIS, SIDIS, and SIA experimental data [25]. The analysis emphasizes in particular the impact of SIDIS data on the sea quark polarizations and resolves the long-standing puzzle regarding the strange helicity shape. As a result of the three subsequent global fits presented in this work, we obtain new and reliable information about the proton spin structure. The results will be summarized in Chapter 6, followed by a discussion about the future of PDF and FF extraction.
CHAPTER 2

High Energy Scattering Observables

Collinear factorization is the theoretical foundation for constructing observables in global QCD analyses of high energy scattering data. In this chapter, we review the formalism to describe DIS, SIDIS, and SIA measurements within this framework. In addition, we give the general expressions for the observables in Mellin moment space and discuss the benefits of implementing the Mellin technique in global QCD fits.

2.1 Deep inelastic scattering

In polarized inclusive DIS, a lepton with spin aligned (↑) or anti-aligned (↓) with its direction of motion scatters from a polarized nucleon target of mass $M$ via the exchange of a virtual photon (see Fig. 2.1). The differential cross section, neglecting the lepton mass, can be expressed theoretically as a contraction of the leptonic tensor $L^{\mu\nu}$ and hadronic tensor $W^{\mu\nu}$,

$$
\frac{d\sigma}{dxdy} = \frac{2\pi y_0^2}{Q^4} L^{\mu\nu} W^{\mu\nu},
$$

(2.1)
FIG. 2.1: Feynman diagram of deep inelastic scattering. The incoming lepton $\ell$ scatters inelastically from the nucleon target $p$ via the exchange of a virtual photon $\gamma^*$. The target remnants fragment into final state hadrons $X$, but only the outgoing lepton $\ell'$ is measured in the final state.

where $Q^2 = -q^2$ is the squared four-momentum transfer, $y = \nu/E = (E - E')/E$ is the lepton fractional energy loss, and $\alpha = e^2/4\pi$ is the electromagnetic fine structure constant. In Eq. (2.1), the dependence on the Bjorken scaling variable $x = Q^2/2M\nu$ is implicit in the hadronic tensor $W^{\mu\nu}$. The lepton-photon vertex in the upper part of Fig. 2.1 is described by the leptonic tensor, which can be computed exactly in quantum electrodynamics (QED) as

$$L_{\mu\nu} = 2(\ell_\mu \ell'_\nu + \ell'_\mu \ell_\nu - \ell_\mu \ell'_\mu g_{\mu\nu} - i\lambda \epsilon_{\mu\alpha\beta} \ell^\alpha \ell'^\beta),$$  

(2.2)

for an incoming and outgoing lepton with four-momenta $\ell_\mu$ and $\ell'_\mu$, respectively. Here $\epsilon_{\mu\alpha\beta}$ is the antisymmetric Levi-Civita tensor and $\lambda = \pm 1$ represents the helicity of the incoming lepton.

On the other hand, the hadronic tensor, which describes the photon-nucleon interaction, is difficult to compute from first principles due to the nonperturbative nature of the bound nucleon. However, respecting current conservation and parity, we can write the
most general form for $W_{\mu\nu}$ as a linear combination of scalar coefficients $F_{1,2}$ and $g_{1,2}$,

$$
W^{\mu\nu} = \left( -g^{\mu\nu} + \frac{q^{\mu}q^{\nu}}{q^2} \right) F_1(x, Q^2)
+ \left( P^{\mu} - q^{\mu} \frac{P \cdot q}{q^2} \right) \left( P^{\nu} - q^{\nu} \frac{P \cdot q}{q^2} \right) \frac{F_2(x, Q^2)}{P \cdot q}
+ i\epsilon_{\mu\nu\alpha\beta} \frac{q^\alpha S^\beta}{P \cdot q} g_1(x, Q^2) + i\epsilon_{\mu\nu\alpha\beta} \frac{q^\alpha}{P \cdot q} \left( S^\beta - P^\beta \frac{S \cdot q}{P \cdot q} \right) g_2(x, Q^2),
$$

(2.3)

where $P^\mu$ and $q^\mu$ are the four-momenta of the nucleon and photon, respectively, and $S^\beta$ is the nucleon spin four-vector, with $S^2 = -M^2$ and $S \cdot P = 0$. The scalar coefficients $F_1(x, Q^2)$, $F_2(x, Q^2)$, $g_1(x, Q^2)$, and $g_2(x, Q^2)$ are known as structure functions, and will be discussed in the context of pQCD later in this section.

Experimental quantities typically measured in polarized DIS are cross section asymmetries, where the difference between different lepton and target spin configurations is observed with respect to the spin averaged cross section. The most general spin asymmetry can be defined in terms of spherical polar angles $\theta^*$ and $\phi^*$, describing the direction of the target polarization relative to the virtual photon momentum vector $q$,

$$
A = \frac{\sigma^\uparrow - \sigma^\downarrow}{\sigma^\uparrow + \sigma^\downarrow} = \frac{\cos \theta^* \sqrt{1 - \epsilon^2} A_1 + \sin \theta^* \cos \phi^* \sqrt{2 \epsilon(1 - \epsilon)} A_2}{1 + \epsilon R},
$$

(2.4)

where $\sigma^{\uparrow/\downarrow} = d\sigma^{\uparrow/\downarrow}/dxdy$ corresponds to Eq. (2.1) for a lepton with helicity $\lambda(\uparrow) = +1$ or $\lambda(\downarrow) = -1$. The general spin asymmetry depends on the ratio $R$ of the longitudinal to transverse photon absorption cross sections, which will be defined in terms of the structure functions later in this section. In addition, Eq. (2.4) depends on the kinematic variable $\epsilon$, which is given by

$$
\epsilon = \frac{2(1 - y) - \frac{1}{2} \gamma^2 y^2}{1 + (1 - y)^2 + \frac{1}{2} \gamma^2 y^2},
$$

(2.5)
with $\gamma^2 = 4M^2x^2/Q^2$. By polarizing the target parallel ($\uparrow\uparrow$) or perpendicular ($\Uparrow\Uparrow$) to the beam direction, Eq. (2.4) can be separated into longitudinal and transverse spin asymmetries,

$$A_{\|} = \frac{\sigma^{\uparrow\uparrow} - \sigma^{\Uparrow\Uparrow}}{\sigma^{\uparrow\uparrow} + \sigma^{\Uparrow\Uparrow}} = D(A_1 + \eta A_2),$$

$$A_\perp = \frac{\sigma^{\downarrow\downarrow} - \sigma^{\uparrow\uparrow}}{\sigma^{\downarrow\downarrow} + \sigma^{\uparrow\uparrow}} = d(A_2 - \zeta A_1),$$

where the photon polarization factors $D$, $d$, $\eta$, and $\zeta$ are defined as

$$D = \frac{y(2 - y)(2 + \gamma^2 y)}{2(1 + \gamma^2) y^2 + (4(1 - y) - \gamma^2 y^2)(1 + R)},$$

$$d = \frac{\sqrt{4(1 - y) - \gamma^2 y^2}}{2 - y} D,$$

$$\eta = \gamma \frac{4(1 - y) - \gamma^2 y^2}{(2 - y)(2 + \gamma^2 y)}, \quad \zeta = \gamma \frac{2 - y}{2 + \gamma^2 y}.$$

The virtual photoproduction asymmetries $A_1$ and $A_2$ that appear in Eqs. (2.4), (2.6), and (2.7) can be decomposed into simple ratios of the spin-dependent to spin-averaged structure functions,

$$A_1 = \frac{(g_1 - \gamma^2 g_2)}{F_1}, \quad A_2 = \gamma \frac{(g_1 + g_2)}{F_1}.$$ 

Extracting these quantities from polarized electron-nucleon scattering requires information about the ratio $R$, which can also be written in terms of the structure functions,

$$R = \frac{(1 + \gamma^2)F_2 - 2xF_1}{2xF_1}.$$ 

The most fundamental observables that can be measured in DIS, then, are the polarized $g_i$ and unpolarized $F_i$ ($i = 1, 2$) structure functions.
Both the spin-averaged and spin-dependent structure functions can be described by a series expansion in powers of $1/Q$, the origin of which will be introduced in Chapter 3. For now, the discussion will focus only on the leading contribution to the structure functions, which are well defined in pQCD. The leading term in $g_1$ is given by a convolution of the polarized PDFs ($\Delta q^+ = \Delta q + \Delta \bar{q}$, $\Delta g$) with the hard scattering coefficients ($\Delta C_{q,g}$),

$$g_1(x, Q^2) = \frac{1}{2} \sum_q e_q^2 [ (\Delta C_q \otimes \Delta q^+)(x, Q^2) + (\Delta C_g \otimes \Delta g)(x, Q^2) ] + \mathcal{O}\left(\frac{1}{Q}\right), \quad (2.11)$$

where $e_q$ is the quark electric charge and $\otimes$ represents the standard convolution integral $C \otimes f = \int_x^1 (d\hat{x}/\hat{x}) C(\hat{x}) f(x/\hat{x})$. In principle, the polarized PDFs and coefficient functions depend on a renormalization scale $\mu_R$ that originates from regulating ultraviolet divergences. Typically this is set to the hard scale $Q$, as was done in Eq. (2.11), but can be varied to estimate theoretical uncertainty. Note also that the expression for the structure function is true to all orders in pQCD since the expansion in $\alpha_s$ is implicit in the hard coefficient functions,

$$\Delta C_i(\hat{x}, Q^2) = \Delta C_i^{(0)}(\hat{x}, Q^2) + \frac{\alpha_s(Q^2)}{4\pi} \Delta C_i^{(1)}(\hat{x}, Q^2) + \mathcal{O}(\alpha_s^2), \quad (2.12)$$

where $\mu_R = Q$ was also set for the strong coupling $\alpha_s$. The leading contribution to the unpolarized structure functions $F_1$ and $F_2$ are similar in form to Eq. (2.11), where the polarized PDFs and coefficients are replaced by the analogous unpolarized functions. Finally, the leading contribution to the $g_2$ structure function is given by the Wandzura-Wilczek relation [26],

$$g_2(x, Q^2) = -g_1(x, Q^2) + \int_x^1 \frac{dz}{z} g_1(z, Q^2) + \mathcal{O}\left(\frac{1}{Q}\right). \quad (2.13)$$
While $g_2$ itself is not necessarily small, it is suppressed by factors of $\gamma$ in the cross section asymmetries (Eq. (2.9)). Consequently, the $g_2$ structure function does not contribute in the Bjorken limit ($Q^2 \to \infty$, finite $x$). In fact, $A_2$ also vanishes in this limit, and the resulting $A_1 = g_1/F_1$ is a simple ratio of the polarized to unpolarized structure functions.

### 2.2 Semi-inclusive deep inelastic scattering

In semi-inclusive DIS, the outgoing struck quark fragments and a single hadron is tagged in the final state (see Fig. 2.2). The polarized cross section asymmetries measured in SIDIS follow directly the discussion from DIS, apart from dependence on an additional kinematic variable $z = p \cdot p_h/p \cdot q$, interpreted as the fraction of the transferred virtual photon momentum $q$ being carried by the outgoing hadron with momentum $p_h$. Experiments also typically measure cross sections that are dependent on the hadron’s transverse momentum $p_{h\perp}$. However, since our concern is only of the collinear distributions, the transverse momentum dependence is integrated out in the SIDIS observables presented in this section.
In the Bjorken limit, the SIDIS virtual photoproduction asymmetry is constructed as a ratio of semi-inclusive structure functions,

\[ A_h^1(x, z, Q^2) = \frac{g_h^1(x, z, Q^2)}{F_h^1(x, z, Q^2)}, \]  

(2.14)

for a process in which a hadron \( h \) is identified in the final state. The semi-inclusive structure functions are subject to power suppressed corrections dependent on the outgoing hadron mass \( (M_h/Q) \), in addition to the \( 1/Q \) and \( M/Q \) terms that arise in DIS. These so-called hadron mass corrections (HMCs) have recently been studied in Ref. [27]; however, since the \( Q^2 \) values of the available experimental data are sufficiently large, the \( 1/Q \) corrections in SIDIS are not considered in this work.

The discussion here will again be restricted only to the leading contribution to the semi-inclusive structure functions. For the polarized \( g_h^1 \) function, it is given by

\[
g_h^1(x, z, Q^2) = \frac{1}{2} \sum_q e_q^2 \left[ (\Delta q(x, Q^2) \otimes \Delta C_{qq}(x, z) \otimes D^h_q(z, Q^2)) 
+ (\Delta q(x, Q^2) \otimes \Delta C_{gq}(x, z) \otimes D^h_g(z, Q^2)) 
+ (\Delta g(x, Q^2) \otimes \Delta C_{qg}(x, z) \otimes D^h_q(z, Q^2)) 
+ (\Delta g(x, Q^2) \otimes \Delta C_{gg}(x, z) \otimes D^h_g(z, Q^2)) \right] + \mathcal{O}\left(\frac{1}{Q}\right).
\]  

(2.15)

Identifying a hadron in the final state introduces a new nonperturbative function, \( D_{q,g}^h \), as a result of factorizing the hard scattering and hadronization distance scales. These are the fragmentation functions (FFs) and can be interpreted at LO as the probability for the struck quark to fragment into a jet containing a hadron \( h \) with fraction \( z \) of the virtual photon momentum. Furthermore, Eq. (2.15) contains off-diagonal terms \( \Delta C_{qg} \) and \( \Delta C_{gq} \) related to the gluon occurring in the initial (\( \Delta g \)) or final (\( D^h_g \)) state. At next-to-leading
order (NLO) in the $\alpha_s$ expansion, all except the diagonal glue-glue term ($\Delta C_{gg}$), which enters at next-to-NLO (NNLO), contribute to the polarized structure function. As in the DIS case, the unpolarized structure function $F_1^h$ is defined similarly to $g_1^h$ with the polarized PDFs and hard scattering coefficients replaced by the unpolarized quantities.

Semi-inclusive DIS plays a key role in global QCD analyses of spin dependent PDFs. Not only does it allow for separation of the quark and anti-quark flavors when combined with analysis of DIS observables, but will have sensitivity to sea quark helicity distributions that are favored in specific charged meson production. However, the determination of polarized PDFs from SIDIS is also strongly dependent on the parameterizations one chooses for the FFs, particularly for kaon production [28]. Therefore, it is important to discuss the QCD process from which much of our knowledge of FFs is obtained.

### 2.3 Single-inclusive $e^+e^-$ annihilation

Single-inclusive hadron production from $e^+e^-$-annihilation (Fig. 2.3) is perhaps the cleanest QCD process to study hadronization. Analogous to PDFs from DIS, SIA observables provide a direct probe to the nonperturbative FFs which describe the formation of

FIG. 2.3: Feynman diagram of single-inclusive $e^+e^-$-annihilation. The electron $e^-$ and positron $e^+$ annihilate and a quark/anti-quark pair is produced from the intermediate photon $\gamma$ or $Z$ boson. The outgoing quarks fragment and a single hadron $h$ is identified in the final state.
mesons and baryons from partons. The experimental observable for an outgoing hadron \( h \) is given by

\[
F_h(z, Q^2) = \frac{1}{\sigma_{\text{tot}}} \frac{d\sigma^h}{dz}(z, Q^2),
\]  

(2.16)

where \( z = 2p_h \cdot q/Q^2 \) is the fraction of the intermediate boson momentum \( q \) carried by the detected hadron with momentum \( p_h \), and \( Q = \sqrt{Q^2} \) is the invariant mass. In the center-of-mass frame, the variable \( z = 2E_h/Q \) can be interpreted instead as the energy fraction of the quark or anti-quark produced in the hard process that is carried by the outgoing hadron with energy \( E_h \).

The differential cross section in Eq. (2.16) is normalized by the total inclusive \( e^+e^- \rightarrow q\bar{q} \) cross section \( \sigma_{\text{tot}} \), which at NLO is

\[
\sigma_{\text{tot}}(Q^2) = \sum_q \frac{4\pi\alpha^2}{Q^2} \tilde{e}_q^2 \left( 1 + \frac{\alpha_s(\mu_R^2)}{\pi} \right) + \mathcal{O}(\alpha_s^2).
\]  

(2.17)

In this expression, \( \alpha = e^2/4\pi \) is the electromagnetic fine structure constant and \( \tilde{e}_q^2 \) is defined as

\[
\tilde{e}_q^2 = e_q^2 + 2e_q g_V^2 g_V^2 \rho_1(Q^2) + (g_A^2 + g_V^2) (g_A^2 + g_V^2) \rho_2(Q^2).
\]  

(2.18)

The coupling factor \( \tilde{e}_q^2 \) is a sum of three terms related to quark-boson coupling. The first is the standard quark-photon coupling given by the quark electric charge \( e_q \). The additional two terms dependent on \( \rho_1 \) and \( \rho_2 \) give the contributions from intermediate \( \gamma Z \) interference.
and $Z$ production, respectively, and are given by

$$
\rho_1(Q^2) = \frac{1}{4 \sin^2 \theta_W \cos^2 \theta_W} \frac{Q^2(M_Z^2 - Q^2)}{(M_Z^2 - Q^2)^2 + M_Z^2 \Gamma_Z^2},
$$

(2.19a)

$$
\rho_2(Q^2) = \frac{1}{(4 \sin^2 \theta_W \cos^2 \theta_W)^2} \frac{Q^4}{(M_Z^2 - Q^2)^2 + M_Z^2 \Gamma_Z^2},
$$

(2.19b)

where $M_Z$ is the mass of the $Z$ boson and $\Gamma_Z$ is its width. The above expressions are also dependent on the weak mixing angle $\theta_W$, where $\sin^2 \theta_W \approx 1/4$. The quark vector and axial vector couplings in Eq. (2.18) are $g^q_V = \frac{1}{2} - \frac{2}{3} \sin^2 \theta_W$ and $g^q_A = +\frac{1}{2}$, respectively, for the up-type quark flavors ($u, c$). For the down-type quark flavors ($d, s, b$), they are given by $g^d_V = -\frac{1}{2} + \frac{2}{3} \sin^2 \theta_W$ and $g^d_A = -\frac{1}{2}$. Lastly, the electron vector and axial vector couplings are defined similarly by $g^e_V = -\frac{1}{2} + 2 \sin^2 \theta_W$ and $g^e_A = -\frac{1}{2}$.

As in previous sections, the observable relevant here (Eq. (2.16)) can be expressed in the collinear factorization framework as a convolution of the hard scattering coefficients $H_i$ with the parton-to-hadron FFs $D_i^h$,

$$
F^h(z, Q^2) \approx F_{\text{coll}}^h(z, Q^2) = \frac{1}{\sigma_{\text{tot}}} \sum_i [H_i \otimes D_i^h](z, Q^2),
$$

(2.20)

where the sum over $i$ runs over all parton flavors $i = u, d, s, \ldots, g$. The FFs and hard coefficients are again dependent on a renormalization scale $\mu_R$ that arises from the renormalization of final state divergences. As was done previously, we have set the renormalization scale $\mu_R$ to the momentum transfer $Q$ in Eq. (2.20).

Many parallels can be drawn about the extraction of FFs from SIA with respect to PDFs from DIS. As in DIS, observables in SIA are sensitive only to the sum of quark and anti-quark flavor FFs, $D_{q+}^h = D_q^h + D_{\bar{q}}^h$, and therefore require additional input from SIDIS or other hadron production processes to separate the individual quark-to-hadron FFs. There is a distinction, however, in the treatment of heavy quark flavors, which are
generated perturbatively in the proton for DIS, but are prominent in SIA due to center-of-
mass energies being much higher than the heavy quark production thresholds. Such topics
will be left for discussion in Chapter 4.

2.4 Observables in Mellin moment space

Since nonperturbative functions are typically determined by experimental data, the
theoretical observables discussed in the previous sections are implemented numerically in
global QCD analyses. In the case where there is a significant amount of experimental data
and many fit parameters, it becomes beneficial to improve the efficiency of the theoretical
calculations. This can be achieved by computing observables in Mellin moment space,
which is considerably faster than numerical calculations in $x$ (or $z$) space [29].

Using the definition of the $N$-th Mellin moment of a function $f(x),$

$$f(N) = \int_0^1 dx \, x^{N-1} f(x),$$

(2.21)
an observable $O(x, Q^2)$ defined by a single convolution integral in $x$ space, e.g. Eqs. (2.11)
or (2.20), can be expressed as a simple product in Mellin space,

$$O(N, Q^2) = \sum_i H_i(N, Q^2) f_i(N, Q^2).$$

(2.22)

Here the $N$-th moment of the observable, $O(N, Q^2)$, is given by general hard scattering
coefficients $H_i$ and nonperturbative functions $f_i$ in Mellin space, summed over the dif-
ferent parton flavors $i = u, d, s, \ldots, g$. Of course, in order to compare with experimental
measurements, Eq. (2.22) must be reverted back to the $x$ space expression $O(x, Q^2).$
The Mellin inversion is performed using contour integration in complex moment space,

\[ \mathcal{O}(x, Q^2) = \frac{1}{2\pi i} \int_C dN x^{-N} \mathcal{O}(N, Q^2), \]  

(2.23)

and is done numerically by defining \( N = c + z e^{i\phi} \), where \( c \) is the point of intersection of the contour with the real axis and is fixed to the right of the rightmost pole. The angle \( \phi \) measures from the real axis to the contour line in complex space at \( c \) and is set to be \( 3\pi/4 \) to assure quick convergence of the integral. Eq. (2.23) can then be expressed as an integration over the variable \( z \),

\[ \mathcal{O}(x, Q^2) = \frac{1}{\pi} \int_0^\infty dz \text{Im} \left[ e^{i\phi} x^{-N} \mathcal{O}(N, Q^2) \right], \]  

(2.24)

where symmetry with respect to the real axis was applied. There are various approaches one could take to evaluate the integral over \( z \), however, the standard method is with a Gaussian quadrature sum,

\[ \mathcal{O}(x, Q^2) \simeq \frac{1}{\pi} \sum_i w_i \text{Im} \left[ e^{i\phi} x^{-N_i} \mathcal{O}(N_i, Q^2) \right], \]  

(2.25)

where \( w_i \) is the Gaussian weight for the \( i \)-th point \( z_i \). This integration method is highly advantageous because it allows for a pre-computation of various theoretical quantities and thus significantly reduces computation time [29]. These are stored as Mellin tables, where the quantity of interest is evaluated at a collection of Mellin points \( (N_i) \) defined by the contour, which can subsequently be called upon in calculations of theoretical observables.

The Mellin moment technique can also be applied to observables dependent on two variables \( x_1 \) and \( x_2 \) (e.g. \( x \) and \( z \) in Eq. (2.15)). The double Mellin moment for a general observable \( \mathcal{O}(x_1, x_2, Q^2) \) that contains two nonperturbative functions \( f_1(x_1) \) and \( f_2(x_2) \) is
given by

\[
\mathcal{O}(N, M, Q^2) = \sum_{i,j} H_{i,j}(N, M, Q^2) f_{1,i}(N, Q^2) f_{2,j}(M, Q^2)
\] (2.26)

where the \(N\)-th and \(M\)-th moment correspond to integrals over \(x_1\) and \(x_2\), respectively. Returning to \(x\) space requires a double Mellin inversion, which is a straightforward extension of Eq. (2.23) and is defined as

\[
\mathcal{O}(x_1, x_2, Q^2) = \frac{1}{(2\pi i)^2} \int dNdM x_1^{-N} x_2^{-M} \mathcal{O}(N, M, Q^2).
\] (2.27)

By defining \(N = c_n + z_n e^{i\phi_n}\) and \(M = c_m + z_m e^{i\phi_m}\), and performing the double Mellin inversion as two subsequent single Mellin inversions, Eq. (2.27) can be expressed as

\[
\mathcal{O}(x_1, x_2, Q^2) = -\frac{1}{2\pi^2} \Re \left[ \int_0^\infty \int_0^\infty dz_n dz_m x_1^{-N} x_2^{-M} \times \left\{ e^{i(\phi_n + \phi_m)} x_2^{-M} \mathcal{O}(N, M, Q^2) - e^{i(\phi_n - \phi_m)} x_2^{-M} \mathcal{O}(N, M^*, Q^2) \right\} \right].
\] (2.28)

The double integration over \(z_n\) and \(z_m\) is then approximated as before by a Gaussian quadrature sum with Gaussian weights \(w_i\) and \(w_j\),

\[
\mathcal{O}(x_1, x_2, Q^2) = -\frac{1}{2\pi^2} \sum_i w_i \sum_j w_j \Re \left[ x_1^{-N_i} \times \left\{ e^{i(\phi_n + \phi_m)} x_2^{-M_j} \mathcal{O}(N_i, M_j, Q^2) - e^{i(\phi_n - \phi_m)} x_2^{-M_j^*} \mathcal{O}(N_i, M_j^*, Q^2) \right\} \right],
\] (2.29)

where the summation occurs first over values of \(M_j = c_m + z_j e^{i\phi_m}\) followed by \(N_i = c_n + z_i e^{i\phi_n}\). Typically the contours for \(N\) and \(M\) are set to be identical such that
$c_n = c_m$ and $\phi_n = \phi_m$. For convenience, the hard coefficient functions needed to compute Eqs. (2.11), (2.15), and (2.20) in Mellin space are given in Appendix A for the $\overline{\text{MS}}$ renormalization scheme [30, 31].

Besides the ability to pre-compute quantities in Mellin space, there are two additional advantages to using the Mellin moment technique in a global QCD analysis. The first is that integration over the kinematic variable $x$ (or $z$) in Mellin space can be computed analytically without spoiling the efficiency of the numerical calculation. This is especially relevant for experimental observables that require an averaging over kinematic bin ranges (excluding $Q^2$ dependence). Consider, for example, an averaging between $x_{\text{min}}$ and $x_{\text{max}}$ for an observable $\mathcal{O}(x, Q^2)$. Since the pre-factor $x^{-N}$ in Eq. (2.23) is the only $x$ dependence, the averaged observable $\langle \mathcal{O} \rangle$ can be written as

$$
\langle \mathcal{O}(x, Q^2) \rangle_{x_{\text{bin}}} = \frac{1}{(x_{\text{max}} - x_{\text{min}})} \frac{1}{2\pi i} \int_C dN \left( \frac{x_{\text{max}}^{1-N} - x_{\text{min}}^{1-N}}{1 - N} \right) \mathcal{O}(N, Q^2),
$$

(2.30)

and the contour integration can be performed using the Gaussian method discussed previously.

Another key aspect of working in Mellin moment space is the application to scale evolution. In global QCD analyses, the nonperturbative distributions that enter into theoretical observables are parameterized at an input scale $Q^2_0$ and must be evaluated at the scale of a given experiment. In the pQCD framework, the scale dependence is governed by the DGLAP equations [32–34], which in $x$ space are given by

$$
\frac{df_i(x, \mu^2)}{d\ln(\mu^2)} = [P_{ij} \otimes f_j](x, \mu^2),
$$

(2.31)

where $f$ is a generic nonperturbative function that depends on a renormalization scale $\mu$ and $P_{ij}$ are the parton $i \to j$ splitting functions. Setting $\mu^2 = Q^2$ then signifies the
dependence of the nonperturbative input on the momentum transfer of a QCD process. For PDF evolution, the variable $x$ is the parton momentum fraction and the splitting functions are space-like ($P_{ij}^S$). When considering the scale dependence of FFs, $x$ is replaced by the kinematic variable $z$ and the splitting functions in Eq. (2.31) become time-like ($P_{ij}^T$).

Solving the integro-differential equations ((2.31)) numerically in $x$ space is highly non-trivial [35–37]. Since convolution integrals become products in Mellin space, scale evolution becomes an ordinary coupled differential equation,

$$\frac{d f_i(N, \mu^2)}{d \ln(\mu^2)} = P_{ij}(N, \mu^2) f_j(N, \mu^2), \quad (2.32)$$

which can be solved using the methods in Ref. [38]. Both the space-like and time-like splitting functions in Mellin space can be found in Appendix B.

Clearly, the Mellin moment technique is an indispensable tool for time-intensive global QCD analyses, such as those that utilize rigorous Monte Carlo statistical methods. This will become even clearer in the following chapter, where multi-dimensional integrals from higher order $1/Q$ and nuclear corrections can be rendered as pre-computed quantities in Mellin space.
CHAPTER 3

Corrections Beyond the Parton Model

In more recent years a wealth of high-precision DIS data at lower energies has become available from Jefferson Lab [39–42], providing new insight into the spin structure of the nucleon. However, many of these new data exist at low values of $Q^2$ and squared final state hadronic mass $W^2$, a phase space region typically excluded by kinematic cuts in global QCD analyses. Furthermore, Jefferson Lab provides fixed-target DIS data on nuclei such as deuterium [42, 43] and $^3\text{He}$ [44–46], which require proper treatment of bound nucleon effects to extract quark spin information. In this chapter, we discuss finite-$Q^2$ and nuclear corrections relevant for experimental observables at Jefferson Lab.

3.1 Higher Twist and Target Mass Corrections in DIS

In the operator product expansion (OPE), a product of two operators at different space-time points can be written as a linear combination of local operators. This framework
allows one to construct hadronic matrix elements in DIS as a series expansion in twist 
\( \tau = d - s \), where the operators are defined by their mass dimension, \( d \), minus spin, \( s \). Higher twist (HT) operators from additional quark or gluon fields in the hard process 
generate terms that are suppressed by powers of \( (1/Q)^{r-2} \) in DIS structure functions. 
Within the same formalism, there are target mass corrections (TMCs) of all orders in \( M/Q \) 
that originate from covariant derivative insertions in leading twist matrix elements [47].

Such corrections can be safely neglected if observables are evaluated in the Bjorken 
limit \( (Q^2 \to \infty) \). On the other hand, when analyzing experimental data at values of mo-
momentum transfer on the order of the hadron mass \( Q \sim M \), corrections from HT operators 
and target mass become sizable and must be addressed. In the first of the three global 
QCD analyses presented in Chapter 5, where low-\( Q^2 \) DIS data from Jefferson Lab are 
included, the HT corrections are treated up to twist-4 in the polarized structure function 
\( g_1 \) and up to twist-3 for \( g_2 \),

\[
\begin{align*}
g_1 &= g_1^{(r_2)} + g_1^{(r_3)} + g_1^{(r_4)} + \text{HT}, \\
g_2 &= g_2^{(r_2)} + g_2^{(r_3)} + \text{HT},
\end{align*}
\]

where the leading twist \( g_1^{(r_2)} \) and \( g_2^{(r_2)} \) are given by Eqs. (2.11) and (2.13), respectively, 
and HT denotes terms of higher twist. Furthermore, TMCs are included for the polarized 
structure functions up to twist-3 for both \( g_1 \) and \( g_2 \). We shall see from the results of the 
global analysis that these terms are sufficient for describing low-\( Q^2 \) data since the twist-4 
contribution is negligible for Jefferson Lab kinematics, and the \( g_2 \) structure function is 
suppressed by a factor \( 1/Q^2 \) in the polarization asymmetries. Following the formalism of
Ref. [48], the target mass corrected $g_1^{(r2)}$ is

$$g_1^{(r2+TMC)}(x, Q^2) = \frac{x}{\xi \rho^2} g_1^{(r2)}(\xi, Q^2) + \frac{(\rho^2 - 1)}{\rho^4} \int_1^x \frac{dz}{z} \left[ \frac{(x + \xi)}{\xi} - \frac{(3 - \rho^2)}{2\rho} \ln \frac{z}{\xi} \right] g_1^{(r2)}(z, Q^2),$$

(3.3)

and the expression for the target mass corrected $g_2^{(r2)}$ is

$$g_2^{(r2+TMC)}(x, Q^2) = -\frac{x}{\xi \rho^3} g_1^{(r2)}(\xi, Q^2) + \frac{1}{\rho^4} \int_1^x \frac{dz}{z} \left[ \frac{x}{\xi} - (\rho^2 - 1) + \frac{3(\rho^2 - 1)}{2\rho} \ln \frac{z}{\xi} \right] g_1^{(r2)}(z, Q^2).$$

(3.4)

The TMCs are controlled by the Nachtmann variable $\xi = 2x/(1 + \rho)$ [47, 49], where $\rho = 1 + \gamma^2$ and the $Q^2$ scale dependence in the leading-twist structure functions is still given by the DGLAP equations, which can be derived in the OPE formalism from renormalized twist-2 operators.

In the limit of large $Q^2$ ($\rho \to 1$ and $\xi \to x$), the polarized structure function $g_1^{(r2+TMC)}$ returns to the massless limit expression $g_1^{(r2)}$ in Eq. (2.11), and the WW relation is recovered for $g_2^{(r2)}$ (Eq. (2.13)). Another observation worth mentioning here is that the target mass corrected structure functions vanish at $\xi = 1$ and are therefore nonzero in the $x \to 1$ limit. This is known in the literature as the “threshold problem” [50–52], and has been a subject of interest in recent studies [53–56]. The issue, however, is relevant only for values of $W^2$ that correspond to the nucleon resonance region, safely below the DIS region considered in global QCD analyses.

Continuing now in the twist series for the polarized structure functions, the twist-3
part of $g_1$ with TMCs is given by [48]

$$
g_1^{(\tau_3+\text{TMC})}(x, Q^2) = \frac{(\rho^2 - 1)}{\rho^3} D(\xi, Q^2) - \frac{(\rho^2 - 1)}{\rho^4} \int_\xi^1 \frac{dz}{z} \left[ 3 - \frac{(3 - \rho^2)}{\rho} \ln \frac{z}{\xi} \right] D(z, Q^2),
$$

(3.5)

and for $g_2$ it is

$$
g_2^{(\tau_3+\text{TMC})}(x, Q^2) = \frac{1}{\rho^3} D(\xi, Q^2) - \frac{1}{\rho^4} \int_\xi^1 \frac{dz}{z} \left[ 3 - 2\rho^2 + \frac{3(\rho^2 - 1)}{\rho} \ln \frac{z}{\xi} \right] D(z, Q^2).
$$

(3.6)

Both are expressed in terms of the function $D$ which is constructed as a sum over twist-3 parton distributions $D_q$,

$$
D(x, Q^2) = \sum_q e_q^2 D_q(x, Q^2).
$$

(3.7)

Theoretically, these twist-3 parton distributions $D_q$ correspond to combinations of quark-gluon operators in the OPE and therefore provide information on nonperturbative quark-gluon interactions. Their scale dependence can be derived from renormalized twist-3 operators in the OPE and is highly nontrivial [57, 58]. We note here that extracting $1/Q^2$ power corrections from the general log($Q^2$) behavior at NLO in the leading twist formalism is particularly challenging to accomplish with the existing data, and therefore distinguishing between different $\alpha_s$ approximations for the higher twist contributions is simply not feasible. For the purpose of this work, the evolution of the function $D$ from the input scale $Q_0^2$ is approximated by the large-$N_c$ limit, where $N_c$ corresponds to the number of active parton colors. Because the power corrections vary sufficiently faster with $Q^2$ than any modification to the large-$N_c$ limit expression for the higher twist evolution (from additional $\alpha_s$ corrections), the results would likely not be sensitive even if the large-$N_c$ $\alpha_s$ corrections were excluded altogether.
In the large-$N_c$ limit, the evolution of the twist-3 function is given in Mellin space as

$$D(N, Q^2) \approx \left( \frac{\alpha_s(Q^2)}{\alpha_s(Q_0^2)} \right)^{\tilde{\gamma}} D(N, Q_0^2), \quad (3.8)$$

where $D(N, Q^2)$ is the Mellin moment of $D(x, Q^2)$ in Eq. (3.7). The exponent of the ratio of strong couplings $\alpha_s$ is the anomalous dimension,

$$\tilde{\gamma} = \frac{1}{(11 - \frac{2}{3}N_f)} \left( \psi(0, N) + \gamma_E - \frac{1}{4} + \frac{1}{2N} \right), \quad (3.9)$$

where $\psi(0, N)$ is the zeroth order polygamma function and $\gamma_E$ is the Euler-Mascheroni constant. Since the twist-3 component of the polarized structure function $g_1$ (Eq. (3.5)) contains an overall factor of $\rho^2 - 1$, it clearly becomes zero in the limit of large $Q^2$. Interestingly, the twist-3 contribution to $g_2$ (Eq. (3.6)) does not become zero in this limit, but instead reduces to

$$g_2^{(\tau_3)}(x, Q^2) = D(x, Q^2) - \int_x^1 \frac{dz}{z} D(z, Q^2), \quad (3.10)$$

an expression similar to the Wandzura-Wilczek relation given by Eq. (2.13) for the $g_2^{(\tau_2)}$ term.

Lastly, the twist-4 term of $g_1$ is constructed at the hadron level,

$$g_1^{(\tau_4)}(x, Q^2) = \frac{H(x, Q^2)}{Q^2}, \quad (3.11)$$

where $H$ is a general function of fit parameters that will be determined by experimental data. In the QCD analysis studying the impact of Jefferson Lab DIS data, the focus is primarily on determining the first two contributions in the twist series of the polarized structure functions. Consequently, both TMCs and $Q^2$ evolution are not considered for
the twist-4 term, which is treated as background for the same reason that is given for the twist-3 evolution approximation.

### 3.1.1 Mellin moments and spin sum rules

As mentioned in the previous chapter, calculating the target-mass corrected structure functions in Mellin space can significantly reduce computation time in a global QCD analysis, since the TMCs can be pre-computed and stored in Mellin tables. Consider, for example, the target-mass corrected twist-2 contribution to \( g_1 \). The expression given in Eq. (3.3) can be rewritten in the Mellin formalism as

\[
g_1^{(\tau_2+\text{TMC})}(x, Q^2) = \frac{1}{2\pi i} \int dN \, g_1^{(\tau_2+\text{TMC})}(N, Q^2) \times \left\{ \frac{x}{\xi^{N+1}\rho^3} + \frac{(\rho^2 - 1)}{\rho^4} \int_\xi^1 \frac{dz}{z^{N+1}} \left[ \frac{(x + \xi)}{\xi} - \frac{(3 - \rho^2)}{2\rho} \ln \frac{z}{\xi} \right] \right\}, \tag{3.12}
\]

where \( g_1^{\tau_2+\text{TMC}}(N, Q^2) \) is the Mellin moment of \( g_1^{\tau_2+\text{TMC}}(x, Q^2) \) defined by Eq. (2.21). The quantity in brackets \( \{ \ldots \} \) is, in general, some function of the kinematics, \( \mathcal{M}(x, N, Q^2) \), that can be computed once beforehand for each value of \( N \) along the Mellin inversion contour.

In fact, certain moments of the polarized structure functions themselves have significance in QCD and are worth mentioning here. The \( N = 1 \) moment of the \( g_2 \) structure function is known as the Burkhardt-Cottingham (BC) sum rule [59],

\[
g_2(1, Q^2) = 0, \tag{3.13}
\]

which can be seen by taking the Mellin moment of the Wandzura-Wilczek relation (Eq. (2.13)). Note that both target-mass corrected twist-2 and twist-3 contributions to the \( g_2 \) structure function, given by Eqs. (3.4) and (3.6), satisfy the BC sum rule. Furthermore, there are
two spin sum rules that are especially relevant for extracting quark polarization contributions to the proton spin. The first is the Bjorken sum rule, which relates the difference between the $N = 1$ moments of the proton and neutron $g_1$ structure functions to the isovector axial charge of the nucleon $g_A$ [60, 61],

$$g_1^p(1, Q^2) - g_1^n(1, Q^2) = \frac{g_A}{6} (1 + \mathcal{O}(\alpha_s)).$$

(3.14)

The other is the Ellis-Jaffe sum rule, which at NLO in $\alpha_s$ is given by [8]

$$g_1^p(1, Q^2) = \frac{1}{36} \left[ 8 \Delta \Sigma(Q^2) + 3g_A + a_8 \right] \left( 1 - \frac{\alpha_s(Q^2)}{\pi} + \mathcal{O}(\alpha_s^2) \right),$$

(3.15)

where $\Delta \Sigma(Q^2) = \sum_q \Delta q^+(1, Q^2)$ is interpreted as the total quark spin contribution to the proton, and $a_8$ is the octet axial charge. Both isovector and octet axial charges are related to the lowest moments of the respective nonsinglet combinations of polarized PDFs,

$$\Delta u^+(1, Q^2) - \Delta d^+(1, Q^2) = g_A,$$

$$\Delta u^+(1, Q^2) + \Delta d^+(1, Q^2) - 2\Delta s^+(1, Q^2) = a_8.$$ 

(3.16)

(3.17)

By measuring the $g_1$ structure function in polarized DIS and using information about the isovector and octet axial charges from weak baryon decays assuming SU(3)$_f$ symmetry, details about the quark polarizations can be extracted. However, there are caveats with using the SU(3)$_f$ value for $a_8$ in global QCD analyses with respect to the proton’s strange quark polarization $\Delta s^+$, which is left for discussion in Chapter 5.

Another quantity of interest is the $d_2$ moment, which is defined as a linear combination
of the $N=3$ moments of the polarized structure functions \[62\],

$$d_2(Q^2) = 2g_1(3, Q^2) + 3g_2(3, Q^2).$$

(3.18)

Similar to the case for the BC sum rule, one can see from the Wandzura-Wilczek relation that the leading twist contributions to the structure functions cancel in the above expression. Therefore, the leading contribution to the $d_2$ moment enters at twist-3 in the OPE, and can be defined entirely in terms of the $N=3$ moments of the twist-3 parton distributions $D_q(3, Q^2)$,

$$d^{(\tau3)}_2(Q^2) = 2 \sum_q e_q^2 D_q(3, Q^2).$$

(3.19)

The $d_2$ moment is of particular interest because it can be related to the nucleon’s electric and magnetic color forces \[63\] and “color polarizability” \[62, 64–66\]. Recently, a high precision experiment from Jefferson Lab provided data on the neutron $d_2$ moment from DIS on a $^3$He target \[45\]. In this case, however, one must treat bound nucleon effects that are inherent in nuclear targets in order to properly extract information about nucleon spin structure.

### 3.2 Nuclear Corrections

Since the discovery of the EMC effect \[67\], it has been known that nucleon parton structure is altered in bound state nuclei. For light nuclei, where information about the nuclear wave functions is better known, these bound state effects can be theoretically accounted for when analyzing lepton-nucleus scattering data. For heavier nuclei, recent efforts have been made to determine nuclear structure functions phenomenologically \[68\].
or directly via nuclear PDFs from global QCD analyses [69–72]. The focus of this section is on the former case, in which a reliable treatment of nuclear effects in the deuteron and $^3$He will be discussed. Such nuclei are required to determine neutron quark structure in lepton-nucleus scattering processes due to the instability of free neutrons.

Typically, scattering from nuclei is treated using the plane wave impulse approximation, where the lepton scatters incoherently from a single nucleon in the nucleus [73, 74]. Effects arising from interactions with multiple nucleons are relevant only for lower values of Bjorken-$x$ ($x \ll 1$) [75] and are not considered here. Under the impulse approximation, corrections from nuclear binding and Fermi motion have been developed by Kulagin et al. using the Weak Binding Approximation (WBA) to compute deuterium [76–78] and $^3$He [79] structure functions in both unpolarized and polarized inclusive reactions. The WBA framework has been used to provide overall good descriptions of nuclear to deuterium structure function ratios for a range of nuclei, and therefore is expected also to work well for light nuclei with the smallest binding energies. The formalism has also been tested against quasielastic (QE) deuterium scattering data (discussed in section 3.2.1 below) and performs fairly well for $Q^2 > 1$ GeV$^2$.

Within the WBA framework, the nucleons are considered to be weakly bound in the nucleus. The interacting bound nucleon with mass $M$ has four momentum $p^\mu = (M + \varepsilon, p)$, where $\varepsilon$ is the separation energy. Furthermore, the system is treated nonrelativistically with $|p|, |\varepsilon| \ll M$. The unpolarized structure function for a light nucleus with mass number $A$ can be defined in the WBA to order $p^2/M^2$ as

$$F_i^A(x, Q^2) = \sum_N \int_x^{MA/M} dy \left[ f_{ij}^N(y, \rho) F_j^N \left( \frac{x}{y}, Q^2 \right) \right], \tag{3.20}$$

for $\rho = \sqrt{1 + \gamma^2}$ and $i, j = L, 2$, where the subscript $L$ denotes the longitudinal structure function $F_L = (1 + \gamma^2)F_2 - 2xF_1$, and $F_j^N$ are the unpolarized nucleon structure functions.
introduced in the previous chapter. Similarly, the polarized nuclear structure functions have the general form

$$g_i^A(x, Q^2) = \sum_N \int_{x}^{M_A/M} dy \left[ \Delta f_{ij}^{N/A}(y, \rho) g_j^N \left( \frac{x}{y}, Q^2 \right) \right], \quad (3.21)$$

where $i, j = 1, 2$. Both are given in terms of a one-dimensional convolution of the nucleon structure functions with the nucleon light-cone momentum distributions $(\Delta) f_{ij}^{N/A}$, or alternatively “smearing functions,” of a given nucleus with mass $M_A$. Moreover, Eqs. (3.20) and (3.21) are summed over all nucleons ($p$ and $n$) in the nucleus and implied is an additional sum over the structure function indices $j$.

The smearing functions for both unpolarized and polarized nuclei can be defined generally as

$$s_{ij}^{N/A}(y_N, \rho) = \int \frac{d^4p}{(2\pi)^4} D_{ij}^{N/A}(\varepsilon, p, \rho) \delta \left( y_N - 1 - \frac{\varepsilon + \rho p_z}{M} \right), \quad (3.22)$$

for $s = f$ or $\Delta f$. They are functions of the kinematic variable $\rho$ and light-cone fraction of momentum $y_N = p \cdot q/M\nu = (M + \varepsilon + \rho p_z)/M$ of the nucleus carried by the probed nucleon. The specification of spin dependency comes from the energy-momentum distributions $D_{ij}^{N/A}$, which are defined by coefficients of the spectral function $\mathcal{P}^{N/A}$ [80],

$$\mathcal{P}^{N/A}(\varepsilon, p, S) = \frac{1}{2} \left[ F_0^{N/A} + F_\sigma^{N/A} \sigma \cdot S + F_t^{N/A} (\hat{p} \cdot S \hat{p} \cdot \sigma - \frac{1}{3} S \cdot \sigma) \right]. \quad (3.23)$$

In this expression, $\sigma$ are the Pauli spin matrices, $S$ is the spin vector defined to point along the $z$-axis, and $\hat{p}$ is a unit vector in the direction of the momentum $\mathbf{p}$. Although not explicitly shown, the coefficients depend on the separation energy $\varepsilon$ and magnitude of the nucleon momentum $|\mathbf{p}|$, $F_{0,\sigma,t}^{N/A} \equiv F_{0,\sigma,t}^{N/A}(\varepsilon, |\mathbf{p}|)$.

For unpolarized nuclei, the energy-momentum distribution of nucleons in the nucleus
is given by the coefficient $F_0^{N/A}$,

$$D_{ij}^{N/A}(\varepsilon, p, \rho) = \left(1 + \frac{\rho p_z}{M}\right) C_{ij} F_0^{N/A}, \quad (3.24)$$

such that the spin-averaged smearing function can be defined as

$$f_{ij}^{N/A}(y_N, \rho) = \int \frac{d^4p}{(2\pi)^4} \left(1 + \frac{\rho p_z}{M}\right) C_{ij} F_0^{N/A} \delta \left(y_N - 1 - \frac{\varepsilon + \rho p_z}{M}\right). \quad (3.25)$$

The elements $C_{ij}$ appearing in Eqs. (3.24) and (3.25) are simply kinematic factors and are given by

$$C_{LL} = 1, \quad (3.26)$$
$$C_{L2} = \frac{\gamma^2 p_1^2}{y_N^2 M^2}, \quad (3.27)$$
$$C_{22} = \frac{1}{\rho^2} \left[1 + \frac{\gamma^2}{2y_N^2 M^2} \left(2p^2 + 3p_1^2\right)\right]. \quad (3.28)$$

In the Bjorken limit ($\gamma^2 \to 0, \rho \to 1$), the off-diagonal $C_{L2}$ term is zero and the smearing functions depend only on the kinematic variable $y_N$. In fact, in this limit the unpolarized smearing functions are normalized per nucleon as

$$\int_0^{M_A/M} dy_N f_{ii}^{N/A}(y_N, 1) = 1, \quad \int_0^{M_A/M} dy_N f_{12}^{N/A}(y_N, 1) = 0, \quad (3.29)$$

such that the diagonal function $f_{11}^{N/A}$ can be interpreted as a probability distribution for a given nucleon to have momentum fraction $y_N$ of the nucleus momentum.

For polarized nuclei, the nucleon energy-momentum distributions are described by the longitudinal $F_\sigma^{N/A}$ and tensor $F_\sigma^{N/A}$ spectral function coefficients. The distributions
required to compute the smearing functions for $g_A^1$ are given by

$$D_{11}^{N/A} = \mathcal{F}_{\sigma}^{N/A} + \frac{3 - \rho^2}{6\rho^2} (3\hat{p}_z^2 - 1) \mathcal{F}_t^{N/A} + \frac{p_z}{\rho M} \left( \mathcal{F}_{\sigma}^{N/A} + \frac{2}{3} \mathcal{F}_t^{N/A} \right) + \frac{p^2}{M^2} \frac{(3 - \rho^2)\hat{p}_z^2 - 1 - \rho^2}{12\rho^2} \left( 3\mathcal{F}_{\sigma}^{N/A} - \mathcal{F}_t^{N/A} \right),$$

(3.30a)

$$D_{12}^{N} = \gamma^2 \left[ -\frac{3\hat{p}_z^2 - 1}{2\rho^2} \mathcal{F}_t^{N/A} + \frac{p_z}{\rho M} \left( \mathcal{F}_{\sigma}^{N/A} + \left( \frac{3}{2}\hat{p}_z^2 - \frac{5}{6} \right) \mathcal{F}_t^{N/A} \right) - \frac{p^2}{M^2} \frac{(1 + \hat{p}_z^2(4\rho^2 - 3)) \mathcal{F}_{\sigma}^{N/A} + 5 + 18\hat{p}_z^4\rho^2 - 5\hat{p}_z^2(3 + 2\rho^2) \mathcal{F}_t^{N/A}}{4\rho^2} \right],$$

(3.30b)

and for the $g_A^2$ smearing functions they are

$$D_{21}^{N} = -\frac{3\hat{p}_z^2 - 1}{2\rho^2} \mathcal{F}_t^{N/A} - \frac{p_z}{\rho M} \left( \mathcal{F}_{\sigma}^{N/A} + \frac{2}{3} \mathcal{F}_t^{N/A} \right) - \frac{p^2}{M^2} \frac{3\hat{p}_z^2 - 1}{12\rho^2} \left( 3\mathcal{F}_{\sigma}^{N/A} - \mathcal{F}_t^{N/A} \right),$$

(3.30c)

$$D_{22}^{N} = \mathcal{F}_{\sigma}^{N/A} + \frac{2\rho^2 - 3}{6\rho^2} (3\hat{p}_z^2 - 1) \mathcal{F}_t^{N/A} + \frac{p_z}{\rho M} \left[ -\gamma^2 \mathcal{F}_{\sigma}^{N/A} + \left( \frac{5}{6} + \frac{1}{3}\rho^2 + \hat{p}_z^2(\frac{3}{2} - \rho^2) \right) \mathcal{F}_t^{N/A} \right] + \frac{p^2}{M^2} \left[ \frac{\hat{p}_z^2(3 - 6\rho^2 + 4\rho^4)}{4\rho^2} - 1 - \frac{2\rho^2}{12\rho^2} \mathcal{F}_{\sigma}^{N/A} + \frac{5 - 2\rho^2(1 + 3\hat{p}_z^2) + 4\hat{p}_z^4\rho^4}{12\rho^2} \left( 3\hat{p}_z^2 - 1 \right) \mathcal{F}_t^{N/A} \right].$$

(3.30d)

Similar to the unpolarized case, the smearing distributions for the polarized structure functions are reduced to functions of one variable $y_N$ in the Bjorken limit, and the off-diagonal $D_{12}^{N/A}$ is clearly zero. The nuclear $g_2$ structure function, on the other hand, still has an off-diagonal contribution from the nucleon $g_1^N$ that remains non-zero even for large $Q^2$. Recall, however, that the $g_2$ contribution to the cross section asymmetry $A_1$ vanishes in this limit, since there is a factor of $\gamma^2$ associated with this term in Eq. (2.9).

Integrating the polarized smearing functions over the momentum fraction $y_N$ in the Bjorken limit give zero for the off-diagonal elements, whereas the diagonal terms,

$$P_i^{N/A} = \int dy \Delta_i^{N/A}(y_N, \rho = 1),$$

(3.31)
are non-zero and can be interpreted as the effective polarization of the nucleons in the nucleus. Defining the \( n \)-th momentum-weighted moment of the spectral coefficients as

\[
F_{m/A(n)}^{N/A} \equiv \int \frac{d^4p}{(2\pi)^4} \left( \frac{p}{M} \right)^n F_{m/A}^{N/A}(\varepsilon, p), \quad m = 0, \sigma, t, \quad (3.32)
\]

the effective polarizations \( P_{i}^{N/A} \) can alternatively be given by

\[
P_{1}^{N/A} = F_{\sigma}^{N/A(0)} - \frac{1}{3} \left( F_{\sigma}^{N/A(2)} - \frac{1}{3} F_{t}^{N/A(2)} \right), \quad (3.33a)
\]

\[
P_{2}^{N/A} = F_{\sigma}^{N/A(0)} - \frac{2}{3} \left( F_{\sigma}^{N/A(2)} - \frac{1}{15} F_{t}^{N/A(2)} \right). \quad (3.33b)
\]

The dominant contribution in Eqs. (3.33) comes from the average nucleon polarization in the nucleus, \( F_{\sigma}^{N/A(0)} \), which can be related to orbital wave function states [77, 79, 81].

Up until this point, the expressions given to compute the nuclear structure functions have been general for any light nucleus. The dependence on the nucleus is contained within the definition of the spectral function coefficients, which are composed from information about the nuclear wave functions. In the following sections, we will discuss in particular two applications involving unpolarized electron-deuteron and polarized electron-\(^3\)He scattering, both of which are relevant for PDF extraction in global QCD analyses.

### 3.2.1 Application to unpolarized electron-deuteron scattering

The unpolarized cross section for an electron scattering inelastically from a deuteron with mass \( M_d \) can be written as a linear combination of the nuclear \( F_1^d \) and \( F_2^d \) structure functions,

\[
\frac{d^2\sigma}{d\Omega dE'} = \sigma_{\text{Mott}} \left( \frac{2}{M_d} \tan^2 \frac{\theta}{2} F_1^d(x, Q^2) + \frac{1}{\nu} F_2^d(x, Q^2) \right), \quad (3.34)
\]
where $\sigma_{\text{Mott}}$ is the Mott cross section describing point-like scattering, $\theta$ is the electron scattering angle, and $\nu = E - E'$ is the electron energy loss. In this expression, the nuclear structure functions are given by Eq. (3.20), where the smearing functions are computed in terms of the deuteron spectral coefficients [76–78],

\[ F_{0}^{N/d} = 4\pi^{3} (\psi_{0}^{2} + \psi_{2}^{2}) \delta(\varepsilon - \varepsilon_{D} + p^{2}/2M), \]

\[ F_{\sigma}^{N/d} = 4\pi^{3} (\psi_{0}^{2} - \psi_{2}^{2}/2) \delta(\varepsilon - \varepsilon_{D} + p^{2}/2M), \]

\[ F_{t}^{N/d} = 4\pi^{3} \frac{3}{2} (\psi_{2} - \sqrt{2}\psi_{0}\psi_{2}) \delta(\varepsilon - \varepsilon_{D} + p^{2}/2M). \] (3.35)

Here $\psi_{0}$ and $\psi_{2}$ correspond to the deuteron S- and D-state wave functions in momentum space, respectively, and $\varepsilon_{D}$ is the deuteron binding energy. Furthermore, isospin symmetry is assumed in the deuteron spectral coefficients such that $f_{ij}^{n/d} = f_{ij}^{d} = f_{ij}^{N/d}$. Although only $F_{0}^{N/d}$ will enter into the unpolarized smearing function calculations, for completeness we give in Eq. (3.35) the coefficients $F_{\sigma}$ and $F_{t}$ required to compute the spin dependent contributions.

Despite the WBA being a systematic treatment of nuclear effects, it can be somewhat difficult to test phenomenologically in the kinematic region of inelastic scattering due to the theoretical uncertainty associated with fitted parton distributions that enter into leading twist structure functions. Even so, there has been much effort to study the impact of nuclear corrections on the inelastic deuteron structure functions [68, 82, 83], and also on the extraction of PDFs from deuteron data in global QCD analyses [84–86]. Quasielastic scattering from the deuteron, where an electron scatters elastically from one of the nucleons in the nucleus, also provides insight into deuteron structure and does not rely on PDF input. Furthermore, there exists a significant amount of data on QE electron-deuteron scattering at a broad range of kinematics [87], making it an ideal process to test the WBA formalism.
In elastic scattering from free nucleons with momentum $p$, the structure functions are given by

$$
F_1^{N(\text{el})}(x, Q^2) = \left[ \frac{1}{2} G_{2MN}^2(Q^2) \right] Q^2 \delta ((p+q)^2 - M^2) \tag{3.36a}
$$

$$
F_2^{N(\text{el})}(x, Q^2) = \left[ \frac{G_{2EN}^2(Q^2) + \tau G_{2MN}^2(Q^2)}{1 + \tau} \right] 2p \cdot q \delta ((p+q)^2 - M^2), \tag{3.36b}
$$

where $G_{EN}$ and $G_{MN}$ are the Sachs electric and magnetic form factors, $q$ is the four momentum transfer by the virtual photon ($Q^2 = -q^2$), and $\tau = Q^2/4M^2$. Kinematically, the QE region corresponds to $x = 1$, as can be seen by the delta function $Q^2\delta((p+q)^2 - M^2) = 2p \cdot q \delta((p+q)^2 - M^2) = \delta(1 - x)$. Quasielastic scattering from the deuteron can be described in the WBA by computing Eq. (3.20) with the nucleon structure functions given above. Assuming the interacting nucleons are on shell ($p^2 = M^2$), the delta function in Eqs. (3.36a) and (3.36b) will remove the convolution integral and evaluate the integrands at $y = x$,

$$
x F_1^{d(QE)}(x, Q^2) = \sum_N \left\{ \frac{1}{2} x f_{11}(x, \rho) G_{2MN}^2(Q^2) + x f_{12}(x, \rho) \left[ \frac{G_{2EN}^2(Q^2) + \tau G_{2MN}^2(Q^2)}{1 + \tau} \right] \right\}, \tag{3.37a}
$$

$$
x F_2^{d(QE)}(x, Q^2) = \sum_N x f_{22}(x, \rho) \left[ \frac{G_{2EN}^2(Q^2) + \tau G_{2MN}^2(Q^2)}{1 + \tau} \right]. \tag{3.37b}
$$

The kinematic region $x \sim 1$ remains the same, but the peak is now broadened over a wider range in $x$ due to the nuclear smearing. The cross section for QE electron-deuteron scattering is then constructed identically to Eq. (3.34) where the inelastic structure functions are substituted by $F_1^{d(QE)}$ and $F_2^{d(QE)}$ given above.

A theoretical prediction of the SLAC quasielastic scattering data from Lung et. al. [91] is given in Figs. 3.1 and 3.2 for various electron beam energies $E$ and scattering angles $\theta$. For comparison, the calculations were performed with the Paris [88], WJC-1 [89],
FIG. 3.1: Quasielastic electron–deuteron scattering cross section. The theoretical predictions are given by the WBA with the Paris [88] (green solid curves), WJC-1 [89] (blue dashed curves), and CD-Bonn [90] (red dot-dashed curves) nucleon-nucleon potentials and compared with the SLAC data from Lung [91] (filled circles) at various energies $E$ (in GeV) and scattering angles $\theta$ (in degrees). The values of squared four-momentum transfer at $x = 1$ is given by $Q^2_0$ in each panel and range from $Q^2_0 \approx 1.75$ to 2.5 GeV$^2$. In the first and last panels, the Bjorken limit calculation (black dotted curves) is shown scaled by a factor of 2 for comparison. (Figure from Ref. [22])
FIG. 3.2: Same as Fig. 3.1 but with $Q_0^2$ between 2.5 and 4 GeV$^2$. (Figure from Ref. [22])
FIG. 3.3: Quasielastic scattering cross section data from Arrington et al. [92] with $Q_0^2$ ranging between 1 and 7 GeV$^2$ compared with the theoretical predictions from the various deuteron wave functions, as in Fig. 3.1. The contributions to the cross sections from QE scattering only (black dotted curves) are also given in each panel. (Figure from Ref. [22])
and CD-Bonn [90] deuteron wave functions. Of course, the QE scattering formulas also require information about the electric and magnetic form factors, which are determined phenomenologically. In these results, the Arrington et al. [93] parameterization was used for the proton and the Bosted [94] function for the neutron. However, no significant change in results were found using parameterizations from Kelly [95], differing only by \( \lesssim 2\% \) for the kinematic range presented here.

Clearly the WBA provides an excellent description of the QE scattering data for the range of kinematics given by the SLAC experimental data. On the other hand, if one uses smearing functions computed in the Bjorken limit \((\rho \to 1)\), the agreement deteriorates significantly as the first and last panels in Fig. 3.1 show. In addition to a narrower QE peak width, the magnitude is \( \approx 2 \) times larger for \( Q^2 \sim 2 \text{ GeV}^2 \). Thus the full, finite-\( Q^2 \) expressions are absolutely necessary to describe the QE region at lower values of \( Q^2 \).

The excellent agreement can again be seen in the comparison with Jefferson Lab’s E89-008 experimental data by Arrington et al. [92] shown in Fig. 3.3. Here the applicability of the WBA is shown for a larger range of \( Q^2 \sim 1 \) to 7 GeV\(^2\). However, as the value of \( Q^2 \) increases, contributions from inelastic scattering become relevant at larger \( x \). In the calculations of the QE cross sections, the inelastic contribution was added by computing Eq. (3.34) with the Bosted-Christy (BC) parameterization of the deuteron structure functions \( F_1^d \) and \( F_2^d \) [96]. A comparison with the cross section of QE scattering alone is shown in Fig. 3.3 and shows a worse agreement of the QE peak as \( Q^2 \) increases, indicating the importance of adding the inelastic contribution to fully describe the scattering data.

Additional comparisons with experimental data can be found in Ref. [22], along with a systematic treatment of off-shell corrections where the nucleon virtuality \((p^2)\) dependence is explicitly taken into account in the nucleon structure functions. The purpose of the discussion here was to briefly illustrate the reliability of the WBA model, which is relevant in order to extract information of PDFs from inelastic electron-deuteron scattering data.
3.2.2 Application to polarized electron-\(^3\)He scattering

Another important aspect of nuclear corrections is the application to scattering processes that involve a \(^3\)He target. Polarized reactions in particular provide crucial information on the spin structure of the neutron. With recent high-precision Jefferson Lab data on \(^3\)He targets [44–46], a proper treatment of nuclear effects has become relevant to reliably determine the polarization of the neutron constituents.

The relevant observables that describe polarized DIS from \(^3\)He targets consist of parallel and perpendicular spin asymmetries which have been discussed previously in Chapter 2. The spin-averaged and spin-dependent \(^3\)He structure functions that enter in Eqs. (2.6) and (2.7) are given in the WBA by Eqs. (3.20) and (3.21), where the light-cone momentum distributions are now expressed in terms of the \(^3\)He spectral coefficients. For the case in which the electron probes one of the protons in the nucleus, the spectral function contains two contributions [79],

\[
\mathcal{F}_m^p(E, \bm{p}) = \mathcal{F}_m^{p(\text{bound})}(\bm{p})\delta (E + \varepsilon_{^3\text{He}} - \varepsilon_d) + \mathcal{F}_m^{p(\text{cont})}(E, \bm{p}),
\]

(3.38)

arising from intermediate bound deuteron states (\(\mathcal{F}_m^{p(\text{bound})}\)) and free nucleon continuum states (\(\mathcal{F}_m^{p(\text{cont})}\)). On the other hand, the neutron spectral function only contains the (pp) continuum scattering states

\[
\mathcal{F}_m^n(E, \bm{p}) = \mathcal{F}_m^{n(\text{cont})}(E, \bm{p}).
\]

(3.39)

Unlike the deuteron, where the spectral functions are written as a simple combination of orbital state wave functions, the \(^3\)He coefficients are highly nontrivial and depend on models constrained by experimental data. Two such models that are commonly used in the literature are from Kievsky et al. (KPSV) [97] and from Schulze and Sauer (SS) [80].
TABLE 3.1: Effective polarization parameters $F_{\sigma/N}^{N/He(0)}$, $F_{\sigma/N}^{N/He(2)}$, $F_{t/N}^{N/He(2)}$ and the average polarizations $P_{1}^{N/He}$ and $P_{2}^{N/He}$ for the neutron and proton, from the KPSV [97] and SS [80] (in parentheses) spectral functions. (Table taken from Ref. [23])

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<th>$F_{\sigma/N}^{N/He(0)}$</th>
<th>$F_{\sigma/N}^{N/He(2)}$</th>
<th>$F_{t/N}^{N/He(2)}$</th>
<th>$P_{1}^{N/He}$</th>
<th>$P_{2}^{N/He}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>neutron</td>
<td>0.856</td>
<td>0.018</td>
<td>0.013</td>
<td>0.851</td>
<td>0.844</td>
</tr>
<tr>
<td></td>
<td>(0.888)</td>
<td>(0.016)</td>
<td>(0.010)</td>
<td>(0.884)</td>
<td>(0.878)</td>
</tr>
<tr>
<td>proton</td>
<td>-0.029</td>
<td>-0.002</td>
<td>0.009</td>
<td>-0.028</td>
<td>-0.028</td>
</tr>
<tr>
<td></td>
<td>(-0.022)</td>
<td>(-0.001)</td>
<td>(0.004)</td>
<td>(-0.021)</td>
<td>(-0.021)</td>
</tr>
</tbody>
</table>

former use a sophisticated variational approach to model the $^3$He wave function, whereas SS solves modified Fadeev equations with three-body forces.

A comparison of the two models is presented in Table 3.1, where values of the integrated spectral functions (Eq. (3.32)) are given along with the effective polarization values $P_{1}^{N/He}$ and $P_{2}^{N/He}$. The average neutron polarization $F_{\sigma/He}^{n/He}$ is by far the largest contribution to the $^3$He polarization, amounting to 86% and 89% for KPSV and SS, respectively. The averaged proton polarization $F_{\sigma/He}^{p/He}$ is small and negative, with $-3\%$ ($-2\%$) for KPSV (SS), indicating an approximate cancellation between the two proton spins in the $^3$He nucleus. This is precisely the reason $^3$He is such an effective scattering target to study neutron polarization.

Overall, the $p^2$-weighted integrals of the spectral coefficients are rather small for both $F_{\sigma}$ and $F_{t}$, reducing the effective polarizations by $<3\%$ for both neutron and proton. Although the tensor moment $F_{t/He}^{p/He(2)}$ for the proton is a sizable, $\approx 10\% - 15\%$ fraction of the average proton polarization, the contribution to $P_{1}$ and $P_{2}$ are negligible due to the suppression factors of $\sim 10$ and $\sim 20$ in Eqs. (3.33). The $<3\%$ contribution from the higher power corrections are especially insignificant when compared to the $\sim 4\%$ and $\sim 15\%$ differences between the $^3$He wave function models [80, 97] for the neutron and proton, respectively.

Before illustrating the effects of the smearing corrections on DIS structure functions
and asymmetries, it is important to briefly discuss contributions from non-nucleonic degrees of freedom. It has long been known that the quark structure of the proton can be altered by a pion cloud effect [98–101]. Similarly, the presence of pions in nuclei has been studied as the origin for the redistribution of quark momentum in nuclei that leads to the EMC effect [102]. Such meson corrections necessarily involve intermediate baryonic states such as the Δ(1232), which can be struck by the lepton probe in DIS processes.

More specifically, DIS from an intermediate Δ in a polarized \(^3\text{He}\) target results in a modified nuclear \(g_1\) structure function,

\[
g_{1}^{\text{He}}(x, Q^2) = g_{1}^{\text{He}}(x, Q^2)|_N + g_{1}^{\text{He}}(x, Q^2)|_\Delta, \tag{3.40}
\]

where the first term is the nucleonic contribution given by Eq. (3.21) and the second is the Δ correction which has been worked out by Bissey et al. [103]. In this framework, Fermi motion of the Δ is neglected and its contribution to \(g_{1}^{\text{He}}\) can be defined in terms of \(N \rightarrow \Delta\) transition structure functions and effective polarizations \(P_{1}^{N\Delta}\),

\[
g_{1}^{\text{He}}(x, Q^2)|_\Delta = 2 \left[ P_{1}^{n\Delta^0}_n g_{1}^{n\Delta^0}(x, Q^2) + P_{1}^{p\Delta^+}_p g_{1}^{p\Delta^+}(x, Q^2) \right]. \tag{3.41}
\]

The \(n \rightarrow \Delta^0\) and \(p \rightarrow \Delta^+\) transition structure functions turn out to be equal in valence quark models [104, 105] that relate them to the nucleon \(g_{1}^n\) and \(g_{1}^p\) structure functions [103],

\[
g_{1}^{n\Delta^0}(x, Q^2) = g_{1}^{p\Delta^+}(x, Q^2) = \frac{2\sqrt{2}}{5} \left[ g_{1}^p(x, Q^2) - 4g_{1}^n(x, Q^2) \right]. \tag{3.42}
\]

To complete the calculation of Eq. (3.41), the sum of the effective polarizations for the
corresponding transitions is given by

$$P_1^n \Delta^0 + P_1^p \Delta^+ = \frac{5}{4\sqrt{2}} \frac{(P_1^n - P_1^p - g_3^{\text{He}}/g_A)(g_1^p(1) - g_1^n(1))}{g_1^p(1) - 4g_1^n(1)}, \quad (3.43)$$

where $g_1^{p,n}(N)$ are the $N = 1$ moments of the polarized structure function, $P_1^{p,n}$ are the nucleon effective polarizations given by Eq. (3.33), and $g_3^{\text{He}}$ is the axial vector charge measured in $^3\text{H}$ $\beta$ decay [106]. Eq. (3.43) is derived from the previous Eqs. (3.40)–(3.42) using the relation between the lowest moment of the isovector structure function for a $^3\text{He}-^3\text{H}$ system and the Bjorken sum rule [60],

$$\frac{g_3^{\text{He}}(1) - g_3^{\text{He}}(1)}{g_1^p(1) - 4g_1^n(1)} = \frac{g_3^{\text{He}}}{g_A}, \quad (3.44)$$

This ratio has been experimentally determined to be $\approx 4\%$ smaller than unity [106] which has been attributed to the admixture of the $\Delta$ isobar in the three-nucleon wave function [107]. Such effects are relevant then to include in polarized DIS structure functions.
In Fig. 3.4, the polarized $g_1$ and $g_2$ DIS structure functions of the free neutron are compared with the $^3$He structure functions with various nuclear corrections. In the effective polarization approximation (EPA), where the light-cone momentum distributions are treated in the large-$Q^2$ and zero binding limits ($\Delta f^N_{ji}/f^{He} \sim \delta(1-y)$, $\Delta f^N_{i\neq j} = 0$), the nuclear structure functions can be constructed as a simple linear combination of the effective polarizations and the polarized nucleon structure functions,

$$g_i^{^3\text{He}}(x, Q^2) = 2P_i^p g_i^p(x, Q^2) + P_i^n g_i^n(x, Q^2), \quad i = 1, 2. \quad (3.45)$$

In this calculation, and all others presented in this section, the nucleon structure functions are computed at leading order with the DSSV parameterization [20] for the polarized PDFs and the KPSV spectral function coefficients [97] for the light-cone momentum distributions. The EPA calculation is compared with the smearing formalism in the Bjorken limit and with the full finite-$Q^2$ convolution given by Eq. (3.21).

In fact, the difference between the EPA and the full finite-$Q^2$ corrected structure functions in Fig 3.4 is shown to be negligible in the $0 < x < 0.5$ region for both $g_1$ and $g_2$, becoming slightly more pronounced at higher $x$, where the structure function is smaller. The contrast between the free neutron and $^3$He structure functions can then be understood simply with the EPA, where $|g_i^{^3\text{He}}| > |g_i^n|$ is a result of the factor $2P_i^p \sim -5\%$ in Eq. (3.45) overcompensating the $\sim 15\%$ reduction in magnitude from $P_i^n$. A quantitatively similar effect is seen for $g_2$, where the sign is reversed compared to $g_1$.

Also shown in Fig 3.4 is the EPA with the contribution from the $\Delta$ (Eq. (3.40)), which shows a considerably larger effect on the polarized structure function in the intermediate $0.1 \lesssim x \lesssim 0.4$ region. At $Q^2 = 5$ GeV$^2$, the DSSV and KPSV values for the polarized PDFs and effective polarizations, respectively, yield a value of $P_1^n \Delta^0 + P_1^p \Delta^+ = -0.0125$ in Eq. (3.43). Note that since there is no analogous Eq. (3.44) for $P_2^N \Delta$, the effect on $g_2$ from
FIG. 3.5: As in Fig. 3.4, but for the polarization asymmetries $A_1$ and $A_2$ of the neutron and $^3$He at $Q^2 = 5$ GeV$^2$, constructed from ratios of the spin-dependent structure functions in Fig. 3.4 and the unpolarized $F_1$ structure function from the NMC parametrization [108]. Note that the $^3$He asymmetries are scaled by a factor $(1 + 2F_p^1/F_n^1)$. (Figure from Ref. [23])

the $\Delta$ contribution to the $^3$He wave function is instead derived from $g_1$ using the WW approximation (Eq. (2.13)).

More notable distinctions between the various nuclear corrections are found in the $^3$He spin asymmetries given in Fig. 3.5. Since the $^3$He asymmetries are substantially smaller than the free neutron asymmetries, as a result of the unpolarized $F_1^n \ll F_1^{^3\text{He}}$ compared to the polarized $g_{1,2}^{^3\text{He}} \approx g_{1,2}^n$ in Eq. (2.9), the calculation of $A_{1,2}^{^3\text{He}}$ is corrected by a factor $(1 + 2F_p^1/F_n^1)$. This compensates for the suppression of the asymmetries from the small proton contribution in $g_{1,2}^{^3\text{He}}$ and allows them to be displayed on the same scale. Of course, since the denominator of the asymmetries depends on the $^3$He spin-averaged structure function $F_1^{^3\text{He}}$, nuclear corrections must be included here as well. This is done using the NMC parameterization [108] of $F_1^p$ and $F_1^n$ with the WBA formalism (Eq. (3.20)).

The effects from the different nuclear corrections in Fig 3.5 for $A_1$ are qualitatively similar to the polarized structure function $g_1$. However, in the large $x > 0.6$ region the full finite-$Q^2$ smearing formalism becomes more relevant to describe the $^3$He asymmetry than the EPA. On the other hand, $A_2^{^3\text{He}}$ shows a much closer agreement with the free
neutron $A_1^n$ in the DIS region. While the $A_2^{3\text{He}}$ is primarily described by the $g_2^{3\text{He}}$ structure function, any difference between $A_2^{3\text{He}}$ and $A_2^n$ will indirectly arise from the nuclear effects in $g_1^{3\text{He}}$ at $Q^2 = 5$ GeV$^2$, as a result of using the WW relation (Eq. (2.13)). Since the nuclear corrections in Fig 3.4 are similar in magnitude and opposite in sign, there is a cancellation between the effects in the polarized structure functions, leading to roughly equivalent scaled $^{3}\text{He}$ and free neutron asymmetries.

To conclude the discussion of nuclear effects, Fig. 3.6 shows the $d_2$ moment computed by Eq. (3.18) with the same nuclear approximations given previously. In addition to using the DSSV polarized PDFs to describe the DIS region, included also is the MAID parameterization [109] for the nucleon resonance region, which is taken here to be $W^2 < 3$ GeV$^2$. Recall, however, that since the leading contribution to the $d_2$ moment is at twist-3, the leading twist PDFs from DSSV will effectively be negligible and the $d_2$ prediction will consist primarily of the resonance region fit from MAID.

As $Q^2$ increases, the magnitude of $d_2$ decreases quickly and the nuclear effects appear
small compared to the free neutron $d_2$ moment. However, the relative size of the nuclear corrections can be seen in the ratio $d_2^{^3\text{He}}/d_2^n$, which rises dramatically with increasing $Q^2$ for all of the nuclear models, ranging from $\approx 2 - 4$ times larger in magnitude than the free neutron case for $Q^2 > 3 \text{ GeV}^2$. As a comparison, contributions to $d_2$ from the quasielastic peak were computed using a straightforward extension of the QE formalism presented in the previous section, where the proton and neutron form factors were taken from Refs. [93] and [95], respectively. The effect is shown in Fig 3.6 and is significantly larger (and opposite in sign) than the inelastic calculation. A more thorough analysis of the $^3\text{He}$ (as well as $^3\text{H}$) QE region will be featured in a forthcoming publication [110].

Overall, it is quite clear that a precise method of including nuclear effects is needed to describe the polarization of the neutron from $^3\text{He}$ data. Although $^3\text{He}$ observables in DIS can be described just as well with the EPA at lower values of $x$, the nuclear effects become increasingly important for the higher-$x$ Jefferson Lab data. In fact, the kinematic phase space of Jefferson Lab data requires a careful treatment of all finite-$Q^2$ corrections from higher twist in addition to the nuclear effects. The practical aspects of including such corrections in global QCD analyses of polarized PDFs will be discussed in the following chapter.
CHAPTER 4

Aspects of Fitting

In the previous chapters, it was shown that high-energy scattering observables can be described in QCD by factorization of the hard scattering and soft nonperturbative regions. Since nonperturbative parton dynamics are encoded in PDFs and FFs, the functions must be determined from experimental data through global QCD analyses. In this chapter, the discussion will focus on the practical aspects of these global QCD studies: optimization of fit parameters, estimation of uncertainties, function parameterization, and experimental observables used in the fitting procedure.

Although we will elaborate on some general fitting methodologies not used in this work, the remaining topics will pertain to three specific analyses performed by the Jefferson Lab Angular Momentum (JAM) collaboration. The first, known as JAM15, is an iterative Monte Carlo (IMC) analysis of quark helicity distributions that studied the impact of Jefferson Lab DIS data on both leading and higher twist distributions [15]. The subsequent global analysis, JAM16, was the first extraction of FFs from SIA observables using Monte Carlo methods [24]. Lastly, the JAM17 analysis was the first-ever simultaneous fit of spin dependent PDFs and FFs, with an emphasis on the impact of SIDIS data on the sea quark...
polarizations [25].

4.1 Bayesian Approach

The key objective in any global QCD fit is to obtain an accurate description of the experimental data with a given model. Statistically speaking, this is accomplished by determining the probability \( P \) of obtaining a specific set of model parameters \( \mathbf{a} = \{a_0, a_1, \ldots, a_n\} \) in a single measurement given knowledge from the data \( D \). This is written \( P(\mathbf{a}|D) \) and can be computed using Bayes' formula,

\[
P(\mathbf{a}|D) = \frac{1}{Z} \mathcal{L}(D|\mathbf{a}) \pi(\mathbf{a}),
\]

where \( Z \) is called the “evidence” parameter and acts as the normalization factor,

\[
Z = \int d^n \mathbf{a} \mathcal{L}(D|\mathbf{a}) \pi(\mathbf{a}).
\]

In these expressions, \( \mathcal{L} \) is the likelihood function and \( \pi \) is the prior probability distribution. The former describes the probability of the data to be inferred from a choice of model parameters, and the latter is the pre-informed probability distribution of the parameters. In the context of the JAM QCD analyses, the prior distribution is set to be flat to avoid bias in parameter optimization. However, it can also be used rather conveniently to restrict regions of parameter space that correspond to unphysical distributions.

With the posterior probability distribution \( P(\mathbf{a}|D) \), we can compute the expectation
value and variance of an observable $O$ that we are interested in,

$$
E[O] = \int d^n a \, \mathcal{P}(a|D) \, O(a), \quad (4.3)
$$

$$
V[O] = \int d^n a \, \mathcal{P}(a|D) \, (O(a) - E[O])^2. \quad (4.4)
$$

Evaluating these integrals is, in fact, nontrivial in global QCD analyses since we do not know a priori the functional form of the posterior distribution. Even if assumptions are made, the collinear distributions are typically parameterized with more than one degree of freedom, rendering the integrals multi-dimensional. Furthermore, the integrations must be performed for each kinematic value at which the observable $O$ is evaluated. Thus computing $E[O]$ and $V[O]$ quickly becomes numerically inefficient and impractical for global QCD fits. The integrals can be estimated statistically, however, in a number of ways.

### 4.2 Method of Maximum Likelihood

Perhaps the most common technique in global QCD studies is the method of maximum likelihood, or more specifically, the method of least squares, where the likelihood function is assumed to be Gaussian in the data,

$$
\mathcal{L}(D|a) = \exp \left[ -\frac{1}{2} \sum_{i}^{N_{\text{dat}}} \left( \frac{D_i - T_i(a)}{\delta D_i} \right)^2 \right]. \quad (4.5)
$$

Here $\delta D_i$ is the uncertainty on the $i$-th data point, $T_i(a)$ is the corresponding model prediction, and the sum runs over all data points $N_{\text{dat}}$. The quantity in the exponential is
the $\chi^2$, which is given by the log-likelihood function,

$$
\chi^2(a) = -2\ln\mathcal{L}(D|a) + C = \frac{1}{2} \sum_{i}^{N_{\text{dat}}} \left( \frac{D_i - T_i(a)}{\delta D_i} \right)^2,
$$

where $C$ is some constant. Note that the expressions given above are specifically for data points that are independent of one another. If the data being considered are statistically correlated, the $\chi^2$ can be written as a product of matrices,

$$
\chi^2(a) = \sum_{i,j} (D_i - T_i(a))(\text{cov}^{-1})_{ij}(D_j - T_j(a)),
$$

where $\text{cov}_{ij} = E[(D_i - E[D_i])(D_j - E[D_j])]$ is the covariance matrix of the data. In either case, the best fit parameters are obtained through $\chi^2$ minimization which, in return, maximizes the likelihood function. The expectation value for an observable is then computed by evaluating the observable with the optimized model parameters $a_0$,

$$
E[\mathcal{O}] = \int d^n a \ P(a|D) \ \mathcal{O}(a) \simeq \mathcal{O}(a_0).
$$

The variance, on the other hand, requires an additional framework to be properly treated in the maximum likelihood method.

### 4.2.1 Hessian Error Propogation

There are several approaches to error estimation when using the method of least squares, but most commonly implemented in PDF analyses is the Hessian technique [111, 112]. Within this framework, the errors are derived by expanding the $\chi^2$ up to second
order about its minimum,

\[ \chi^2(a) \approx \chi^2(a_0) + \sum_{i,j} \Delta a_i H_{ij} \Delta a_j, \tag{4.9} \]

where \( \Delta a_i(\Delta a_j) \) is the difference between the \( i(j) \)-th parameter and its corresponding minimized value, and \( H_{ij} \) is the Hessian matrix defined as

\[ H_{ij} = \frac{1}{2} \left. \frac{\partial^2 \chi^2(a)}{\partial a_i \partial a_j} \right|_{a=a_0}. \tag{4.10} \]

In fact, the Hessian is equivalent to the inverse of the covariance matrix of the parameters, \( H_{ij} \equiv C^{-1}_{ij} = E[(a_i - E[a_i])(a_j - E[a_j])]^{-1} \), which can be obtained from the \( \chi^2 \) minimization procedure. As a result of expanding the \( \chi^2 \), the probability distribution \( \mathcal{P}(a|D) \) is proportional to the exponential of the second order term,

\[ \mathcal{P}(a|D) \propto \exp \left( -\frac{1}{2} \chi^2(a) \right) \propto \exp \left( -\frac{1}{2} \sum_{i,j} \Delta a_i H_{ij} \Delta a_j \right). \tag{4.11} \]

Assuming a linear approximation for the observable \( \mathcal{O} \),

\[ \mathcal{O}(a) \approx \mathcal{O}(a_0) + \sum_i \Delta a_i \frac{\partial \mathcal{O}}{\partial a_i}, \tag{4.12} \]

the formula for the variance \( V \) given in Eq. (4.4) can then be approximated by,

\[ V[\mathcal{O}] \approx \frac{1}{(2\pi)^{n/2}} \int d^n a \exp \left[ -\frac{1}{2} \sum_{i,j} \Delta a_i H_{ij} \Delta a_j \right] \left( \sum_{k,l} \frac{\partial \mathcal{O}}{\partial a_k} \frac{\partial \mathcal{O}}{\partial a_l} \Delta a_k \Delta a_l \right). \tag{4.13} \]

where \( 1/(2\pi)^{n/2} \) is the standard \( n \)-dimensional Gaussian normalization. This expression doesn’t appear any simpler since the integration is still present and the derivatives of the observables with respect to each parameter must be known. However, Eq. (4.13) can be
further reduced if one diagonalizes the Hessian matrix and expresses the formula in terms of the eigenvalues and eigenvectors of the parameter space.

By diagonalizing the Hessian matrix, the parameter displacements $\Delta a_i$ can be written as a linear combination of eigendirections $\hat{e}_{i,k}$,

$$\Delta a_i = \sum_k \frac{t_k}{\sqrt{\lambda_k}} \hat{e}_{i,k}, \quad (4.14)$$

where $\lambda_k$ are the Hessian eigenvalues, $\sum_j H_{ij} \hat{e}_{j,k} = \lambda_k \hat{e}_{i,k}$, and $t_k$ is the length along eigendirection $k$. Using the fact that the eigenvectors $\hat{e}$ are orthonormal, Eq. (4.13) can be reduced to

$$V[\mathcal{O}] \approx \sum_k t_k^2 \left( \frac{\partial \mathcal{O}}{\partial t_k} \right)^2 \approx \sum_k \left( \frac{\mathcal{O}(t_k = +1) - \mathcal{O}(t_k = -1)}{2} \right)^2, \quad (4.15)$$

where the final result was obtained by instead traversing back-to-back in scaled eigendirections such that $\mathcal{O}(t_k = \pm 1) \equiv \mathcal{O}(a_0 \pm \sqrt{\lambda_k} \hat{e}_k)$. This corresponds to a shift in the minimum $\chi^2$ by one unit ($\Delta \chi^2 = 1$), or equivalently a 68% confidence level for a Gaussian distribution. In summary then, one simply needs to compute the inverse of the covariance (i.e. Hessian) matrix of the parameters, obtain its eigenvalues and then shift the parameters according to Eq. (4.15) for each eigendirection.

Although Hessian error propagation provides a systematic treatment of uncertainties for the method of least squares, the assumptions being made can be problematic for global QCD analyses. For example, the behavior of $\Delta \chi^2$ along the eigendirections is presumed to be quadratic. In practice, function parameters that are difficult to constrain will have relatively flat directions that correspond to large eigenvalues, causing the computation of the Hessian matrix to be numerically unstable. To remedy this, the uncontrolled parameter values are fixed at the cost of potentially biasing the fit results.
Furthermore, the choice of $\Delta \chi^2 = 1$ for the eigendirection shift can lead to underestimated uncertainties due to the insufficiency of the linear approximation in Eq. (4.12). This is accounted for by multiplying Eq. (4.15) with a tolerance parameter $T^2$, the choice for which is somewhat arbitrary and varies among different global studies, leading to a rather ambiguous reflection of the true uncertainties. However, all of the assumptions that are discussed here can be avoided altogether using Monte Carlo methods to evaluate the integrals in Eq. (4.4).

4.3 Monte Carlo Techniques

When the number of model parameters and experimental measurements becomes increasingly large, a more rigorous statistical approach is needed to properly extract physical information in global QCD fits. While Monte Carlo (MC) techniques are often used in this respect, they come with the cost of being computationally more expensive. Despite this, such procedures can provide indispensable tools for error estimation.

The primary objective for any MC method is to obtain a precise representation of the probability distribution $P(a|D)$ such that the expectation value and variance integrations can be approximated by weighted sums,

$$E[\mathcal{O}] \simeq \sum_k w_k \mathcal{O}(a_k),$$

$$V[\mathcal{O}] \simeq \sum_k w_k (\mathcal{O}(a_k) - E[\mathcal{O}])^2,$$

where $w_k$ is the weight for the $k$-th parameter set $a_k$ and the sum of over all weights is one, $\sum_k w_k = 1$. The set of parameters and their corresponding weights is called the sample distribution of $P(a|D)$, and obtaining such information is dependent on the MC technique used.
4.3.1 Data Resampling and Cross Validation

One particular way of obtaining a sample distribution \( \{ w_k, a_k \} \) is by resampling the experimental data using Gaussian smearing and performing a sufficiently large number of \( \chi^2 \) minimizations. For each fit, the pseudo-data set can be constructed as,

\[
D_{k,i}^{(\text{pseudo})} = D_{i}^{(\text{exp})} + \delta D_{i}^{(\text{exp})} R_{k,i},
\]

where \( D_{k,i} \) is the \( i \)-th data point in the \( k \)-th pseudo-data set, \( \delta D_{i}^{(\text{exp})} \) is the corresponding uncertainty from the original data \( D_{i}^{(\text{exp})} \), and \( R_{k,i} \) is a randomly chosen number from the standard normal distribution. The \( \chi^2 \) minimization procedure is then typically performed with a gradient descent algorithm. Upon obtaining an adequate number of optimal parameters \( a_{0,k} \), the sample distribution is then composed of \( N \) equally weighted parameter sets \( \{ w_k = 1/N, a_{0,k} \} \) such that

\[
E[\mathcal{O}] \simeq \frac{1}{N} \sum_k^N \mathcal{O}(a_{0,k}),
\]

\[
V[\mathcal{O}] \simeq \frac{1}{N} \sum_k^N (\mathcal{O}(a_{0,k}) - E[\mathcal{O}])^2.
\]

There is, however, one significant disadvantage when using an MC technique with \( \chi^2 \) minimization to handle a heavily parameterized model. In such case, the \( \chi^2 \) for a given fit can be significantly less than one, indicating an over-fitting of the pseudo-data. The presence of over-fitting also appears as sharp peaks in the probability distribution \( P(a|D) \).

Fortunately, there is a systematic way to prevent such behavior. For each pseudo-data set assembled by Gaussian resampling, a partition can be made to form separate training and validation sets. The parameters can then be optimized with the training set, and at each step in the \( \chi^2 \) minimization procedure, the trained parameters are used to compute
the validation set $\chi^2$. Initially, the $\chi^2$ for both fractions will decrease as the minimization progresses. However, there will be a point in which the validation $\chi^2$ begins to increase as the training set $\chi^2$ continues decreasing, signaling over-fitting of the data. The optimized parameters are then chosen as the set that minimizes the validation $\chi^2$.

This procedure, known as cross-validation (CV), is used with data resampling in the JAM global QCD analyses. Besides seeing a deterioration of the validation $\chi^2$ in the minimization procedure, over-fitting is also present if the difference between the training and validation $\chi^2$ is too large. This occurs when the training partition of the data does not sufficiently represent the full data set. In JAM, an additional criteria for selecting the minimized parameters in JAM is given by

$$\left| \frac{\chi^2_{\text{dof}}^{(\text{training})}}{\text{dof}} - \frac{\chi^2_{\text{dof}}^{(\text{validation})}}{\text{dof}} \right| < 2\epsilon, \quad (4.21)$$

where we set $\epsilon$ to be one standard deviation of the ideal noncentral $\chi^2_{\text{dof}}$ distribution. This particular choice is based on the fact that the distribution of $\chi^2$ values obtained after fitting the resampled data will follow a noncentral $\chi^2$ probability density,

$$P(\chi^2; n, \lambda) = \frac{1}{2} \exp \left[ -\frac{1}{2} (\chi^2 + \lambda) \right] \left( \frac{\chi^2}{\lambda} \right)^{(n-2)/4} I_{n/2-1}(\sqrt{\lambda\chi^2}), \quad (4.22)$$

where $n$ is the number of degrees of freedom ($\approx$ number of data points $N_{\text{dat}}$) and $I_{n/2-1}$ is the modified Bessel function of the first kind. Because of resampling, the distribution of $\chi^2$ values will peak at $\chi^2_{\text{dof}} \sim 2$ due to the non-centrality parameter $\lambda \simeq 2n$, which is given by the sum of the expectation values $E$ of the $\chi^2$ for individual data points, $\lambda = \sum_{i}^{N_{\text{dat}}} E[\chi^2_i]$.

The only significant disadvantage of using the CV technique is that the resulting sample distribution can depend on the choice of partition fraction. There are more sophisticated methods of CV [113–115] that can be used to obtain a less ambiguous representation
of the posterior probability distribution, but these were found to be numerically impractical to implement in the JAM global analyses. Instead, the methodology was improved by introducing an iterative procedure.

### 4.3.2 Iterative Monte Carlo (IMC)

Due to the complexity of the $\chi^2$ topology, there can be many local minima in which the gradient descent algorithms can get stuck. In this case, collecting an ensemble of fits from data resampling and cross validation may not yield an adequate description of the posterior probability distribution. As a solution, the JAM global QCD analyses of spin-dependent PDFs and FFs used an iterative methodology based on data resampling and cross validation.

In Fig. 4.1, a workflow diagram of the iterative Monte Carlo (IMC) technique is shown. The guess parameters that enter a given least-squares fit, which we call the “priors”, are chosen in the initial iteration from flat sampling of the parameter space. Note that since $P(a|D)$ can be multimodal, it is important to have various starting points to adequately explore the parameter space. The fits are then performed with the resampled data (pseudo-data) that have been partitioned 50/50 into training and validation sets. In the JAM analyses, we use the Levenberg-Marquardt lmdiff algorithm [116] to minimize the training $\chi^2$, and the set of optimized parameters, which we call “posteriors”, are chosen according to the CV criteria described in the previous section. From the collection of fit results, a sampler is created and new priors are generated to act as initial guesses for another iteration of $\chi^2$ minimization.

The choice of sampler is not unique in the IMC methodology and has evolved over the course of the JAM global fits. In JAM15, the spin-dependent PDF parameters were collected and sampled from directly for the next iteration of fits. The drawback of this
FIG. 4.1: Workflow of the iterative Monte Carlo fitting strategy. In the upper diagram (red lines) an iteration begins at the prior sampler and a given number of fits are performed generating an ensemble of posteriors. After the initial iteration, with a flat sampler, the generated posteriors are used to construct a multivariate Gaussian sampler for the next iteration. The lower diagram (with blue lines) summarizes the workflow that transforms a given prior into a final posterior. (Figure from Ref. [24])

sampling method in particular is that parameters which became pinned in a local minimum can stay there for subsequent iterations, although data resampling certainly decreases the chances of this occurring. In the JAM16 Monte Carlo analysis of pion and kaon FFs, the parameter central values and covariance matrix were used to construct a multi-variate Gaussian distribution from which the next set of parameters are chosen.

Lastly, the combined polarized PDF and FF analysis sampled from a distribution obtained by Kernel Density Estimation (KDE) [117, 118]. This method provides a non-parametric way to determine a multidimensional probability density function of the pa-
FIG. 4.2: Mean and two-sided standard deviations of the $\chi^2_{dof}$ distribution as a function of the iteration number for the training (blue points) and validation (red points) data sets, compared with the mean (dashed horizontal line at $\chi^2_{dof} = 2$) and standard deviation (yellow band) for the ideal noncentral $\chi^2_{dof}$ distribution. (Figure from Ref. [15])

Parameters from a given sample distribution with size $N$. In KDE, the density function is given by [118]

$$f_N(\mathbf{a}) = \frac{1}{N} \sum_k^n \prod_i \frac{1}{h_i(N)} K_i \left( \frac{a_i - a_{i,k}}{h_i(N)} \right),$$

(4.23)

where the sum is over members of the posterior ensemble and the product is over the different parameters $\mathbf{a} = \{a_0, a_1, \ldots, a_n\}$ such that $a_{i,k}$ is the $i$-th parameter in the $k$-th sample member. The parameter dependent kernel $K$ is chosen to be Gaussian in the JAM17 analysis and therefore is similar to the sampling method used in JAM16. However, there is freedom given for the choice of the bandwidth, or smoothness, parameter $h$ that determines how well the features of the distribution are defined. In fact, this parameter can heavily influence the shape of the resulting distribution regardless of the functional
form of the kernel. In the JAM17 analysis, the final results were obtained using Scott’s Rule [119] for the bandwidth value, \( h_i(N) = h(N) = N^{-1/5} \).

The stopping criteria for the iterative process also varies slightly between JAM15 and the subsequent global fits. The final results of JAM15 were obtained by computing the training and validation set \( \chi^2 \) with the optimized parameters after each iteration. The results are illustrated in Fig. 4.2, where the mean and two-sided standard deviations of the training and validation \( \chi^2 \) are shown along with the mean and standard deviation of the ideal noncentral \( \chi^2_{\text{dof}} \) distribution. After six iterations, the agreement with the noncentral \( \chi^2 \) value is stable, indicating statistical convergence.

Although the \( \chi^2 \) distributions across the iterations do provide some insight to the stability of the uncertainties for the fitted distributions, this criterion does not depend explicitly on the function parameters. Therefore, in JAM16 and JAM17 we instead consider what can be interpreted as the hypervolume that encompasses the posteriors in parameter
space $V$, 

$$V = \prod_i \sqrt{W_i},$$  \hspace{1cm} (4.24)

using the eigenvalues $W_i$ of the covariance matrix. In computing Eq. (4.24) for each iteration, the convergence of the sample distribution $\{w_k, a_k\}$ is more directly determined.

The result for JAM16 is shown in Fig. 4.3, where the prior volume $V$ (constructed from the posteriors of the previous iteration) for pions and kaons are given for each iteration which contain 200 fits in the IMC procedure. A large statistical fluctuation of the prior volume is seen for the first $\sim 10$ iterations, followed by stability at $\sim 20$ iterations as indicated by the shaded bands. Once the region of interest has been isolated by the iterative process, a final iteration containing $10^4$ fits is performed to increase the statistics of our final sample. An identical convergence criterion is used for the JAM17 combined analysis and therefore is not shown here.

In summary, IMC is a statistically rigorous PDF and FF extraction method that improves on the basic data resampling and CV procedures. Although iterating thousands of $\chi^2$ minimizations to obtain a precise representation of the posterior probability distribution is computationally intensive, it is necessary to remove any arbitrariness or assumptions that come with a combined maximum likelihood and Hessian method.

### 4.3.3 Nested Sampling

Another MC method that has more recently become relevant for the JAM collaboration is nested sampling [120, 121]. Although this technique is not used to obtain the results presented in Chapter 5, it has been applied in a recent JAM analysis [122] and will be pertinent for an upcoming simultaneous global fit of unpolarized and polarized scattering data. It is nonetheless important to discuss briefly as an alternative to the data
resampling and CV approach discussed in the previous section.

For our purpose, nested sampling is used to obtain the sample distribution \( \{ w_k, a_k \} \) as a byproduct of estimating the evidence integral \( Z \) given by Eq. (4.2). This is cleverly done via a statistical mapping of the multi-dimensional integration over the prior volume to a single dimension \([120],\)

\[
Z = \int d^n a \, \mathcal{L}(D|a) \pi(a) = \int_0^1 dX \mathcal{L}(X).
\]  
\[(4.25)\]

The one-dimensional integration is then approximated using a simple numerical integration method,

\[
Z \simeq \sum_i w_i \mathcal{L}_i,
\]  
\[(4.26)\]

such as the trapezoidal rule, i.e. \( w_i = \frac{1}{2} (X_{i-1} - X_{i+1}) \), where the points \( X_i \) correspond to a set of parameters that are from the prior volume. Although the values for \( X_i \) for a chosen set of parameters are unknown, they are sorted according to \( X_i = t_i X_{i-1} \), with \( \mathcal{L}(X_i) < \mathcal{L}(X_{i-1}) \), such that \( t_i \) can be statistically estimated.

The algorithm then is rather straightforward. The first step is to initialize \( \mathcal{L}_0 = 0 \) for \( X_0 = 1 \) and sample randomly \( N \) number of active points, where the \( N \) points are organized to have monotonically increasing likelihood values \( \mathcal{L}_0 < \mathcal{L}_1 < \ldots < \mathcal{L}_N \). A sample is then taken from the prior volume and the corresponding likelihood value is computed. The new point is sorted within the list of \( N \) active points and the lowest likelihood value \( \mathcal{L}_i \) is removed. Each time this occurs, the prior volume will shrink approximately by a factor of \( \exp(-1/N) \) such that the lowest likelihood value will have a corresponding value \( X_i = \exp(-i/N) \). The procedure is then iterated until the entire prior volume has been explored.
Eventually, the region of maximum likelihood will be isolated and the procedure will be terminated once a particular criterion, typically based on the spacing of the $X$ values, is met. At this point, the sample distribution is comprised of the set of points in $X$ that were removed by the sorting algorithm, with corresponding weights $w_i$. Following Eqs. (4.1), (4.2), and (4.4), it can be shown that the weights in Eq. (4.17) from nested sampling are

$$w_i = \frac{1}{Z} \frac{1}{2} \sum_{i} \left( X_{i-1} - X_{i+1} \right) C_i,$$

where the trapezoidal sum is used and $Z$ is given by Eq. (4.26). Note that the normalized weights will then be distributed such that the largest contributions will come from the region of maximum likelihood.

Nested sampling is a powerful MC method for estimating the probability $P(a|D)$. Instead of relying on parameter optimization through gradient descent algorithms, the procedure provides a systematic way of exploring the multi-dimensional likelihood topology. Furthermore, the algorithm can be parallelized to increase the numerical efficiency. This aspect in particular is crucial for global QCD analyses that contain a significant number of fit parameters and data sets.

### 4.4 Parameterizations

Now that the JAM fitting methodology has been described, the discussion will continue to specific details about the $\chi^2$ calculation, namely, the parameterization of the nonperturbative distributions. Recall that the theoretical predictions for the various scattering processes are computed in the collinear factorization framework outlined in Chapter 2. Information about the experimental data sets used in the JAM global analyses will be left for the following section.

The functional form for all of the spin-dependent PDFs and FFs extracted in the JAM global fits is given at the initial scale $Q^2_0 = 1 \text{ GeV}^2$ and can be generalized with a
template function $T$,

$$T(x; a) = \frac{M x^a (1 - x)^b (1 + c \sqrt{x} + dx)}{\beta(n + a, 1 + b) + c\beta(n + \frac{1}{2} + a, 1 + b) + d\beta(n + 1 + a, 1 + b)}, \quad (4.27)$$

where $x$ is a general kinematic variable, $a = \{M, a, b, c, d\}$ are the fit parameters, and $\beta$ is the Euler beta function, which can be evaluated for any finite, nonzero $n$. For spin PDFs, the variable $x$ will correspond to the parton momentum fraction, whereas for FFs the kinematic variable is the hadron momentum fraction $z_h$. The corresponding template function in Mellin space is given by a ratio of beta functions,

$$T(N; a) = \frac{\beta(N + a, 1 + b) + c\beta(N + \frac{1}{2} + a, 1 + b) + d\beta(N + 1 + a, 1 + b)}{\beta(n + a, 1 + b) + c\beta(n + \frac{1}{2} + a, 1 + b) + d\beta(n + 1 + a, 1 + b)}, \quad (4.28)$$

where $T(N; a)$ is the $N$-th Mellin moment of Eq. (4.27). In the JAM15 analysis only, the template function was simplified instead to fit the overall normalization parameter $N$ such that $T(x; a) = N x^a (1 - x)^b (1 + c \sqrt{x} + dx)$. Equating this with Eq. (4.27), one can derive a simple relationship between $N$ and $a$ such that the two forms are equivalent. However, Eq. (4.27) is more beneficial to use in that a specific choice for the factor $n$ in the denominator allows us to interpret $M$ as a physical quantity related to the moments of the PDFs or FFs. This is clear from Eq. (4.28) in the case where $N = n$. The choice for $n$ in the JAM global QCD analysis will be discussed in the following.

4.4.1 Helicity distributions and higher twist

Since polarized DIS is sensitive only to the sum of quark and anti-quark helicity distributions $\Delta q^+ = \Delta q + \Delta \bar{q}$, we parameterize in JAM15 the $\Delta u^+$, $\Delta d^+$, $\Delta s^+$ and $\Delta g$ flavors with a single function, i.e. $\Delta q^+, \Delta g = T(x; a_{q^+, g})$. In principle, the $\Delta u^+$ and $\Delta d^+$ distributions will have contributions from both valence and sea quarks, suggesting the need
for two template functions. The polynomial terms $c$ and $d$ that are included in Eq. (4.27), however, are sufficiently flexible to describe the DIS data. Note that while the $a$ and $b$ parameters govern the $x \to 0$ and $x \to 1$ behavior, respectively, the $c$ and $d$ parameters are needed to allow a possible sign change of the distributions. The twist-3 $D_q$ distributions introduced in Eq. (3.7) were parameterized identically to the leading twist distributions in JAM15 for both $u$ and $d$ flavors, as well as the twist-4 structure functions for proton and neutron $H_{p,n}$ given in Eq. (3.11).

In JAM17, the combined spin PDF and FF analysis fit only the leading twist spin PDF distributions along with the FFs. Furthermore, the addition of SIDIS data allowed for a separation of the quark and anti-quark distributions. For this purpose, we parameterize $\Delta\bar{u}$, $\Delta\bar{d}$, and $\Delta\bar{s}$ in addition to the $\Delta q^+$ and $\Delta g$ from JAM15. We also fixed $d = 0$ for all of the collinear spin PDFs since we found significant anti-correlation between $c$ and $d$ and only one sign changing parameter is necessary. This also helped to reduce the significant amount of parameters coming from the combined PDF and FF functions. Lastly, because Eq. (4.27) is used exactly in JAM17, the choice of $n = 0$ is made so that the fit parameter $M$ corresponds to the lowest moment of the helicity distributions, $\Delta q(1)$, at the input scale.

In fact, this value for $n$ has rather important implications for the spin structure of the proton, since the lowest moment of the helicity distributions can be interpreted as the spin contribution from the parton flavor. In addition to insensitivity to the individual quark and anti-quark helicity distributions, the wealth of DIS data only provide information on the appropriate combination of all quark flavors. Information about the strange helicity $\Delta s^+$ then comes from additional SU(3) flavor constraints given by Eq. (3.17) which relates the non-singlet combination of moments to the axial vector charges. In JAM15, we impose such constraints with $g_A = 1.269(3)$ and $a_8 = 0.586(31)$ coming from weak neutron and hyperon decays, respectively. On the other hand, the addition of SIDIS observables allows
an empirical determination of these quantities, and in JAM17 we therefore perform the fits without the SU(3)$_f$ constraints.

4.4.2 Fragmentation functions

Similar to DIS, observables in SIA can only provide information about the sum of the quark and anti-quark FFs. We therefore parameterize in JAM16 the $D_q^+ = D_q^h + D_q^b$ functions for the light $u, d$ and $s$ quarks, as well as $D_g^h$, at the input scale with at least one template function (Eq. (4.27)), setting parameters $c = d = 0$, and choosing $n = 1$ such that the $M$ parameter corresponds to the average momentum fraction $z$. Furthermore, the heavy charm and bottom quark FFs, $D_{c^+}$ and $D_{b^+}$, are parameterized at their mass thresholds, $m_c = 1.43$ GeV and $m_b = 4.3$ GeV, and thus are activated discontinuously in the zero-mass variable flavor evolution scheme. Lastly, we use charge conjugation symmetry to relate $D_q^+ = D_q^- + D_q^g$, and $D_g^+ = D_g^- + D_g^h$.

For pions, the $u^+$ and $d^+$ FFs are related by isospin symmetry. We note here that existing data is currently not sensitive to the difference between $u$ in $\pi^+$ and $d$ in $\pi^-$, especially since the mass difference between the positively and negatively charged pions is much smaller than that between protons and neutrons. Since the isospin differences in the nucleon are expected to be of the order $1 - 2\%$ [123], they are also not distinguished in the polarized PDF parameterization given above. The light $u^+$ and $d^+$ FFs are assigned two independent shapes to represent both the favored and unfavored fragmentation process, e.g. $u \rightarrow \pi^+$ and $\bar{u} \rightarrow \pi^+$, respectively,

$$D_{u^+}^{\pi^+} = D_{d^+}^{\pi^+} = T(z; a_{u,d}^{\pi}) + T(z; b_{u,d}^{\pi}).$$

The two different parameter sets $a_{u,d}^{\pi}$ and $b_{u,d}^{\pi}$ allow flexibility to distinguish the favored and unfavored distributions that are different in behavior and magnitude. The remaining
flavors for pion production are simply given by a single template $D_{s^+,c^+,b^+,g} = T(z; a_{s,c,b,g}^\pi)$.

On the other hand, the distributions that contain the favored process in kaon production, $u^+$ and $s^+$, are parameterized independently due to the mass difference between the up and strange quarks. They are each given two shapes $D_{u^+,d^+,c^+,g} = T(z; a_{u,d,c,b,g}^K)$ and $D_{s^+,d^+,c^+,g} = T(z; a_{s,d,c,b,g}^K)$ for the same reasons as in pion production. The remaining kaon distributions are parameterized with only a single function $D_{d^+,c^+,b^+,g} = T(z; a_{d,c,b,g}^K)$.

In JAM17, we separate the light quark $q^+$ distributions by parameterizing the unfavored quark-to-hadron FFs with a single template. In fact, only one additional function is necessary to constrain the individual flavors in pion and kaon production. For the pion FFs, we parameterize $D_{u^+} = D_{d^+} = T(z; a_{u,d}^\pi)$, which can be derived from isospin and charge conjugation symmetry. The kaon FFs will have additional fit parameters from $D_{s^+}$. The remaining unfavorable light quark distributions are given by $D_{s^+} = (1/2)D_{s^+}^\pi$ and $D_{u^+} = (1/2)D_{d^+}^K$, where the latter is because of the similarity in mass between the $u$ and $d$ quarks. Similar assumptions are made also for the heavy quarks, $D_{c^+} = (1/2)D_{c^+}^h$ and $D_{b^+} = (1/2)D_{b^+}^h$.

### 4.4.3 Penalties and prior information

As mentioned previously, the IMC procedure begins by flat sampling a sufficiently wide region of parameter space to use as guess parameters in $\chi^2$ minimization. In the JAM global QCD analyses, the leading twist PDF distributions are sampled in the range $a \in [-1, 0]$ for the low-$x$ behavior. For the $x \rightarrow 1$ behavior, we sample from $b \in [2, 5]$ for $\Delta u^+$ and $\Delta d^+$ and $b \in [2, 10]$ for $\Delta s^+$ and $\Delta g$. The larger range for the sea distributions $\Delta s^+$ and $\Delta g$ is necessary to reflect a suppression in the large-$x$ region, whereas the $\Delta u^+$ and $\Delta d^+$ have valence contributions and therefore will be less suppressed. Lastly, the sign changing $c$ and $d$ parameters are sampled between values of $-1$ and $1$ and the normalization of the
$\Delta q^+$ and $\Delta g$ are chosen such that the first moment moments of the singlet distribution $\Delta \Sigma(Q_0^2)$ and gluon $\Delta G(Q_0^2) = \Delta g(1, Q^2)$ are equal to 0.5.

Since the shapes for the higher twist distributions studied in JAM15 are less known, the flat sampling regions were set to be slightly more flexible to allow for harder distributions. The higher twist contributions are more relevant at low-$W$ or high-$x$ for fixed $Q^2$, and therefore we sampled $a \in [-1, 1]$ for both twist-3 and twist-4 distributions. The $b, c$ and $d$ parameter ranges are given to be the same as $\Delta u^+$ and $\Delta d^+$. Moreover, as a test of whether we can obtain a signal for higher twist at all from the DIS data, we started the normalizations $\mathcal{N}$ at zero.

The initial flat sampling ranges for the pion and kaon FFs are very similar to the leading twist PDFs. The functions that contain favored components have an upper bound on the $a$ and $b$ sampling regions set equal to that of $\Delta u^+$ and $\Delta d^+$ which have valence contributions. Furthermore, the unfavored quark-to-hadron FFs are parameterized similar to the sea distributions in the proton. On the other hand, the lower bounds for $a$ and $b$ are given by $a > -1.9$ and $b > 0$ such that the first moment of the FFs are finite integrable.

It is important to note that although ranges for all of the distributions are given for initial sampling, the optimized parameters can be distributed outside these regions if the data prefer. In principle, it doesn’t matter where the MC fits start from, as the iterative process will eventually guide the parameters to the region of maximum likelihood. However, to prevent unphysical distributions (e.g. $b < 0$), the JAM15 and JAM16 analyses included hard penalties in the $\chi^2$ if the parameters move outside a physical value. Consequently, this also increases the yield of optimized parameters that are used in the sampler for the next iteration.

The issue with hard $\chi^2$ penalties, however, is that there will be a significant build up of samples at the physical boundaries, potentially biasing the priors of the subsequent iteration. Furthermore, it is possible that parameters navigate through unphysical regions.
of parameter space to reach the true $\chi^2$ minimum. In the combined JAM17 analysis, then, the likelihood function was defined to include Gaussian prior distributions such that the $\chi^2$ has the form

$$
\chi^2 = \sum_i \left( \frac{D_i - T_i(a)}{\delta D_i} \right)^2 + \sum_{\ell} \left( \frac{a_\ell - \mu_\ell}{\sigma_\ell} \right)^2,
$$

(4.30)

where $a_\ell$ is the $\ell$-th fit parameter that is distributed with mean $\mu_\ell$ and width $\sigma_\ell$. The additional term in the $\chi^2$ can heavily bias a global analysis if one chooses $\sigma$ to be too small. For the purpose of preventing unphysical distributions, the prior distributions were set such that they are essentially flat in the regions of interest outlined in this section, and then fall rapidly outside these parameter ranges. The effect allows us to avoid hard boundaries in the $\chi^2$ while still increasing the number of posteriors needed to construct an efficient sampler for the following iteration.

### 4.5 Experimental Data

The final aspect of the $\chi^2$ function yet to be considered is the input from experimental data and uncertainties. The treatment of the latter is a rather involved topic and therefore will only be discussed as it relates to the JAM QCD analyses. Up until this point, the $\chi^2$ has been defined in terms of the uncorrelated uncertainties $\delta D_i$. In practice, experiments will often have correlated systematic uncertainties that must be treated separately.

The JAM global fits incorporate correlated uncertainties by including a normalization factor $N_i^{(e)}$ in the $\chi^2$,

$$
\chi^2(a) = \sum_{\epsilon} \left[ \sum_i \left( \frac{D_i^{(e)} - T_i^{(e)}(a)/N_i^{(e)}}{\delta D_i^{(e)}} \right)^2 + \sum_k \left( \frac{r_k^{(e)}}{\delta r_k^{(e)}} \right)^2 \right],
$$

(4.31)
where in this expression we have made explicit the sum over the experimental sets \((e)\).

The normalization factor \(N_i^{(e)}\) is given by

\[
N_i^{(e)} = 1 - \frac{1}{D_i^{(e)}} \sum_k r_k^{(e)} \beta_{k,i}^{(e)},
\]

(4.32)

where \(\beta_{k,i}^{(e)}\) is the \(k\)-th correlated point-to-point systematic uncertainty and \(r_k^{(e)}\) is a corresponding fit parameter that controls the magnitude of the normalization. As a consequence of fitting the additional \(r_k^{(e)}\) parameters, a penalty is given by the quadrature sum of these values in Eq. (4.33) to limit the size of the data shifts. Since pseudo-data is used as the input for the \(\chi^2\) minimization, we use instead the Pearson’s \(\chi^2\),

\[
\chi^2(a) = \sum_e \left[ \sum_i \left( \frac{D_i^{(e)}}{\delta D_i^{(e)}} - \frac{E[T_i^{(e)}(a)/N_i^{(e)}]}{N_i^{(e)}} \right)^2 \right],
\]

(4.33)

to determine the goodness-of-fit with respect to the original experimental data \(D_i^{(e)}\), where \(E[T_i^{(e)}(a)/N_i^{(e)}]\) is the expectation value of the shifted theory values.

### 4.5.1 Deep inelastic scattering observables

The JAM15 and JAM17 global analyses of spin-dependent PDFs use all available inclusive DIS world data that pass the kinematic cuts on \(Q^2\) and the invariant final state mass \(W^2 = M^2 + Q^2(1-x)/x\). The data consist of various leptons scattering from proton, deuteron, and \(^3\)He targets. In Fig. 4.4, the region of kinematic phase space covered by the experiments are shown with the \(W^2 = 4\) GeV\(^2\) and 10 GeV\(^2\) boundaries. For a cut at \(W^2 = 10\) GeV\(^2\), most of the data from EMC [124], SMC [125, 126], COMPASS [127–129], SLAC [130–137] and HERMES [138–140] are included. At the lower boundary, additional high-precision data from Jefferson Lab’s Hall A [44, 45, 141] and CLAS [41–43]
collaborations become available.

In the JAM15 global QCD fit, a cut was made at $W^2 = 4 \text{ GeV}^2$ and $Q^2 = 1 \text{ GeV}^2$. This choice was made based on a series of IMC analyses that were performed with varying cuts on $W^2$ and $Q^2$ and included the higher order corrections described in Chapter 3. The resulting $\chi^2_{\text{dof}}$ values are given in Tables 4.1 and 4.2. For a fixed value of $Q^2 = 1 \text{ GeV}^2$, lowering $W^2$ from 10 GeV$^2$ to 4 GeV$^2$ dramatically increases the number of data points from $\sim 1000$ to $\sim 2500$, most of which come from Jefferson Lab. Within this range, the increase in the $\chi^2_{\text{dof}}$ is not significant. However, upon decreasing the $W^2$ cut to 3.5 GeV$^2$,
TABLE 4.2: Dependence of the global fits on the cut on the four-momentum transfer squared, $Q^2_{\text{cut}}$, for a fixed $W^2_{\text{cut}} = 4 \text{ GeV}^2$. The $\chi^2_{\text{dof}}$ values and number of points included by the different $Q^2$ cuts are listed, with the JAM15 fit values indicated in boldface. (Figure from Ref. [15])

<table>
<thead>
<tr>
<th>$Q^2_{\text{cut}}$ (GeV$^2$)</th>
<th>1.0</th>
<th>2.0</th>
<th>4.0</th>
</tr>
</thead>
<tbody>
<tr>
<td># points</td>
<td>2515</td>
<td>1421</td>
<td>611</td>
</tr>
<tr>
<td>$\chi^2_{\text{dof}}$</td>
<td>1.07</td>
<td>1.08</td>
<td>0.95</td>
</tr>
</tbody>
</table>

a more substantial deterioration of the $\chi^2$ is seen. This is not entirely surprising, since as $W^2$ decreases, the nucleon resonance region will become more present, rendering the DIS formalism inadequate.

Of course, using the $\chi^2$ as the only indicator for the quality of the fit is not sufficient. For this reason, we also compute particular moments of the PDFs and higher twist distributions for the $W^2$ and $Q^2$ ranges of 3.5 to 6 GeV$^2$ and 1 to 4 GeV$^2$, respectively. The results are shows in Figs. 4.5 and 4.6 for the single moment $\Delta \Sigma(Q^2)$, the gluon moment $\Delta G(Q^2)$, as well as the proton and neutron $d_2$ and twist-4 $h(= H(3, Q^2))$ moments. Moreover, the $x$-weighted integrals were computed in the range of experimental data, i.e. $x \in [0.001, 0.8]$, to avoid extrapolation.

The dependence of the moments on $W^2$ is relatively stable down to 3.5 GeV$^2$, except for $\Delta \Sigma$ and the third moment of the proton twist-4 distribution $h_p$. The former increases by roughly one standard deviation, whereas the twist-4 moment decreases dramatically, albeit with larger uncertainties. Note, however, that the twist-4 moment overall is essentially negligible, and hence any change will be significant at such values. Nevertheless, such variation can indicate the presence of higher twist from the nucleon resonance region. This is further supported by the decrease of uncertainties for several higher twist moments, namely $d_2^p$ and $h_n$. The reduction of uncertainties can also be attributed to the significant increase in data points as $W^2$ and $Q^2$ are varied. Although the moments in Fig. 4.6 are stable, lowering the $Q^2$ cut adds $\sim 1900$ data points between 4 and 1 GeV$^2$, which has the
FIG. 4.5: Dependence on $W_{\text{cut}}^2$ of several moments of twist-2 PDFs ($\Delta \Sigma$ and $\Delta G$), the twist-3 $d_2$ moments, and the third moments $h_p$ and $h_n$ of the twist-4 distributions of the proton and neutron. All fits use $Q_{\text{cut}}^2 = 1 \text{ GeV}^2$, and the moments are truncated moments evaluated in the measured region between $x = 0.001$ and 0.8. (Figure from Ref. [15])

Effect of decreasing the moment uncertainties, particularly for $\Delta \Sigma$ and $\Delta G$.

Overall, the purpose of this exercise was to include as much DIS data as possible without extending into the resonance region, and therefore the cut at $W^2 = 4 \text{ GeV}^2$ is chosen for the JAM15 analysis. Finally, since the variation in $Q^2$ is small for both the $\chi^2$ and moments, we choose to exclude data below 1 GeV$^2$, which is typical in global QCD fits of helicity distributions.

The polarized DIS observables considered in the JAM analyses are the cross section spin asymmetries introduced in Chapter 2. In particular, we fit the longitudinal (Eq. (2.6)) and transverse (Eq. (2.7)) spin asymmetries where available, rather than the virtual photoproduction asymmetries (Eq. (2.9)) which rely on assumptions about the ratio $R$ in order to determine. While the majority of asymmetry data are given from proton or light nuclei targets, we also include neutron asymmetry data from HERMES [139], which is
FIG. 4.6: As in Fig. 4.5, but for varying values of $Q^2_{\text{cut}}$ between 1 and 4 GeV$^2$, for a fixed $W^2_{\text{cut}} = 4$ GeV$^2$. (Figure from Ref. [15])

extracted from polarized positron-$^3$He scattering. To compute the unpolarized structure functions in the denominators of the asymmetries, we use the CJ12 unpolarized PDF parameterization [84].

While most of the transverse spin asymmetries were measured with a target polarization that was $90^\circ$ relative to the beam direction, the SLAC E115x experiment [137] provided DIS data with a target polarization that was $92.4^\circ$. Furthermore, the definitions for $\theta^*$ and $\phi^*$ were affected due to one of the three spectrometers being located on the opposite side of the beam line. The resulting transverse asymmetry, which we denote $\tilde{A}_{\perp}$, is then computed from Eq. (2.4) with the average $\theta^*$ and $\phi^*$ values for each kinematic bin.

The treatment of the correlated systematic uncertainties for most experiments is rather straightforward. Typically, an overall normalization constant is given by a collection of multiplicative factors that correct the raw experimental data, e.g. the dilution factor and uncertainties in the beam and target polarizations. In this case, the normal-
ization constant was taken for the ratio of $\frac{\beta_{k,i}^{(e)}}{D_i^{(e)}}$ in Eq. (4.32). However, since this information was not available for the recent proton and deuteron data from CLAS [41–43], a different procedure was used.

For the eg1-dvcs data [42], the systematic uncertainties that were given for each kinematic bin originate completely from correlated normalization uncertainties. In this case, we simply used this value for the single point-to-point correlated uncertainty $\beta_{1,i}$, with the overall sign being set to that of the corresponding data point. The proton eg1b data [41], on the other hand, had a small, 3% normalization uncertainty, which we assigned for all kinematic bins but in addition added the systematic errors in quadrature with the uncorrelated statistical uncertainties, $\delta D_i^{(e)}$. Since the eg1b deuteron data [43] had much larger correlated normalization uncertainties ($\sim 14\%$ for the 5.7 GeV data and $\sim 7\%$ for the 4.2 GeV data), they were subtracted from the systematic errors and the remainder was added in quadrature to the statistical uncertainties.

### 4.5.2 Single-inclusive $e^+e^-$ annihilation observables

In the JAM16 and JAM17 global QCD analyses, all available data sets for charged pion and kaon production from single inclusive $e^+e^-$-annihilation were included to constrain the FF distributions. In particular, we fit LEP data from the OPAL [142, 143], ALEPH [144], and DELPHI [145, 146] Collaborations at CERN, TASSO [147–149] and ARGUS [150] collaboration data from DESY, data from the TPC [151–153], HRS [154], SLD [155], and BaBar [156] Collaborations at SLAC, and also from the TOPAZ [157] and Belle [158, 159] collaborations at KEK, for a total of 459 $\pi^\pm$ data points and 391 $K^\pm$ data points. Roughly half of these are at center-of-mass energies near the $Z$-boson pole, $Q \approx M_Z$, and the remainder extend down to energies just below the $\Upsilon(4S)$ resonance, $Q \approx 10.5$ GeV, provided by Belle, BaBar, and ARGUS. The correlated systematic uncertainties
are presented by most of the experiments as overall normalization uncertainties, and are therefore treated as such in the minimization procedure. The systematic errors from the remaining experiments are treated as uncorrelated and added in quadrature with the statistical uncertainties.

The experimental observables are typically given by Eq. (2.16), where the cross section consists of a sum over all quark-to-hadron flavors. However, the TPC, OPAL, DELPHI, and SLD experiments in particular distinguish between light-quark and heavy-quark \( e^+e^- \rightarrow q\bar{q} \rightarrow hX \) events. The process for obtaining the tagged heavy-quark events varies for each experiment, but the tracks are typically more easily identified due to the large difference in quark mass. Distinguishing the light quarks, on the other hand, is much more difficult. The OPAL experiment is the only experiment to provide the separate probabilities for the \( u, d, \) and \( s \) quark-to-hadron fragmentation. In any case, the flavor-tagged data are especially useful to constrain the individual quark-to-hadron FFs.

We also include in the JAM analyses the most recent Belle [158] and BaBar [156] data that extend the kinematic range of world data to high \( z \) at low \( Q^2 \). The Belle measurements are presented as \( d\sigma^h/dz \) and therefore must be divided by the total cross section \( \sigma_{\text{tot}} \) given by Eq. (2.17). However, an additional correction must be made to account for the variation of the fragmentation energy scale \( Q/2 \) due to effects from initial-state (ISR) and final-state (FSR) photon radiation. Consequently, one must multiply the total cross section by 0.64616(3), the estimated ISR/FSR correction factor [159]. The BaBar data consist of “prompt” and “conventional” data sets corresponding to lifetimes of primary hadrons or decay products being shorter than \( 10^{-11} \) s or approximately \( (1 - 3) \times 10^{-11} \) s, respectively. Although the difference is negligible for kaon production, the prompt cross sections are larger in magnitude for pion production than the conventional set. In the JAM16 analysis, we study the impact of both sets on the global fits, but in the subsequent JAM17 fit we use only the “prompt” data set which is numerically closer to the LEP data after \( Q^2 \) evolution.
Lastly, to avoid kinematic regions beyond the collinear factorization framework or that are sensitive to resummations of large logarithms from soft-gluon radiation, we exclude data at low \( z \). In principle, a kinematic cut on \( z \) will depend on the scale \( Q \) and hadron mass \( m_h \). In the JAM16 and JAM17 global QCD analysis, we reflect this dependence by applying a cut at \( z > 0.1 \) for energies \( Q < M_Z \) and \( z > 0.05 \) for data at the \( Z \)-boson pole. Since hadron mass effects are more relevant at low \( z \) for the heavier kaon meson, we exclude low-\( Q \) data from ARGUS and BaBar below \( z \sim 0.2 \).

### 4.5.3 Semi-inclusive deep-inelastic observables

In the JAM17 global QCD analysis, a simultaneous fit of helicity distributions and FFs was performed using all available SIDIS spin asymmetry data (Eq. (2.14)), in addition to the DIS and SIA observables listed previously. The total of \( \approx 150 \) SIDIS data points include HERMES measurements of \( \pi^\pm \) production from the proton [160], \( \pi^\pm \) and \( K^\pm \) production from the deuteron [160], as well as charged pion and kaon production from muon-proton [161] and muon-deuterium [161, 162] scattering from the COMPASS Collaboration.

Since the focus of the JAM17 analysis was to study the impact of SIDIS data on the leading twist helicity distributions, we only include DIS and SIDIS measurements at \( W^2 > 10 \text{ GeV}^2 \) with \( Q^2 > 1 \text{ GeV}^2 \), which is necessary to avoid contamination from higher twist effects. Although much of the DIS data is removed, including all Jefferson Lab measurements, virtually all of the SIDIS data is still available to fit. Furthermore, to limit the number of fit parameters in the combined analysis, we fix the normalization parameters \( r_k^{(e)} \) to their respective values from the DIS and SIA only fits, and do not treat correlated systematic uncertainties in the SIDIS data. Instead, the systematic uncertainties are added in quadrature to the statistical errors, leading to slightly overestimated uncertain-
ties. However, in the region of $x$ we are interested in ($x \gtrsim 0.1$) the SIDIS uncertainties are mostly dominated by the uncorrelated statistical errors.

All of the components of the $\chi^2$ have now been discussed. The parameterization for the theoretical predictions, the world scattering data included in the IMC fitting procedure, and the systematic treatment of experimental uncertainties are all that is needed to extract reliable information of the nonperturbative distributions in a global QCD study. In the following Chapter, the results from the three sequential Monte Carlo global analyses performed by JAM are presented.
CHAPTER 5

Results from JAM Global QCD Analyses

Using the IMC methodology described in the previous chapter, the JAM collaboration successfully performed a series of global QCD studies to obtain vital information about the spin structure of the proton (see Table 5.1). The JAM15 analysis [15] provided the foundation for our understanding of the proton’s quark and gluon helicity distributions by including all available inclusive DIS data and treating systematically higher twist and nuclear effects. Naturally, a subsequent analysis was planned to consider experimental observables from semi-inclusive DIS to constrain the sea quark polarizations and resolve the discrepancy in the strange helicity shape, which was shown to be different between global fits with only inclusive DIS data and those with both DIS and SIDIS observables.

However, using a fixed parameterization of FFs for the SIDIS spin asymmetries was not ideal since our aim was to adequately minimize bias, and the available FFs were known to impact the shape of the strange distribution [16, 21, 28]. We therefore first performed an IMC study of pion and kaon FFs from SIA data [24]. This allowed us to
then fit simultaneously the parton spin distributions and FFs in a combined global QCD analysis of DIS, SIDIS, and SIA experimental data [25]. In this chapter, we present the results from these recent JAM extractions of spin PDFs and FFs as they were completed chronologically, and discuss their implications regarding the proton spin structure.

\section*{5.1 Iterative Monte Carlo Analysis of Spin PDFs}

The resulting $\chi^2_{\text{dof}}$ for each experiment included in the JAM IMC analysis of inclusive DIS is listed in Table 5.2. Overall, the fit gave a reasonable $\chi^2_{\text{dof}}$ of 1.07 for a total of 2515 data points. The agreement of our fit with each experimental data set is further illustrated in Figs. 5.1 to 5.9, where the various spin asymmetries are shown explicitly as a function of $x$ for different $Q^2$ intervals in the range from 1 to $\sim 100$ GeV$^2$. In these figures, all of the data and corresponding uncertainties are shifted by the fitted point-to-point
TABLE 5.2: Inclusive DIS data sets used in the JAM15 global PDF analysis, indicating the observables fitted, the targets used, the number of data points in each experiment, and the respective \( \chi^2_{\text{res}} \) values. (Table from Ref. [15])

<table>
<thead>
<tr>
<th>experiment</th>
<th>reference</th>
<th>observable</th>
<th>target</th>
<th># points</th>
<th>( \chi^2_{\text{res}} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>EMC</td>
<td>[124]</td>
<td>A1</td>
<td>p</td>
<td>10</td>
<td>0.40</td>
</tr>
<tr>
<td>SMC</td>
<td>[125]</td>
<td>A1</td>
<td>p</td>
<td>12</td>
<td>0.47</td>
</tr>
<tr>
<td>SMC</td>
<td>[125]</td>
<td>A1</td>
<td>d</td>
<td>12</td>
<td>1.62</td>
</tr>
<tr>
<td>SMC</td>
<td>[126]</td>
<td>A1</td>
<td>p</td>
<td>8</td>
<td>1.26</td>
</tr>
<tr>
<td>SMC</td>
<td>[126]</td>
<td>A1</td>
<td>d</td>
<td>8</td>
<td>0.57</td>
</tr>
<tr>
<td>COMPASS</td>
<td>[127]</td>
<td>A1</td>
<td>p</td>
<td>15</td>
<td>0.92</td>
</tr>
<tr>
<td>COMPASS</td>
<td>[128]</td>
<td>A1</td>
<td>d</td>
<td>15</td>
<td>0.67</td>
</tr>
<tr>
<td>COMPASS</td>
<td>[129]</td>
<td>A1</td>
<td>p</td>
<td>51</td>
<td>0.76</td>
</tr>
<tr>
<td>SLAC E80/E130</td>
<td>[130]</td>
<td>A1</td>
<td>p</td>
<td>22</td>
<td>0.59</td>
</tr>
<tr>
<td>SLAC E142</td>
<td>[131]</td>
<td>A1</td>
<td>(^3\text{He})</td>
<td>8</td>
<td>0.49</td>
</tr>
<tr>
<td>SLAC E142</td>
<td>[131]</td>
<td>A2</td>
<td>(^3\text{He})</td>
<td>8</td>
<td>0.60</td>
</tr>
<tr>
<td>SLAC E143</td>
<td>[132]</td>
<td>A1(_j)</td>
<td>p</td>
<td>81</td>
<td>0.80</td>
</tr>
<tr>
<td>SLAC E143</td>
<td>[132]</td>
<td>A1(_j)</td>
<td>d</td>
<td>81</td>
<td>1.12</td>
</tr>
<tr>
<td>SLAC E143</td>
<td>[132]</td>
<td>A1(_L)</td>
<td>p</td>
<td>48</td>
<td>0.89</td>
</tr>
<tr>
<td>SLAC E143</td>
<td>[132]</td>
<td>A1(_L)</td>
<td>d</td>
<td>48</td>
<td>0.91</td>
</tr>
<tr>
<td>SLAC E154</td>
<td>[133]</td>
<td>A1(_j)</td>
<td>(^3\text{He})</td>
<td>18</td>
<td>0.51</td>
</tr>
<tr>
<td>SLAC E154</td>
<td>[133]</td>
<td>A1(_L)</td>
<td>(^3\text{He})</td>
<td>18</td>
<td>0.97</td>
</tr>
<tr>
<td>SLAC E155</td>
<td>[134]</td>
<td>A1</td>
<td>p</td>
<td>71</td>
<td>1.20</td>
</tr>
<tr>
<td>SLAC E155</td>
<td>[135]</td>
<td>A1</td>
<td>d</td>
<td>71</td>
<td>1.05</td>
</tr>
<tr>
<td>SLAC E155</td>
<td>[136]</td>
<td>A1(_L)</td>
<td>p</td>
<td>65</td>
<td>0.99</td>
</tr>
<tr>
<td>SLAC E155</td>
<td>[136]</td>
<td>A1(_L)</td>
<td>d</td>
<td>65</td>
<td>1.52</td>
</tr>
<tr>
<td>SLAC E155x</td>
<td>[137]</td>
<td>(\bar{A}_1)</td>
<td>p</td>
<td>116</td>
<td>1.27</td>
</tr>
<tr>
<td>SLAC E155x</td>
<td>[137]</td>
<td>(\bar{A}_1)</td>
<td>d</td>
<td>115</td>
<td>0.83</td>
</tr>
<tr>
<td>HERMES</td>
<td>[138]</td>
<td>A1(_j)</td>
<td>&quot;n&quot;</td>
<td>9</td>
<td>0.25</td>
</tr>
<tr>
<td>HERMES</td>
<td>[139]</td>
<td>A1(_j)</td>
<td>p</td>
<td>35</td>
<td>0.47</td>
</tr>
<tr>
<td>HERMES</td>
<td>[139]</td>
<td>A1(_j)</td>
<td>d</td>
<td>35</td>
<td>0.94</td>
</tr>
<tr>
<td>HERMES</td>
<td>[140]</td>
<td>A2</td>
<td>p</td>
<td>19</td>
<td>0.93</td>
</tr>
<tr>
<td>JLab E99-117</td>
<td>[141]</td>
<td>A1(_j)</td>
<td>(^3\text{He})</td>
<td>3</td>
<td>0.27</td>
</tr>
<tr>
<td>JLab E99-117</td>
<td>[141]</td>
<td>A1(_L)</td>
<td>(^3\text{He})</td>
<td>3</td>
<td>1.58</td>
</tr>
<tr>
<td>JLab E06-014</td>
<td>[44]</td>
<td>A1(_j)</td>
<td>(^3\text{He})</td>
<td>14</td>
<td>2.12</td>
</tr>
<tr>
<td>JLab E06-014</td>
<td>[45]</td>
<td>A1(_L)</td>
<td>(^3\text{He})</td>
<td>14</td>
<td>1.06</td>
</tr>
<tr>
<td>JLab eg1-dvcs</td>
<td>[42]</td>
<td>A1</td>
<td>p</td>
<td>195</td>
<td>1.52</td>
</tr>
<tr>
<td>JLab eg1-dvcs</td>
<td>[42]</td>
<td>A1(_j)</td>
<td>d</td>
<td>114</td>
<td>0.94</td>
</tr>
<tr>
<td>JLab eg1b</td>
<td>[41]</td>
<td>A1(_j)</td>
<td>p</td>
<td>890</td>
<td>1.11</td>
</tr>
<tr>
<td>JLab eg1b</td>
<td>[43]</td>
<td>A1(_j)</td>
<td>d</td>
<td>218</td>
<td>1.02</td>
</tr>
<tr>
<td>total</td>
<td></td>
<td></td>
<td></td>
<td>2515</td>
<td>1.07</td>
</tr>
</tbody>
</table>

normalizations \( N_i^{(e)} \) introduced in the previous chapter,

\[
\bar{D}_i^{(e)} = N_i^{(e)} D^{(e)}, \quad (5.1)
\]

\[
\delta \bar{D}_i^{(e)} = N_i^{(e)} \delta D^{(e)}. \quad (5.2)
\]

The magnitudes of such shifts are given by the differences \( \bar{D}^{(e)} - D^{(e)} \) and are illustrated by the syst(±) bands in each panel. In addition to the JAM15 central values and uncertainties, we also give the spin asymmetries computed only with the leading twist-2 structure.
functions, including TMCs.

Overall, the proton longitudinal polarization asymmetries from EMC [124], SMC [125, 126], COMPASS [127, 129], SLAC [130, 132, 134], and HERMES [139] shown in Fig. 5.1 are in good agreement with the fit results with almost all of the $\chi^2_{\text{dof}}$ being less than one. Only the SMC [126] and SLAC E155 [134] experiments indicate a slightly worse agreement with a $\chi^2_{\text{dof}} > 1.2$ over the range of $x$ and $Q^2$ given by the data. The proton transverse asymmetries in Fig. 5.2 are also well described by the JAM15 results, with all but the SLAC155x [137]
The fit to eg1b gave an overall signal for non-zero higher twist in the Jefferson Lab data from the CLAS eg1-dvcs [42] and eg1b [41] experiments, illustrated in Figs. 5.3 and 5.4. The signal for non-zero higher twist in the SLAC E143 [132] measurement of for $x \gtrsim 0.2$ at $Q^2 \sim 1.0$ GeV$^2$, and slightly positive higher twist effects in the large-$x$ $A^p_\perp$ data.

The difference between the leading twist contributions and the full JAM15 result is more evident in the Jefferson Lab data from the CLAS eg1-dvcs [42] and eg1b [41] experiments, illustrated in Figs. 5.3 and 5.4. The signal for non-zero higher twist in eg1-dvcs $A^p_\parallel$ is given by the decrease of the full fit result at lower $Q^2 \lesssim 2$ GeV$^2$ for larger $x \gtrsim 0.2$, where higher twist effects are expected to be present. Similar contributions are seen in the eg1b data, where very small bin widths in $x$ and $Q^2$ are given for $\sim 900$ points. The fit to eg1b gave an overall $\chi^2_{\text{dof}} = 1.11$, indicating a relatively good agreement for both

---

FIG. 5.2: Proton transverse polarization asymmetries $A^p_\perp$ and $A^p_\parallel$ from SLAC [132, 136, 137] and HERMES [140]. The curves and legends are as in Fig. 5.1. (Figure from Ref. [15])
the $E = 4.2$ and $5.7$ GeV data.

However, a large positive systematic shift is seen for the eg1b data as indicated by the syst(+) band in Fig. 5.4. Such effects can be attributed to a strong pull from the eg1-dvcs $6.0$ GeV measurements, which have extremely small statistical errors and therefore dominate the $\chi^2$ fit to Jefferson Lab data. Of course, this also means the data will be significantly more difficult to fit in a global analysis, as indicated by the large $\chi^2_{dof} = 1.52$ for the entire eg1-dvcs data set. Moreover, a possible tension between the $E = 4.8$ and $6$ GeV data may exist due to the full fit result lying below the lower energy data points. It is possible that the $6$ GeV measurements from eg1-dvcs have underestimated systematic uncertainties which would lead to such issues between the different energy data sets.
The comparisons of the JAM15 results with the deuteron longitudinal and transverse asymmetries are shown in Figs. 5.5 and 5.6. Since the uncertainties are generally larger for scattering from the deuteron, most of the data can be accommodated in the fit. Only the SMC $A_1^d$ data [125] and E155 $A_1^d$ [135] data are not as well described by the fitted asymmetries, with $\chi^2_{\text{dof}} = 1.26$ and 1.52, respectively. The disagreement with SMC is primarily in the low-$x$ region ($x \lesssim 0.1$) where the errors are very small, whereas the large E155 $\chi^2$ arises from a significant fluctuation of the data values, particularly at larger $Q^2$. Similar to the case of scattering from the proton, negligible higher twist effects are seen for the $A_1^d$ and $A_1^d$ asymmetries. Slight differences between the full JAM15 fit and leading twist only contributions are present at higher $x$ values in the $A_1^d$ asymmetries. However, given the uncertainties in this region, the higher twist effects here are insignificant.

FIG. 5.4: Proton longitudinal polarization asymmetries $A_1^p$ from the eg1b [41] experiment at Jefferson Lab. The curves and legends are as in Fig. 5.3. (Figure from Ref. [15])
FIG. 5.5: Deuteron longitudinal polarization asymmetries $A^L_p$ and $A^L_t$ from SMC [125, 126], COMPASS [127], SLAC [132, 135] and HERMES [139] experiments. The curves and legends are as in Fig. 5.1. (Figure from Ref. [15])

FIG. 5.6: Deuteron transverse polarization asymmetries $A^T_p$ from SLAC [132, 136, 137] data. The curves and legends are as in Fig. 5.1. (Figure from Ref. [15])
FIG. 5.7: Deuteron longitudinal polarization asymmetries $A_\parallel^d$ from the eg1-dvcs [42] experiment at Jefferson Lab’s Hall B. The curves and legends are as in Fig. 5.3. (Figure from Ref. [15])

FIG. 5.8: Deuteron longitudinal polarization asymmetries $A_\parallel^d$ from the eg1b [43] experiment at Jefferson Lab. The curves and legends are as in Fig. 5.3. (Figure from Ref. [15])
Lastly, the experimental asymmetries from polarized electron-\(^3\)He scattering are shown in Fig. 5.9. The polarized \(^3\)He asymmetries come from the SLAC E142 [131] and E154 [133] experiments as well as Jefferson Lab’s E99-117 [141] and E06-014 [44, 45] experiments from Hall A. Overall, the JAM15 fit result is compatible with the longitudinal asymmetry data, except for the low-\(x\) measurements in E06-014 which lead to the data set having a \(\chi^2_{\text{dof}} = 2.12\). Similar agreement is seen in the transverse spin asymmetries, where all but
FIG. 5.10: Comparison of the JAM15 IMC fits (red curves, with the average indicated by the black solid curve) with corresponding fits excluding all Jefferson Lab data (yellow curves, with the average given by the black dashed curve) for the twist-2 PDFs $\Delta u^+$, $\Delta d^+$, $\Delta s^+$, and $\Delta g$, the twist-3 distributions $D_u$ and $D_d$, and the twist-4 functions $H_p$ and $H_n$ at $Q^2 = 1$ GeV$^2$. Note that $x$ times the distribution is shown. For illustration each distribution is represented by a random sample of 50 fits. (Figure from Ref. [15])

the E99-117 data ($\chi^2_{\text{dof}} \gtrsim 1.5$) have reasonable $\chi^2_{\text{dof}}$. The apparent disagreement with the E99-117 data is mainly due to a single datum in a set that consists of only 3 data points. Finally, the signal for non-negligible higher twist contributions is again not present in the fit to $A_{\text{He}}^H$ data. However, there is some slightly negative higher twist effects given by the lower-$Q^2$ E06-014 measurements.
5.1.1 Impact of Jefferson Lab data

To determine the impact of Jefferson Lab data on the leading and higher twist distributions, we performed separately a global IMC fit to inclusive DIS measurements that were not from the CLAS [41–43] and Hall A [44, 45, 141] experiments. The results are displayed in Fig 5.10, where the twist-2 $\Delta u^+$, $\Delta d^+$, $\Delta s^+$, and $\Delta g$ helicity distributions, twist-3 $D_u$ and $D_d$, as well as the twist-4 $H_p$ and $H_n$ functions are given at the input scale $Q^2 = 1$ GeV$^2$ for both the full JAM15 fit result and the global fit without Jefferson Lab data. Although the complete analysis resulted in $\sim 8000$ final posteriors, the figure shows a random sample of 50 for illustration purposes.

The most defining feature of comparison between the two IMC fit results is the reduction of uncertainties in the region $0.1 \lesssim x \lesssim 0.7$, particularly for the leading twist $\Delta u^+$ and $\Delta d^+$ distributions. This is not entirely surprising, since much of the high precision Jefferson Lab data fall in this kinematic range and the $\Delta u^+$ and $\Delta d^+$ helicity distributions are the leading contributions to the DIS asymmetries. On the other hand, there is also a decrease of the uncertainty bands in the low-$x$ region of these spin PDFs. This result is an effect of anti-correlation between the high- and low-$x$ regions, which is partly caused by the weak baryon constraints (Eq. (3.17)) implemented in this analysis. Since the Jefferson Lab data prefer a slightly larger $\Delta u^+$ at intermediate- to large-$x$ values, the anti-correlation induces a suppression of the distribution in the low-$x$ region. A very similar argument can be made for the $\Delta d^+$ PDF.

The impact of Jefferson Lab data on the $\Delta s^+$ distribution can also be attributed to anti-correlation effects. Since inclusive DIS is not sensitive to the strange polarization, the information must rely on the input from weak baryon decays. As a result, the decrease in the $\Delta d^+$ distribution induces an increase in the $\Delta s^+$ PDF at $x \sim 0.2$ in order to both satisfy the SU(3)$_f$ constraint and maintain a quality fit to the asymmetry values. Note
that the reduction of the uncertainty bands is also primarily due to the decrease in the 
$\Delta u^+$ and $\Delta d^+$ uncertainties.

Inclusive DIS is also not very sensitive to the gluon helicity distribution, which enters only at NLO in the QCD formalism. It can also be determined indirectly through $Q^2$ evolution, but both are relatively weak constraints, as can be seen by the larger uncertainties in Fig. 5.10. However, the increased statistical precision of measurements from Jefferson Lab seems to provide some indication for a more positive $\Delta g$ in the intermediate-$x$ region. Perhaps not surprisingly, there is no effect at low $x$ outside the kinematic region covered by the CLAS and Hall A experiments.

The significant amount of low $Q$ data certainly provide more information about the twist-3 $D_u$ and $D_d$ distributions. While the former stays positive for $x \gtrsim 0.1$ between the two independent fits, the $D_d$ distribution changes sign completely and becomes negative when Jefferson Lab measurements are included. Both then reflect the sign from their respective twist-2 functions and decrease in error with the additional high $x$, low $Q$ data. The effect of uncertainty reduction is again seen for the twist-4 $H_p$ and $H_n$ distributions when including the additional Jefferson Lab data. Both of these twist-4 functions are consistent with zero, which therefore indicates that the higher twist effects in DIS asymmetries are dominated by the twist-3 contributions.

### 5.1.2 JAM15 Distributions and Moments

The final spin-dependent PDFs and higher twist distributions from the full IMC analysis are displayed in Fig. 5.11 for $Q^2 = 1 \text{ GeV}^2$. While a random sample of 100 fits is given to illustrate the Monte Carlo aspect of the analysis, the central values and standard deviations given in Fig. 5.11 are computed using the full, $\sim 8000$ fits and Eqs. 4.17 with $w_k = 1/N$. Both the $\Delta u^+$ and $\Delta d^+$ are well constrained by the inclusive DIS data, as
indicated by the relatively small error bands. This is further supported by the values of their lowest moments at the same scale, \( \Delta u(1) = 0.82 \pm 0.01 \) and \( \Delta d^+(1) = -0.42 \pm 0.01 \), listed in Table 5.3 for the truncated integrals in \( x \), which include only the region of \( x \) covered by experiment, i.e. \( x \in [0.001, 0.8] \). However, extrapolating in \( x \) to compute the full integral results in an insignificant change to the moments.

The strange polarization \( \Delta s^+ \) is determined to be negative over all \( x \), with the lowest moment being \( \Delta s^+(1) = -0.10 \pm 0.01 \), which comes directly from the SU(3)\(_f\) symmetry value for the octet axial charge in Eq. (3.17). As a result, the total quark contribution to the proton spin is then \( \Delta \Sigma = 0.28 \pm 0.04 \) over the full range in \( x \), although the truncated value \( 0.31 \pm 0.03 \) is not significantly different. In fact, most of the quark contributions have little contribution from the extrapolated low- and high-\( x \) regions, as can be seen

\[ \frac{x}{u^+}, \frac{x}{d^+}, \frac{x}{s^+}, \frac{x}{g} \]

\[ \frac{x}{Du}, \frac{x}{Dd}, \frac{x}{Hp}, \frac{x}{Hn} \]
TABLE 5.3: Lowest moments of the twist-2 PDFs $\Delta u^+, \Delta d^+, \Delta s^+$, $\Delta \Sigma$ and $\Delta G$, the twist-3 $d_p^2$ and $d_n^2$ moments, and the $x^2$-weighted moments $h_p$ and $h_n$ of the twist-4 distributions. The truncated moments in the measured region $x \in [0.001, 0.8]$ and the extrapolated full moments are shown at $Q^2 = 1$ GeV$^2$. (Table from Ref. [15])

<table>
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<th>moment</th>
<th>truncated</th>
<th>full</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\Delta u^+$</td>
<td>$0.82 \pm 0.01$</td>
<td>$0.83 \pm 0.01$</td>
</tr>
<tr>
<td>$\Delta d^+$</td>
<td>$-0.42 \pm 0.01$</td>
<td>$-0.44 \pm 0.01$</td>
</tr>
<tr>
<td>$\Delta s^+$</td>
<td>$-0.10 \pm 0.01$</td>
<td>$-0.10 \pm 0.01$</td>
</tr>
<tr>
<td>$\Delta \Sigma$</td>
<td>$0.31 \pm 0.03$</td>
<td>$0.28 \pm 0.04$</td>
</tr>
<tr>
<td>$\Delta G$</td>
<td>$0.5 \pm 0.4$</td>
<td>$1 \pm 15$</td>
</tr>
<tr>
<td>$d_p^2$</td>
<td>$0.011 \pm 0.004$</td>
<td>$0.011 \pm 0.004$</td>
</tr>
<tr>
<td>$d_n^2$</td>
<td>$-0.002 \pm 0.002$</td>
<td>$-0.002 \pm 0.002$</td>
</tr>
<tr>
<td>$h_p$</td>
<td>$-0.000 \pm 0.001$</td>
<td>$0.000 \pm 0.001$</td>
</tr>
<tr>
<td>$h_n$</td>
<td>$0.001 \pm 0.002$</td>
<td>$0.001 \pm 0.003$</td>
</tr>
</tbody>
</table>

in Table 5.3. The gluon polarization, on the other hand, is clearly unconstrained with a moment $\Delta G = 0.5 \pm 0.4$ for the measured region. Including the extrapolated region doubles this value, and increases the uncertainty by a factor $\sim 40$. Additional input from polarized $pp$ collision data that are more sensitive to the gluon helicity is needed to better constrain its distribution and moment.

In Fig. 5.12, we compare our leading twist $\Delta q^+$ and $\Delta g$ distributions to other global PDF parameterizations. The BB10 [18] and JAM13 [163] analyses, the latter being the very first JAM Collaboration fit (the author was not in the collaboration at that time), use only inclusive DIS data to determine the helicity distributions. Distributions from LSS10 [21] and DSSV09 [20] were obtained using additional information from semi-inclusive DIS. Furthermore, the DSSV09 analysis and other parameterizations from AAC09 [19] and NNPDF14 [17] included jet and pion production data from polarized $pp$ scattering at RHIC. The NNPDF group also considered $W$ boson production data to help constrain the anti-quark polarizations.

Overall, the shapes and magnitudes of the $\Delta u^+$ and $\Delta d^+$ distributions are similar to the other global fits. The former distribution is slightly larger in magnitude at the
peak. However, the spread is relatively small with respect to the $\Delta d^+$ magnitude. Here the JAM15 result is smaller at $x \sim 0.2$ than most parameterizations of $\Delta d^+$. In fact, the peak is similar in size to the “reference fit” in the JAM13 analysis [163] which did not consider nuclear smearing or higher twist corrections. The additional high precision data from Jefferson Lab therefore counteracts the nuclear and finite-$Q^2$ effects since the final JAM13 result shown in Fig. 5.12 is significantly more negative in the intermediate $x$ region.

The strange polarization $\Delta s^+$ is slightly harder with a negative peak at $x \sim 0.2$. With additional information on the $\Delta u^+$ and $\Delta d^+$, the distribution is the result of correlation effects partly induced by the weak baryon constraints. It is similar to the other parameterizations except for the DSSV09 and LSS10 $\Delta s^+$ functions, which change sign to become positive at $x \sim 0.1$. These two analyses in particular include kaon production data from...
SIDIS, observables that are sensitive to the strange helicity distribution but require information about the strange to kaon FFs. The resolution of this discrepancy between the DIS only and the combined DIS and SIDIS results for $\Delta s^+$ will be left for the final section of this chapter. Nevertheless, the strange moment is roughly the same, and the resulting flavor singlet moment $\Delta \Sigma$ is relatively stable between each of the analyses, ranging from $\Delta \Sigma = 0.24$ from NNPDF14 [17] to $\Delta \Sigma = 0.34$ from BB10 [18] at $Q^2 = 1$ GeV$^2$.

The difficulty in constraining the gluon polarization is again seen by the variation of the different parameterizations in Fig. 5.12. Here most of the distributions are positive in the intermediate $x$ region, some changing sign at low $x$ to become negative. Although we allow for the possibility for a sign change, we find the $\Delta g$ to be strictly positive. Interestingly, our result is qualitatively similar in the intermediate $x$ region to analyses that include polarized $pp$ collision data. In fact, the most recent global fit by de Florian et al. [13], which contains recent jet data from RHIC, also determines a positive gluon with no indication for a sign change.

Continuing now to the higher twist contributions, the final JAM15 twist-3 $D_u$ and $D_d$ distributions are clearly non-zero in Fig. 5.11 with positive and negative signs, respectively. We find for the 3rd moment of these quantities, which is relevant for computing the $d_2$ moment, values of $D_u(3, Q^2) = 0.013 \pm 0.005$ and $D_d(3, Q^2) = -0.005 \pm 0.003$ at $Q^2 = 1$ GeV$^2$. Combining these values with the squared electric charges, we find a neutron twist-3 contribution that is relatively small compared to the proton. This is evident from studying the effect of higher twist on the proton spin asymmetries from CLAS [41, 42], where the differences between the leading twist only and full results are larger than that for the effective neutron target asymmetries, i.e. from $^3$He and deuterium. The $d_2$ moment is then determined reliably from the twist-3 PDFs since the $x$-weighted integrals of the twist-4 distributions $h_p = H_p(3)$ and $h_n = H_n(3)$, listed in Table 5.3, are effectively zero and do not contribute.
FIG. 5.13: $d_2$ moments of the proton (red curves and symbols) and neutron (blue curves and symbols) computed from the JAM15 twist-3 $D_u$ and $D_d$ distributions and compared with (a) lattice QCD calculations [164], and (b) moments extracted from the $g_1$ and $g_2$ structure functions from several SLAC [137] and Jefferson Lab [45, 46, 165, 166] experiments (filled symbols), with the JAM15 results (open symbols and dotted error bars) corresponding to the experimentally measured regions. The E155x results include extrapolations into unmeasured regions at low and high $x$, while the Jefferson Lab results are mostly from the resonance region. (Figure from Ref. [15])

In Fig. 5.13a, we illustrate the $Q^2$ dependence of the $d_2$ moment for the proton and neutron between $Q^2 = 1$ and 5 GeV$^2$. The $d_2$ values at $Q^2 = 1$ GeV$^2$ are given in Table 5.3 and are computed from the twist-3 PDFs without TMCs, Eq. (3.19), where we drop the “($\tau 3$)” label to simplify notation. Note, however, that the experimental $d_2$ values will in principle contain all higher twist and target mass corrections. Over the $Q^2$ range, the proton $d_2$ moment is a sizeable, 1-2 $\sigma$ away from zero and slowly decreases from $Q^2$. The neutron $d_2$ moment is small and negative, but compatible with zero within uncertainties. Interestingly, without Jefferson Lab data, the positive $D_d$ distribution in Fig. 5.10 would render the neutron $d_2$ moment positive while the proton $d_2$ value would essentially remain unchanged albeit with larger uncertainties. The negative $d_2$ value is therefore driven by the additional information from high precision electron-$^3$He scattering at Jefferson Lab.

Our phenomenological value for the $d_2$ moments are also compared with that obtained
TABLE 5.4: $d_2$ moments of the proton and neutron $g_{1,2}$ structure functions from the SLAC E155x [137] and Jefferson Lab RSS [165, 166], E01-012 [46] and E06-014 [45] experiments, compared with the $d_2$ moments computed from the JAM15 twist-3 $D_{u,d}$ distributions. The $Q^2$ values and the $W$ and $x$ ranges for each experiment are given. The E155x $d_2$ values include extrapolations into unmeasured regions, while the others are truncated moments over the measured regions only. The errors on the JAM15 values are given to the relevant number of significant figures, while the experimental results are quoted from the respective publications. 

(Table from Ref. [15])

<table>
<thead>
<tr>
<th>experiment</th>
<th>ref.</th>
<th>target</th>
<th>$Q^2$ (GeV$^2$)</th>
<th>$W$ range (GeV)</th>
<th>$x$ range</th>
<th>$d_2$(JAM15)</th>
<th>$d_2$(exp.)</th>
</tr>
</thead>
<tbody>
<tr>
<td>E155x</td>
<td>[137]</td>
<td>p</td>
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<td>$&gt; M$</td>
<td>[0, 1]</td>
<td>0.007(3)</td>
<td>0.0032(17)</td>
</tr>
<tr>
<td></td>
<td>[137]</td>
<td>n</td>
<td>5.00</td>
<td>$&gt; M$</td>
<td>[0, 1]</td>
<td>-0.001(2)</td>
<td>0.0079(48)</td>
</tr>
<tr>
<td>RSS</td>
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<td>p</td>
<td>1.30</td>
<td>[1.06, 2.01]</td>
<td>[0.29, 0.84]</td>
<td>0.009(3)</td>
<td>0.0057(9)</td>
</tr>
<tr>
<td></td>
<td>[166]</td>
<td>p</td>
<td>1.28</td>
<td>[1.08, 1.91]</td>
<td>[0.32, 0.82]</td>
<td>0.008(3)</td>
<td>0.0037(5)</td>
</tr>
<tr>
<td></td>
<td>[166]</td>
<td>n</td>
<td>1.28</td>
<td>[1.08, 1.91]</td>
<td>[0.32, 0.82]</td>
<td>-0.001(2)</td>
<td>0.0015(12)</td>
</tr>
<tr>
<td>E01-012</td>
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<td>[1.04, 1.38]</td>
<td>[0.54, 0.86]</td>
<td>-0.000(1)</td>
<td>0.00186(156)</td>
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<td></td>
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<td>[1.07, 1.50]</td>
<td>[0.64, 0.90]</td>
<td>0.000(1)</td>
<td>-0.00055(118)</td>
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<td></td>
<td>[46]</td>
<td>n</td>
<td>3.00</td>
<td>[1.10, 1.61]</td>
<td>[0.64, 0.90]</td>
<td>0.000(1)</td>
<td>0.00080(137)</td>
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<tr>
<td>E06-014</td>
<td>[45]</td>
<td>n</td>
<td>3.21</td>
<td>[1.11, 3.24]</td>
<td>[0.25, 0.90]</td>
<td>-0.001(1)</td>
<td>-0.00261(79)</td>
</tr>
<tr>
<td></td>
<td>[45]</td>
<td>n</td>
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<td>[1.17, 3.72]</td>
<td>[0.25, 0.90]</td>
<td>-0.001(1)</td>
<td>0.00004(83)</td>
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</table>

by first principle calculations of matrix elements of local twist-3 operators in lattice QCD from the QCDSF/UKQCD Collaboration [164]. The results are displayed in Fig. 5.13a, where the simulations give $d_2^p = 0.004(5)$ and $d_2^n = -0.001(3)$ at $Q^2 = 5$ GeV$^2$. Their values agree well within uncertainties with our JAM15 extraction.

In Fig. 5.13b and Table 5.4 we compare our $d_2$ results with moments determined from experimental measurements of the $g_1$ and $g_2$ structure functions. We compute the relevant $x$-weighted integrals over the region measured by experiment, except for the SLAC E155x experiment which reported a value that extrapolated to $x = 0$ and $x = 1$. It’s important to note that the experimental moments are strictly determined from the nucleon resonance region, except for the Jefferson Lab E06-014 value [44], which contains a small contribution from the region of DIS. Furthermore, our calculation does not include contributions from elastic scattering, discussed briefly in Chapter 3. Therefore, the comparison should not be
taken too literally, but instead should be viewed as a test of quark-hadron duality [167].

Remarkably, most of the experimental extractions of $d_2$ agree well with our results from the global fit within errors. Only the lower-$Q^2$ $d_2^p$ from RSS and E155x $d_2^n$ moments are significantly different in magnitude from the JAM15 result, the latter being opposite in sign but with large uncertainties. Upcoming experiments from Jefferson Lab at 12 GeV may be able to provide better constraints of the neutron $d_2$ moment up to $Q^2 \approx 6$ GeV$^2$.

In summary, the JAM15 global fit provides a unique insight into proton spin structure by including high precision Jefferson Lab data and systematically treating nuclear and higher twist corrections. Although the leading-twist helicity distributions were studied in detail, not much can be said about the separate quark and anti-quark PDFs from inclusive DIS. Before discussing the JAM analysis that included SIDIS observables which do allow such separation, however, it is important to discuss the non-perturbative FFs that are relevant in experiments that measure final state mesons. In the following section, we present the results from the JAM global IMC fit of FFs to pion and kaon production data in $e^+e^-$-annihilation collisions.

### 5.2 Iterative Monte Carlo Analysis of FFs

In Table 5.5, the resulting $\chi^2/N_{\text{dat}}$ are listed for each experimental data set along with their respective observable type, energy $Q$, and fitted normalization parameter $N^{(e)}$. Furthermore, the normalized distribution of $\sim 10^4$ posteriors as a function of $\chi^2/N_{\text{dat}}$ for the training, validation and combined sets are given fits in Fig. 5.14. Recall that in this case, the $\chi^2$ will peak at 2 in the ideal Gaussian limit due to the non-centrality parameter in Eq. (4.22). However, inconsistencies in the data sets can lead to a shift of the $\chi^2/N_{\text{dat}}$ to be larger than 2, as is evident for pion production where the distribution peak is around 2.5. On the other hand, the distribution peak for kaon production is at $\sim 2.1$, much closer
TABLE 5.5: Single-inclusive $e^+e^-$ annihilation experiments used in this analysis, including the type of observable (inclusive or tagged), center-of-mass energy $Q$, number of data points $N_{\text{dat}}$, average fitted correlated normalization (when different from “1”), and $\chi^2$ values for pion and kaon production. Note that the normalization factors for the TASSO data, indicated by (*) in the table, are in the range $0.976 - 1.184$ for pions and $0.891 - 1.033$ for kaons. For the BaBar pion data [156] the “prompt” data set is used in the fit discussed in this paper, with normalization and $\chi^2$ values obtained using the “conventional” data set in parentheses. (Table from Ref. [24])

<table>
<thead>
<tr>
<th>experiment</th>
<th>ref.</th>
<th>observable</th>
<th>$Q$ (GeV)</th>
<th>$N_{\text{dat}}$</th>
<th>$\chi^2$</th>
<th>kaons $N_{\text{dat}}$</th>
<th>$\chi^2$</th>
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<td>ARGUS</td>
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<td>35 1.024(1.058)</td>
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<tr>
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<tr>
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<tr>
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<td>30.2(40.4)</td>
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<td>74.6(61.9)</td>
<td>28 0.992 134.1</td>
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<td>599.3(671.2)</td>
<td>391 1.31(1.46)</td>
<td>395.0 1.01</td>
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This does not necessarily mean the data sets are compatible, since the kaon data sets contain much larger statistical uncertainties than pion production and can therefore be more easily accommodated in the global fit.

A direct comparison of the fitted SIA cross sections with the corresponding experimental values is displayed as ratios of data to theory in Figs. 5.15 and 5.16. For the lower energy data, $Q \lesssim 30$ GeV, the theory provides a decent description of the data within the relatively large uncertainties, except for a few sets from TPC, HRS, and TOPAZ which differ by $\sim 5 - 10\%$. The recent high-precision data from Belle and BaBar in particular show relatively good agreement with the global fit results, and are consistent with the
FIG. 5.14: Normalized yield of IMC fits versus $\chi^2/N_{\text{dat}}$ for the training (blue forward hashed), validation (green backward hashed), and combined (red dotted) samples for $\pi$ (left panel) and $K$ production (right panel). (Figure from Ref. [24])

older ARGUS data [150] from DESY. However, the Belle pion data [158, 159] require a sizeable $\sim 10\%$ normalization shift, which perhaps can be attributed to underestimated initial state radiation effects [159] in the cross section normalization. Regardless, this should not in any way affect the shapes of the extracted FFs in our global analysis.

For the experimental data at the $Z$ boson mass, $Q = M_Z$, where the errors are typically smaller, an overall good agreement with the fit results is also obtained. There are, however, some discrepancies between large-$z$ spectra, particularly between the DELPHI [145, 146] and SLD [155] data sets for both inclusive and $uds$-tagged observables at $z \gtrsim 0.4$. In this case, the DELPHI data are systematically above the fitted cross sections whereas the SLD data lies below the results. A better agreement between these sets is for the heavy flavor tagged results, where there are only slight differences in the data at the largest $z$ values, which have large errors. Although most of the flavor tagged data simply distinguish the light $u, d, s$ flavors from the heavy quarks $c$ and $b$, the OPAL experiment [142, 143]
FIG. 5.15: Ratio of experimental single-inclusive $e^+e^-$ cross sections to the fitted values versus $z$ (or $z_{\text{min}}$ for OPAL data [142, 143]) for pion production. The experimental uncertainties are indicated by the black points, with the fitted uncertainties denoted by the red bands. For the BaBar data [156] the prompt data set is used. (Figure from Ref. [24])
FIG. 5.16: As in Fig. 5.15, but for kaon production. (Figure from Ref. [24])
provides integrated cross sections from $z_{\text{min}}$ to 1 for each flavor separately. While the heavy quark data, particularly the $b$-tagged samples in pion production, have large $\chi^2$ values, the unfavored $d$-to-kaon data are well described. In contrast, the unfavored $s$-to-pion data show worse agreement with the theoretical values.

It is important to note that all of the OPAL observables require a significant normalization shift of $\approx 20\%$. With the large $\chi^2$ values for the specific cases described above, one may question whether to include the OPAL flavor tagged data at all in the global fit, and if so, whether the theoretical interpretation is correct. However, since the OPAL experiment quotes integrated quantities, the data will primarily affect the overall normalization of the extracted FFs, with little information on $z$ dependence coming from different $z_{\text{min}}$ limits. Nevertheless, it is important to include all information from SIA to determine the FFs, and OPAL provides valuable constraints on the individual quark-to-hadron distributions to which inclusive observables are not sensitive.

Overall, the final $\chi^2/N_{\text{dat}}$ is $\approx 1.31$ for the entire pion production data. This value increases to $\chi^2/N_{\text{dat}} = 1.46$ when substituting the prompt BaBar pion data with the conventional set. The slightly worse $\chi^2$ comes mostly from the differences in the fit to both BaBar and TPC inclusive data. Interestingly, the Belle data seem to prefer the conventional BaBar set, since the $\chi^2$ decreases and the normalization shift is closer in value to that needed for BaBar. This can be understood by noting that the BaBar conventional cross sections are $\sim 10\%$ larger in value than the prompt, which are smaller than the Belle data and therefore do not require as large of a normalization.

The overall description of the kaon production data is slightly better than for pions, primarily due to the kaon data having larger uncertainties. Similar to the pion case, we see a $\sim 10\%$ decrease in the TPC experimental cross section values [151–153] with respect to the resulting JAM fit. On the other hand, a significantly smaller value for the normalization parameter is needed to describe the Belle data [158, 159]. Furthermore, there
is less discrepancy in the large-$z$ region as opposed to that discussed previously for pion production, where only the SLD heavy flavor tagged data indicate a significant deviation from the theory. Once again the individual flavor separation from OPAL [142, 143] require an $\approx 10-15\%$ normalization to accommodate in the fit. Despite a roughly 10% decrease in the data to theory ratio for the DELPHI inclusive and flavor tagged observables [145, 146], which did not have a normalization fit parameter, the high energy data are described relatively well. As a result, the final JAM fit to kaon data gave $\chi^2/N_{\text{dat}} = 1.01$. 

FIG. 5.17: Fragmentation functions for $u^+, d^+, s^+, c^+, b^+$ and $g$ into $\pi^+$ (red bands) and $K^+$ (blue bands) mesons as a function of $z$ at the input scale ($Q^2 = 1 \text{ GeV}^2$ for light quark flavors and gluon, $Q^2 = m_q^2$ for the heavy quarks $q = c$ and $b$). A random sample of 100 posteriors (yellow curves for $\pi^+$, green for $K^+$) is shown together with the mean and variance (red and blue bands). (Figure from Ref. [24])
5.2.1 JAM16 Fragmentation Functions

The final set of fragmentation functions extracted from the IMC procedure is presented in Fig. 5.17. The distributions are given at the input scales, which correspond to $Q^2 = 1 \text{ GeV}^2$ for the light $u, d, s,$ and $g$ parton flavors and $Q^2 = m_q^2$ for the heavy $c$ and $b$ quarks. A random sample of 100 posteriors is shown with the central values and uncertainties computed from Eqs. 4.17 with $N_{\text{pos}} = 200$ selected posteriors that give an adequate description of the full $10^4$ fit results.

Generally all of the distributions, except for $s^+ \rightarrow \pi^+$, are larger in magnitude than the corresponding kaon functions for a majority of the $z$ values. Since we imposed exact isospin symmetry in parameterizing the pion FFs, the $D_{u^+}^{\pi^+}$ and $D_{d^+}^{\pi^+}$ distributions are identical. Furthermore, the distributions give the leading contributions to the pion SIA cross sections at larger $z$ values, $z \gtrsim 0.2$, since they contain the favored $u \rightarrow \pi^+$ and $\bar{d} \rightarrow \pi^+$ processes. On the other hand, the $D_{s^+}^{\pi^+}$ FF is completely unfavored and is much smaller in magnitude with a peak at $z \sim 0.3 - 0.4$. Recall that $D_{s^+}^{\pi^+}$ is given by a single shape whereas the $u^+$ and $d^+$ to $\pi^+$ FFs are parameterized with two functions to reflect both the favored and unfavored processes. Analogous to the strange helicity distribution from DIS, pion observables in SIA have little sensitivity to the unfavored $s^+$ distribution. However, in this case the small amount of flavor tagged data can provide some information.

In comparing the heavier $s^+, c^+$ and $b^+$ distributions, we find that these generally become softer with increasing quark mass. The $c^+$ and $b^+$ FFs to pions show somewhat singular behavior at $z \lesssim 0.1$, but are similar in magnitude to the light quark functions when evolved to the same scale. Lastly, pion production from gluons is described by the $D_g^{\pi^+}$ FF, which peaks strongly at $z \approx 0.25$ at the input scale, and has larger uncertainties than the favored $u^+$ and $d^+$ distributions. Similar to the gluon spin-dependent PDF in DIS, the gluon FF is constrained through $Q^2$ evolution and higher order $\alpha_s$ corrections.
in the SIA cross sections. Although the experimental SIA cross sections are given for a significantly large range of center-of-mass energies, additional information from hadron production in $pp$ collisions is preferred to better constrain the $D_h^\pi^+$ distribution.

In the kaon production sector, the JAM results again show a reflection of the meson valence structure with $u^+$ and $s^+$ to $K^+$ distributions dominating at larger $z$ values. However, in this case, the $D_{u^+}^{K^+}$ and $D_{s^+}^{K^+}$ FFs, which are parameterized with two shape functions, are fit independently due to the larger difference in quark mass. As a result, we find $D_{s^+}^{K^+} \gtrsim D_{u^+}^{K^+}$ at large $z$ values. The unfavored $d^+$ to kaon FF exhibits behavior similar to the unfavored $s^+$ to pion function, peaking instead at $z \sim 0.25$ with much smaller magnitude and larger errors. For the heavy $c^+$ and $b^+$ FFs, we find the peaks slightly shifted to larger $z$ compared to the pion case, but again similar in magnitude to the light flavor distributions. Finally, the gluon to kaon FF is very small at input scale with a peak at $z \approx 0.85$, which is consistent with previous analyses [168].

Such behavior of the $D_h^h$ and other unfavored FF shapes is curious and can lead one to question whether our extractions contain artifacts of the fitting methodology, or whether they represent physical distributions. To determine the answer, we display in Fig. 5.18 some of the steps in the IMC procedure, where the first and last rows correspond to the initial and final fitting stages, respectively. Here the distributions for both pions and kaons are given at the input scale as a function of $z$. The individual curves represent the priors for each iteration which, upon minimizing the $\chi^2$, result in the central values and standard deviations shown in Fig. 5.18. In the first row, the large spread in the priors is given by a flat sampling of the parameter space, but is significantly reduced after just a single iteration of fits, particularly for the distributions for which the SIA data are most sensitive. The unfavored distributions, on the other hand, require more iterations to reach stability in their shapes, e.g. the $s^+$ to $\pi^+$ distribution. After $\approx 30$ iterations, the FF shapes have roughly converged, which is further supported by the stability in the prior
FIG. 5.18: Iterative convergence of the $\pi^+$ (red bands) and $K^+$ (blue bands) fragmentation functions for the $u^+$, $d^+$, $s^+$, $c^+$, $b^+$ and $g$ flavors (in individual columns) at the input scale. The first row shows the initial flat priors (single yellow curves for $\pi^+$ and green curves for $K^+$) and their corresponding posteriors (error bands). The second and third row are selected intermediate snapshots of the IMC chain, and the last row shows the priors and posteriors of the final IMC iteration. (Figure from Ref. [24])
It’s important to note that since the lowest experimental center-of-mass energies are at $\approx 100$ GeV$^2$, the FFs displayed previously at the input scale are not directly comparable to experimental data. In fact, many of the distribution peaks seen in Fig. 5.17 become washed out after evolution. This is illustrated in Fig. 5.19, where the different flavor FFs are computed at $Q^2 = 1, 10, \text{ and } 100$ GeV$^2$ in addition to the mass of the $Z$-boson $Q^2 = M_Z^2$. Note that since the heavy quark FFs are parameterized at their mass thresholds, the distributions are zero below these values.

Our final JAM FFs are compared with those extracted from other global QCD analyses, particularly from HKNS [168] and DSS [169], in Fig. 5.20. Overall, the shapes are qualitatively similar among the different parameterizations, however, there are several dif-
FIG. 5.20: Comparison of the JAM fragmentation functions (solid curves) for $\pi^+$ (red curves) and $K^+$ (blue curves) with the HKNS [168] (dashed curves) and DSS [169] (dotted curves) parametrizations at the input scale $Q^2 = 1$ GeV$^2$ for the light quark and gluon distributions, and $Q^2 = 10$ and 20 GeV$^2$ for the $c^+$ and $b^+$ flavors, respectively. (Figure from Ref. [24])

...ferences in magnitude that are important to discuss. For pion production, the leading $u^+$ and $d^+$ distributions are similar in size to HKNS at intermediate to high $z$ values, but becomes larger by $\sim 20 - 30\%$ in the region of $z \lesssim 0.3$. The $s^+$ to $\pi^+$ FF peak is shifted to the right relative to both HKNS and DSS, but is comparable in size. For the gluon FF to pions, our result is given by a much larger and narrower peak than the previous fits, but is located at approximately the same $z$ value, $z \approx 0.25$.

Turning now to the kaon FFs, we find the favored $D_{u^+}^{K^+}$ and $D_{s^+}^{K^+}$ functions similar in magnitude to HKNS and DSS, with the former quark-to-hadron FF being closer to HKNS and the latter to DSS. More specifically, the up-to-kaon distribution is about $\sim 20 - 30\%$ above the HKNS function, and is significantly larger than the DSS parameterization, especially for the region $z \lesssim 0.6$. In contrast, the JAM $s^+$ to $K^+$ FF can be seen between
FIG. 5.21: Comparison of the JAM fragmentation functions (solid curves) for $\pi^+$ (red curves) and $K^+$ (blue curves) with the HKNS [168] (dashed curves), DSS [169] (dotted curves) and AKK [170] (dot-dashed curves) evolved to a common scale $Q^2 = M_Z^2$. Note that the fragmentation functions $D(z)$ are shown rather than $zD(z)$. (Figure from Ref. [24])

the two other global fits. Here the distribution is compatible with DSS at large $z \gtrsim 0.5$, but differs in the intermediate-$z$ region. It’s important to note that both $D_{u+}^{K^+}$ and $D_{s+}^{K^+}$ distributions play a crucial role in strange quark spin PDF extractions [16, 28]. In our result, we do not find as significant of a difference in magnitude between the two FFs as in the DSS global fit.

Lastly, the behavior of the gluon to kaon distribution at the input scale is similar between the various analyses. In particular, the JAM distribution is comparable in magnitude to the DSS parameterization which is significantly smaller than the HKNS function. The peak at larger $z$ with respect to the $D_{g}^{\pi^+}$ distribution can be attributed to the higher energy requirement for $g \to s\bar{s}$ splittings for kaon production relative to $g \to u\bar{u}$ or $g \to d\bar{d}$ creations to form pions in reactions at the input energy scale. Regardless, such character-
process | target | \(N_{\text{dat}}\) | \(\chi^2\)
--- | --- | --- | ---
DIS | \(p, d, ^3\text{He}\) | 854 | 854.8
SIA \((\pi^\pm)\) | | 459 | 600.1
SIA \((K^\pm)\) | | 391 | 397.0
SIDIS \((\pi^\pm)\) | HERMES [160] | \(d\) | 18 | 28.1
| HERMES [160] | \(p\) | 18 | 14.2
| COMPASS [162] | \(d\) | 20 | 8.0
| COMPASS [161] | \(p\) | 24 | 18.2
SIDIS \((K^\pm)\) | HERMES [160] | \(d\) | 27 | 18.3
| COMPASS [162] | \(d\) | 20 | 18.7
| COMPASS [161] | \(p\) | 24 | 12.3

**Total:** | | 1855 | 1969.7

**TABLE 5.6:** Summary of \(\chi^2\) values and number of data points \(N_{\text{dat}}\) for the various processes used in this analysis. (Table from Ref. [25])

This is essentially removed after evolving the gluon distributions to the \(Z\)-boson pole. This is illustrated in Fig. 5.21, where the previous HKNS [168] and DSS [169] parameterizations are compared on a logarithmic scale with AKK [170] and the present JAM global fit for the various parton-to-hadron FFs. Overall, we find a qualitative agreement between JAM and the other distributions, with AKK typically being larger at smaller \(z\) values. At large \(z\), the spread between the different analyses is more visible.

### 5.3 Simultaneous Extraction of PDFs and FFs

Now that fragmentation functions have been successfully extracted in a JAM IMC analysis of SIA data, they can be utilized to help constrain the quark helicity distributions in semi-inclusive DIS. The resulting \(\chi^2\) values for the JAM global QCD analysis of DIS, SIDIS, and SIA experimental data, fitting simultaneously the spin PDFs and FFs, is summarized in Table 5.6. Since the focus of this analysis was to study the impact of SIDIS data on the leading twist PDFs, we exclude data below \(W^2 = 10\ \text{GeV}^2\) and \(Q^2 = 1\)
FIG. 5.22: Proton and deuteron longitudinal polarization asymmetries $A_{1}^{\pi^\pm}$ for charged pion and kaon production from the HERMES [139] and COMPASS [127, 129] experiments. The data are compared with the pion asymmetries (red solid curves) and kaon asymmetries (blue solid curves) from the JAM17 global fit (with bands indicating 1σ uncertainties).

GeV$^2$ to avoid contamination from higher twist effects. While this decreases the total number of DIS points from $\approx 2500$ fitted in JAM15 to $\approx 850$, much of which are from Jefferson Lab experiments, the SIDIS data are essentially unaffected.

The agreement overall between the combined fit results and the various experimental data sets is rather good. In fact, there is little change in the description of the DIS asymmetries and SIA cross sections from the previous JAM15 and JAM16 analyses. Since semi-inclusive DIS is a new fitted observable, we list separately the $\chi^2$ for pion and kaon production from the HERMES [160] and COMPASS [161, 162] experiments and illustrate
in Fig. 5.22 the comparison of the fit results with the SIDIS asymmetries. In general the fit results are compatible with the experimental asymmetries, though the statistical errors are rather large, particularly as \( x \) increases. Recall that the CJ12 parameterization for the unpolarized PDFs are used in the denominator for the unpolarized structure functions. A relative difference of \( \sim 2 - 5\% \) in the asymmetry values was found by substituting the CJ12 functions with the MMHT14 global fit PDF [171], a negligible deviation with respect to the experimental errors. Overall, we find for pion asymmetries a value \( \chi^2 = 68.2/80 \) and \( \chi^2 = 49.3/71 \) for kaon production.

### 5.3.1 JAM17 Spin PDFs and Fragmentation Functions

In Fig. 5.23, the central values and standard deviations of the leading twist PDFs from the combined IMC analysis are presented. Since semi-inclusive DIS observables are not particularly sensitive to the gluon helicity distribution, the extracted distribution shape is essentially the same as in JAM15 and therefore is not shown here. In fact, the large \( \Delta u^+ \) and \( \Delta d^+ \) distributions are also very similar to that of JAM15, with only a slight shift of the peaks to larger \( x \). While the \( \Delta u^+ \) PDFs in Fig. 5.24 are compatible within their uncertainties, the \( \Delta d^+ \) from the combined fit is larger in magnitude. This can be attributed to an anti-correlation with the \( \Delta s^+ \), which is found to be less negative, and therefore is compensated by \( \Delta d^+ \) to maintain a good description of the asymmetry data. Furthermore, the uncertainty for the present extraction of \( \Delta d^+ \) is slightly larger since the wealth of high-precision Jefferson Lab data was not available after the kinematic cuts.

Also displayed in Fig. 5.23 are the results for the sum and difference of the light sea quark polarizations \( \Delta \bar{u} \) and \( \Delta \bar{d} \), which can now be determined from the SIDIS observables. While both are consistent with zero within relatively large uncertainties, the sea asymmetry shows a slight preference to be positive in the region \( x \approx 0.01 - 0.1 \). Interestingly,
our phenomenological extraction of the isovector sea polarization agrees qualitatively with some non-perturbative model calculations [172, 173], as well as some lattice QCD predictions [174, 175], where the light flavor difference is determined to be larger than the isoscalar combination, $\Delta \bar{u} + \Delta \bar{d}$. The result is also similar to the DSSV09 parameterization [20], which is shown in Fig. 5.23 to lie just inside the $1\sigma$ uncertainty of our extraction.

The indication for a nonzero sea asymmetry at low $x$ can be attributed to several different observables in SIDIS that are sensitive to $\Delta \bar{u}$ and $\Delta \bar{d}$. As an example, we show in Fig. 5.24 the COMPASS asymmetry values [161] for $\pi^-$ production, $A_{1\pi}^+$, which in principle...
FIG. 5.24: Semi-inclusive polarization asymmetries $A_{1p}^{\pi^-}$ from COMPASS [161] (left) and $A_{1d}^{K^-}$ from HERMES [160] (right) compared with the full JAM17 fit (red curves and band) and with the result assuming $\Delta \bar{q} = \Delta \bar{u} = \Delta \bar{d} = 0$ (for $A_{1p}^{\pi^-}$) and the (negative) $\Delta s^+$ from JAM15 [15] (for $A_{1d}^{K^-}$). (Figure from Ref. [25])

provides the most information on the $\bar{u}$ helicity distribution due to the $\pi^-$ valence structure. In addition to the full fit result, we also compute $A_{1p}^{\pi^-}$ with zero sea quark polarization $\Delta \bar{u} = \Delta \bar{d} = 0$. Perhaps not surprisingly, the comparison reveals a small difference between the two results in the region of $x$ that produces a nonzero isovector sea polarization. Such contributions are found in other observables sensitive to the up and down sea spin PDFs.

As was mentioned briefly in the discussion of the $\Delta d^+$ distribution, the strange polarization shown in Fig. 5.23 is determined to be less negative in the intermediate-$x$ region. The inclusion of SIDIS data removes the prominent negative distribution peak determined in the JAM15 DIS-only analysis and instead suggests a possible change in sign for the strange helicity shape, within relatively large uncertainties. In fact, the origin of this difference can be identified by the $K^-$ tagged deuteron asymmetry, $A_{1d}^{K^-}$, from HERMES [160] and COMPASS [162]. Theoretically, this observable is expected to provide the most information on the strange helicity distribution $\Delta s$, since not only is it weighted by the favored $D_s^{K^-}$ FF, but nuclear effects in deuterium reduce the large $\Delta u$ contributions in the scattering cross sections. Since the $\Delta u$ PDF is the dominant contribution in the $K^+$ asymmetries, a precise extraction of the strange helicity from $A_{1}^{K^+}$ data is impractical.
given the current size of experimental uncertainties.

Indeed, the HERMES deuteron $K^-$ production data [160] are highly sensitive to $\Delta s$, as is illustrated in Fig. 5.24. In addition to the full JAM17 fit result, a calculation of the polarization asymmetry is performed with a negative $\Delta s^+$ from the JAM15 analysis. Clearly the description of the SIDIS experimental data deteriorates with the JAM15 strange PDF, increasing the $\chi^2$ from 5.7 to 18.5 for 9 data points. Compared to the same observable from COMPASS [162], where the experimental errors are slightly larger than that of HERMES, a $\chi^2$ increase of 12.0 to 18.5 is determined for 10 data points. Interestingly, a small effect is also seen for the COMPASS $K^-$ data on protons [161], which is not measured in HERMES. Here the $\chi^2$ almost doubles from 4.8 to 9.0 for 12 data points.

We also present in Fig. 5.23 the strange quark asymmetry $\Delta s^-$, which in principle can be determined from high precision SIDIS kaon data. One might expect this quantity to be zero from perturbatively generated strange quarks in the proton, and indeed this assumption is made in most global analyses which set $\Delta s = \Delta \bar{s}$. However, nonperturbative effects from chiral symmetry breaking can lead to a nonzero difference [176–178]. As Fig. 5.23 shows, the signal for a nonzero $\Delta s^-$ is very weak and extracting such information from available SIDIS data is simply not realistic.

The extraction of the strange helicity distribution also relies heavily on the choice of FFs in the fit to SIDIS asymmetries [16, 21, 28]. We avoid this issue entirely by fitting the FFs simultaneously with the spin PDFs. The results for the FFs are displayed in Fig. 5.25 for a choice of scale relevant to SIDIS data, $Q^2 = 5 \text{ GeV}^2$. Furthermore, we only show the quark flavors that SIDIS pion and kaon observables impact directly. As Fig. 5.25 indicates, the $u^+$ to $\pi^+$ distribution is well constrained, although mostly by the wealth of SIA data as was seen in the JAM16 global fit. The unfavored $D_\bar{u}^{\pi^+}$, on the other hand, is primarily determined by pion production in SIDIS and is not as well determined. For kaons, a similar difference in the uncertainties between the favored and unfavored distributions is seen in
FIG. 5.25: Fragmentation functions $zD_q^h$ to $\pi^+$ (left panel) and $K^+$ (right panel) for $u^+$ (blue), $\bar{u}$ (green), $s^+$ (red) and $s$ (grey) at $Q^2 = 5$ GeV$^2$ for the JAM17 analysis. Random samples of 50 posteriors are shown with the mean and variance, and compared with the $s^+ \to K^+$ FFs from DSS [169] (dashed) and HKNS [168] (dotted). (Figure from Ref. [25])

Fig. 5.25. In this case, the size of the 1$\sigma$ error for $D_{s}^{K^+}$ is larger with respect to the favored $D_{u}^{K^+}$ or $D_{s}^{K^+}$ distributions due to the larger uncertainties associated with kaon data.

The impact of SIDIS on $D_{s}^{K^+}$ is minimal within uncertainties, only slightly increasing the distribution in the low-$z$ region compared to the JAM16 SIA-only result. Compared to the previous HKNS [168] and DSS [169] global fits, the JAM17 result is similar in magnitude to the DSS parameterization, particularly for higher $z$ values, while the HKNS function is significantly lower. Such characteristics of the $s^+$ to $K^+$ FF have, as mentioned previously, significant consequences for the extraction of $\Delta s^+$. In particular, the smaller $D_{s}^{K^+}$ from HKNS allows a negative $\Delta s^+(x)$ at $x \sim 0.1$ in a global fit of DIS and SIDIS data, consistent with analyses of DIS data alone. Interestingly, our extraction of the kaon FFs also agree qualitatively with a recent NJL-Jet model calculation [179], where $D_{s}^{K^+} > D_{u}^{K^+}$ at large $z$. Overall, the light quark $D_{q^+}$ distributions for both pions and kaons, including the heavy flavor and gluon FFs which are not shown, remain relatively unaffected by the SIDIS observables.
5.3.2 Resolution of the Strange Polarization Discrepancy

The puzzling difference between the different strange helicity shapes introduced by the DSSV09 global fit is still very much present in the simultaneous PDF and FF analysis discussed here. While it is known that negatively charged kaons from lepton-deuterium scattering is the leading cause for the shift in the $x$ dependence of $\Delta s^+$, the negative shape frequently extracted in analyses of DIS data is yet to be fully understood. The resolution of this so-called “strange polarization puzzle” [16, 28] depends on several different key factors.

Perhaps not surprisingly, imposing the weak baryon constraints with the SU(3)$_f$ value for the octet axial charge $a_8$ results in the largest effect on the strange helicity distribution from polarized DIS. More specifically, since the $\Delta u^+$ and $\Delta d^+$ PDFs are well determined by the DIS data, the value for the lowest moment of the strange distribution, $\Delta s(1) \sim -0.1$ at $Q^2_0 = 1 \text{ GeV}^2$, is automatically induced by the SU(3)$_f$ constraint, which drives the shape to be negative across all $x$ values. In fact, we have confirmed that removing these constraints results in a strange helicity distribution that can be fixed to zero at the input scale with no impact on the $\chi^2$ values of the analysis. The polarized DIS data alone, in combination with $Q^2$ evolution, are therefore largely insensitive to the strange polarization.

While the values for the non-singlet quark combinations in Eq. (3.17) generate a nonzero value for the integral of the strange distribution, the $x$-dependent features can be understood by examining the impact of low-$x$ DIS data, where a larger contribution from sea quarks is expected in spin asymmetry measurements. Indeed, we find that a positive-like strange, as in the DSSV09 parameterization, remains qualitatively unchanged in an analysis of DIS data with low-$x$ ($x \lesssim 0.2$) measurements excluded. Interestingly, the effect can be attributed specifically to the lowest 5 bins from COMPASS deuterium data, which appear to favor a negative strange polarization close to zero. With input from
weak baryon decays, this has the consequence of shifting the negative polarization to the intermediate $x$ region in order to satisfy the SU(3) axial charge value. Finally, large-$x$ shape parameters in global fits are typically restricted to values $b \approx 6 - 10$ to reflect a suppression of the sea distributions, which then artificially produces the peak of $\Delta s^+$ at $x \sim 0.1$ where available DIS data have no direct sensitivity.

The resolution, therefore, is to include observables that directly impact $\Delta s^+$ while simultaneously relaxing the SU(3) constraints. In doing so, one can extract a truly physical strange helicity distribution that adequately describes all spin asymmetry measurements. Note, however, that this doesn’t necessarily mean the SU(3) symmetry relation is violated, as Fig. 5.23 illustrates. Here we isolate posterior samples consistent with the octet axial charge measured in weak hyperon decays and compute the central value for $\Delta s^+(x)$. The result still prefers to be positive at $x \sim 0.1$, but the lowest moment $\Delta s^+(1) \sim -0.1$ is now generated by the low-$x$ region. While this may disagree with COMPASS deuterium data for $x \lesssim 0.2$, the errors are not small enough to impact the $\chi^2$ minimization procedure significantly. On the other hand, our final result gives a value $\Delta s^+(1) = -0.03(10)$ that is small and negative but has larger uncertainty. Interestingly, this value agrees with a recent lattice QCD simulation which determined $\Delta s^\text{latt}(1) = -0.02(1)$ at $Q^2 \approx 7$ GeV$^2$ [180].

5.3.3 Lowest Moments of Spin PDF Combinations

The more positive $\Delta s^+$ moment extracted from the JAM17 combined fit results in a $\approx 20\%$ decrease in the central value of the octet axial charge, $a_8 = 0.46(21)$, compared to that obtained from hyperon decays assuming SU(3)$_f$ symmetry, $a_8 = 0.586(21)$. While this has been suggested in earlier theoretical studies [181], the degree of SU(3) breaking from our phenomenological analysis is inconclusive given the significantly large uncertainty. However, as Fig. 5.26 demonstrates, the peak of the normalized sample distribution as a
function of the octet axial charge was determined by flat sampling the prior distributions in the range $a_8 \in [-0.2, 1.2]$. The experimental data therefore clearly indicate the preference for the $a_8$ value, though higher precision kaon data are needed to reduce the error.

Of course, the strange moment also directly impacts the spin content of the proton from quarks and anti-quarks, $\Delta \Sigma$. In this analysis, the smaller $\Delta s^+$ moment leads to a value $\Delta \Sigma = 0.36(9)$ that is $\approx 25\%$ larger at the input scale [181], although this is compatible with the JAM15 global fit result [15] within the relatively large uncertainty. Much of this error is due to the uncertainty in $\Delta s^+$, since we find much smaller $1\sigma$ error bands for the leading $\Delta u^+$ and $\Delta d^+$ distributions. This is further supported by the moment of the non-singlet combination $\Delta u^+ - \Delta d^+$, illustrated in Fig. 5.26. From our combined fit, we obtain a value for the triplet axial charge $a_3 \equiv g_A = 1.24(4)$. Compared to the value measured from weak neutron decays, $g_A = 1.269(3)$, our phenomenological extraction
is a remarkable confirmation of SU(2)$_f$ symmetry to almost 2%. Lastly, we display in Fig. 5.26 the lowest moment of the light antiquark asymmetry across the normalized sample distribution. Our result indicates a preference for a larger $\Delta\bar{u}$, $\Delta\bar{u} - \Delta\bar{d} = 0.05(8)$, but is compatible with zero within uncertainties. Additional information from $W^{\pm}$ asymmetries in $pp$ collisions from PHENIX [182] and STAR [183], both of which also indicate a slightly positive asymmetry in the $x \sim 0.15$ region, are needed to confirm a possible nonzero signal.
CHAPTER 6

Conclusion and Outlook

Although the nonperturbative nature of bound state hadrons currently prohibits a purely theoretical description of hadron structure within QCD, factorization of the perturbative and nonperturbative regions in high energy scattering processes allows us to extract information on the hadron’s quark and gluon dynamics from experimental data. Global QCD analyses, such as those presented in this work, are therefore extraordinarily useful for providing fundamental information about the composition and formation of atomic nuclei. Since the functions that inherit the nonperturbative behavior are, by definition, universal, they can be determined from different types of particle scattering processes that are sensitive to various aspects of hadron structure.

The spin structure of the proton has been of particular interest to the global fitting community in recent decades, following the original EMC result that indicated a surprisingly small spin contribution from the proton’s quark constituents. A significant amount of polarized DIS data from experiments around the world has been effective in determining the valence up and down helicity distributions in the proton. Moreover, additional measurements from polarized semi-inclusive DIS and $pp$ scattering are now becoming available.
to constrain the sea quark and gluon polarizations. By including such information together with an improved theoretical formalism and fitting methodology, our understanding of the proton spin structure from global QCD analyses significantly improves.

In this work, all of the components necessary for a robust extraction of the spin-dependent PDFs and parton-to-hadron FFs have been discussed. In Chapter 2, the theoretical formulas for DIS, semi-inclusive DIS, and single inclusive $e^+e^-$ annihilation observables were given at NLO in the perturbative expansion in $\alpha_s$, followed by a generalization of the observables to Mellin space and a discussion of $Q^2$ evolution. The subsequent chapter considered corrections beyond the parton model description of DIS, namely power corrections of order $1/Q$ from higher twist and $M^2/Q^2$ from target mass. Also outlined was a systematic treatment of nuclear effects, which is necessary to determine quark structure information from lepton-nucleus scattering, and their application to electron-deuteron and electron-$^3$He reactions specifically. In Chapter 4, the key features of global QCD fits were described in detail. In addition to exploring the various fitting methodologies, we explained the parameterization of the PDFs and FFs, the experimental data sets required to optimize the parameters, and the treatment of the correlated systematic uncertainties. In the end, three global QCD analyses performed by the JAM Collaboration were successful in obtaining crucial information about hadronization and proton spin structure.

6.1 Summary of Results

In the JAM15 analysis [15], one of the essential goals was to maximize the available experimental information needed to constrain the helicity distributions. By systematically studying the goodness-of-fit $\chi^2$ and stability of particular moments of the extracted distributions, the squared four-momentum transfer $Q_{\text{cut}}^2 = 1$ GeV$^2$ and final state mass $W_{\text{cut}}^2 = 4$ GeV$^2$ were found to be the limit in which our perturbative QCD formulas were
applicable in the global fit. As a result, a wealth of high precision Jefferson Lab DIS data were utilized in the JAM analysis, which had the general effect of reducing the extracted leading twist and higher twist distribution uncertainties.

Overall, the collection of inclusive DIS data sets are described rather well by the fitted spin asymmetries in JAM15, with an overall $\chi^2_{\text{dof}} = 1.07$. The resulting $\Delta u^+$ and $\Delta d^+$ are consistent with previous analyses, with the latter being slightly less negative and softer in the $x \sim 0.1$ region with the additional Jefferson Lab data. This, of course, is correlated with the strange helicity $\Delta s^+$, which is found to be strictly negative and slightly harder than previous fits. For the gluon distribution, our result is positive in the intermediate $x$ region, similar to the distribution obtained in Ref. [13]. However, since $\Delta g$ in DIS arises primarily through $Q^2$ evolution and higher order effects, its uncertainties are rather large, particularly for $x \lesssim 0.1$.

The impact of the Jefferson Lab data is more clearly illustrated in the higher twist sector, where nonzero twist-3 $D_u$ and $D_d$ distributions were obtained from the high-precision proton and deuteron asymmetries from CLAS in Hall B [41–43] and $^3$He asymmetries from Hall A [44, 45]. While the $D_u$ distribution qualitatively remained the same with the inclusion of Jefferson Lab data, the twist-3 $D_d$ function flipped sign to become negative for all $x$. As a result, the neutron $d_2$ moment is slightly negative but consistent with zero within uncertainties, while the proton $d_2$ moment is relatively large and positive. Interestingly, our $d_2$ results agree with the lattice QCD calculation at $Q^2 = 5 \text{ GeV}^2$, as well many resonance region extractions, but disagrees with the SLAC E155x experimental value [137] which is larger in magnitude and opposite in sign.

In the following JAM16 analysis [24], the first Monte Carlo analysis of fragmentation functions from charged pion and kaon production in single inclusive $e^+e^-$ annihilation was performed. In addition to the abundant experimental data at the $Z$-boson pole, we include the new high precision measurements from Belle [158, 159] and BaBar [156] at $Q \sim 10$
GeV, which extend to the higher values in the hadron momentum fraction $z$. Despite some tension between the DELPHI [145, 146] and SLD [155] pion measurements at large-$z$ values, a good overall agreement was obtained with both the low and high center-of-mass energy spectra. The fit to the kaon data was significantly better with a $\chi^2$ closer to unity, although this is mostly a result of the larger experimental uncertainties which rendered possible tensions less evident.

With the exception of the unfavored $s^+ \text{ and } g$ FFs to pions, the extracted distributions are found to be similar to previous determinations of pion FFs. For the $D_g^{\pi^+}$ distribution, the resulting shape was more strongly peaked than the HKNS [168] and DSS [169] parameterizations, while the $D_s^{\pi^+}$ FF was shifted to slightly larger $z$ values. More noticeable differences between our global fit and previous extractions are seen in the kaon sector. Here we find a larger magnitude for the favored $u^+ \text{ to } K^+$ FF at low to moderate $z$ compared to DSS. Moreover, while the $D_{s+}^{K^+}$ distribution is similar in magnitude to DSS for $z \gtrsim 0.5$, our more flexible parameterization resulted in a significantly different shape at low $z$. The small $D_g^{K^+}$ FF, on the other hand, is compatible with the DSS global fit, both peaking at large $z$ values. In any case, many of the differences between the various FF parameterizations are washed out after evolving to the $Z$-boson mass, where much of the experimental data exist. Here, only the unfavored $s^+ \text{ and } g$ to pion FFs are still shown to be noticeably different.

Lastly, a first-ever combined spin PDF and FF extraction was accomplished in an analysis of available DIS, SIDIS, and SIA data. To avoid higher twist contributions, only data above $W^2 = 10 \text{ GeV}^2$ were included in the global fit. Overall, a good description of the SIDIS data sets were achieved, as well as for the DIS and SIA observables where the fit quality was not significantly affected by the additional information from SIDIS. The leading $\Delta u^+$ and $\Delta d^+$ PDFs are found to be consistent with the previous JAM15 results across most $x$ values. With the additional SIDIS data, $\Delta d^+$ became slightly more negative.
at \( x \sim 0.2 \) as a result of the \( \Delta s^+ \) distribution becoming smaller in the same region.

Perhaps the most impactful result in the JAM17 analysis was the resolution of the long-standing strange polarization puzzle. By carefully examining various fit results, we’ve determined the negative strange polarization in DIS-only analyses is artificially constructed from the SU(3)\(_f\) constraint, low \( x \) COMPASS deuterium data, and parameterization bias arising from fixing shape parameters. The resolution, therefore, is to remove the input of the isovector and octet axial charges from weak baryon decays while simultaneously fitting observables sensitive to the \( \Delta s^+ \) distribution. In SIDIS, we find the \( A_{1,d}^{K^-} \) asymmetries to have the largest sensitivity to the strange helicity shape and prefer a distribution shape that is small and perhaps positive in the intermediate \( x \) region.

The uncertainties on the strange helicity distribution are determined to be rather large and indicates the need for higher precision kaon production data in SIDIS. This is further supported by the lowest moment, \( \Delta s^+(1) = -0.03(10) \), which in turn inflates the 1\( \sigma \) errors for \( \Delta \Sigma \) and octet axial charge \( a_8 \). Nevertheless, our value for the total quark spin contribution is larger but consistent with previous analyses. Furthermore, flat sampling the values of \( a_8 \) in our IMC analysis results in a distribution that peaks at \( \sim 20\% \) SU(3) symmetry violation. For the isovector sea polarization we find a distribution that is slightly positive in the \( x \lesssim 0.1 \) region. The moment also indicates a slightly positive light sea asymmetry with \( \Delta \bar{u}(1) - \Delta \bar{d}(1) = 0.05(8) \), however, both quantities are consistent with zero within uncertainties.

6.2 Future of PDF and FF Extraction

As more experimental information becomes available, uncertainties for the various sea quark and gluon distributions will decrease and an improved picture of the proton’s collinear spin structure will emerge. While the need for higher precision polarized SIDIS
data is rather clear from our JAM17 analysis, available data on other scattering processes that are sensitive to the quark and gluon helicity structure can be included. More specifically, experiments that measure longitudinal single-spin asymmetries in $W^\pm$ production from polarized $pp$ scattering [182, 183] provide valuable information about the light anti-quark polarizations, $\Delta \bar{u}$ and $\Delta \bar{d}$. Furthermore, inclusive jet [11] and pion [12, 184] production from $pp$ collisions at RHIC would help determine the weakly constrained $\Delta g$ PDF in our analyses. All such observables will be included in future JAM IMC analyses, in addition to unpolarized SIDIS to help reduce the individual quark and anti-quark FF uncertainties.

On the theoretical front, there are several improvements that will be necessary to describe increasingly precise data. In future JAM global fits, we will be including NNLO [185, 186] and small-$x$ [187, 188] corrections to the formalism presented in Chapter 2. While the former simply improves the precision of the pQCD calculation, the latter will be beneficial for polarized PDF extractions in the absence of small-$x$ data. In addition, resummation of large logarithms that appear in the hard scattering coefficients are necessary to describe observables at higher $x$ values, where the effect is most relevant. Lastly, since our analyses use the zero-mass variable-flavor-number-scheme (ZM-VFNS), treatment of the heavy flavor masses in the QCD formalism will be necessary to properly describe heavy quark production. The ACOT renormalization scheme [189, 190] in particular is known to improve the agreement with HERA data at low $Q^2$ [190], where corrections of order $m^2/Q^2$ are relevant in the $F_L$ structure function, and will be implemented in upcoming JAM global studies.

The future of PDF and FF extraction will not only rely on including additional experimental observables or theoretical improvements, however, but also a robust methodology. While single $\chi^2$ minimization procedures have been quite successful in determining non-perturbative distributions in the past, such techniques are rather treacherous for global
analyses that contain a substantial amount of fit parameters and experimental measurements. In this case, reliable error estimation should instead be based on utilizing Monte Carlo methods to evaluate the Bayesian expectation and variance integrals. Such techniques are particularly useful for handling incompatible data sets, in addition to exploring the multi-dimensional $\chi^2$ or likelihood topology. Additional data analysis and statistical tools, such as complex machine learning algorithms, can also be implemented to minimize bias and extract the optimized functions efficiently.

The work presented here certainly took crucial steps in this direction, introducing an iterative Monte Carlo fitting procedure and simultaneously treating spin PDFs and FFs. However, the unpolarized PDFs in the denominator of DIS and SIDIS asymmetries were fixed, which can influence the fit results. While the unpolarized PDFs were found to play an insignificant role in the JAM17 analysis, it is nevertheless proper to treat simultaneously all non-perturbative input functions in global QCD studies. A forthcoming JAM analysis [191] will aim to accomplish this in a global fit to both unpolarized and polarized experimental observables. Such types of QCD studies, in combination with increasing theoretical precision and reliable Monte Carlo fitting methodologies, will ultimately take precedence in efforts to determine the proton spin structure.
APPENDIX A

Hard Scattering Coefficients in Mellin Space

In this appendix the hard coefficient functions in Mellin moment space are given for the scattering observables discussed in Chapter 2. For convenience, we also give the unpolarized DIS and SIDIS coefficients necessary to compute the spin asymmetries. At leading order in $\alpha_s$ the coefficients in Mellin space are simply equal to one. The relevant NLO coefficients depend on the analytic continuation of harmonic sums $S_1(N)$ and $S_2(N)$ to complex values of $N$ \[192\],

$$S_1(N) = \sum_{j=1}^{N} \frac{1}{j} \quad \rightarrow \quad \gamma_E + \psi^{(0)}_{N+1},$$

$$S_2(N) = \sum_{j=1}^{N} \frac{1}{j^2} \quad \rightarrow \quad \zeta(2) - \psi^{(1)}_{N+1},$$

where $\gamma_E$ is the Euler-Mascheroni constant and $\zeta$ is the Riemann zeta function. The $m$-th derivative of the polygamma function $\psi^{(m)}_{N}$ that appear in the above expressions is given...
by

\[ \psi_{N}^{(m)} = \frac{d^{m} \psi_{N}}{dN^{m}} = \frac{d^{m+1} \ln \Gamma(N)}{dN^{m+1}}. \tag{A.3} \]

In DIS, the NLO quark coefficient for the \( g_{1}^{(r2)} \) structure function (Eq. (2.11)) in Mellin space is [193, 194]

\[ \Delta C_{q}^{(1)}(N, Q^{2}) = C_{F} \left[ 2S_{1}^{2}(N) - 2S_{2}(N) + 2S_{1}(N) \left( \frac{3}{2} + \frac{1}{N+1} - \frac{1}{N} \right) - \frac{2}{N(N+1)} + \frac{3}{N} + \frac{2}{N^{2}} - 9 \right], \tag{A.4} \]

while for the gluon one has

\[ \Delta C_{g}^{(1)}(N, Q^{2}) = 2 \frac{(N-1)(1-N-NS_{1}(N))}{N^{2}(N+1)}, \tag{A.5} \]

where \( C_{F} = 4/3 \). The unpolarized scattering coefficients for the \( F_{2} \) and \( F_{L} \equiv (1+\gamma^{2})F_{2} - 2xF_{1} \) structure functions are given by [195]

\[ C_{2,q}^{(1)}(N, Q^{2}) = C_{F} \left[ 2S_{1}^{2}(N) - 2S_{2}(N) + 2S_{1}(N) \left( \frac{3}{2} - \frac{1}{N(N+1)} \right) + \frac{3}{N} + \frac{4}{N+1} + \frac{2}{N^{2}} - 9 \right], \tag{A.6} \]

\[ C_{L,q}^{(1)}(N, Q^{2}) = C_{F} \frac{4}{N+1}. \tag{A.7} \]
for the quark contributions and

\[
C^{(1)}_{2g}(N, Q^2) = -2T_R \left[ S_1(N) \frac{N^2 + N + 2}{N(N + 1)(N + 2)} + \frac{1}{N} - \frac{1}{N^2} \right.
\]
\[
- \frac{6}{N + 1} + \frac{6}{N + 2}\right], \tag{A.8}
\]

\[
C^{(1)}_{Lg}(N, Q^2) = \frac{8T_R}{(N + 1)(N + 2)}, \tag{A.9}
\]

for the gluon terms, where \( T_R = 1/2 \). In semi-inclusive DIS, the NLO coefficients for \( g_1^h \) (Eq. (2.15)) in Mellin space are given by [29]

\[
\Delta C^{(1)}_{qq}(N, M, Q^2) = C_F \left[ -8 - \frac{1}{M^2} + \frac{2}{(M + 1)^2} + \frac{1}{N^2} + \frac{(1 + M + N)^2 - 1}{M(M + 1)(N)(N + 1)} \right.
\]
\[
+ 3S_2(M) - S_2(N) + (S_1(N) + S_1(M)) \left( S_1(M) + S_1(N) 
\right.
\]
\[
- \frac{1}{M(M + 1)} - \frac{1}{N(N + 1)} \right], \tag{A.10}
\]

\[
\Delta C^{(1)}_{gq}(N, M, Q^2) = C_F \left[ \frac{2 - 2M - 9M^2 + M^3 - M^4 + M^5}{M^2(M - 1)^2(M + 1)^2} + \frac{2M}{N(M + 1)(M - 1)} \right.
\]
\[
- \frac{2 - M + M^2}{M(M + 1)(M - 1)(N + 1)} \right.
\]
\[
- (S_1(M) + S_1(N)) \frac{2 + M + M^2}{M(M + 1)(M - 1)} 
\]
\[
- \frac{2}{M(M + 1)(N + 1)} \right], \tag{A.11}
\]

\[
\Delta C^{(1)}_{qq}(N, M, Q^2) = T_R \left[ \frac{(N - 1)}{N(N + 1)} \left( \frac{1}{M - 1} - \frac{1}{M} + \frac{1}{N} - S_1(M) - S_1(N) \right) \right], \tag{A.12}
\]
and similarly for the $F^h_1$ and $F_L$ structure functions by

\begin{align}
C^{(1)}_{1,qq}(N, M, Q^2) &= \Delta C^{(1)}_{qq} + C_F \frac{2}{M(M+1)N(N+1)}, \\
C^{(1)}_{1,qg}(N, M, Q^2) &= \Delta C^{(1)}_{qg} + C_F \frac{2}{(M+1)N(N+1)}, \\
C^{(1)}_{1,gq}(N, M, Q^2) &= T_R \left[ \frac{2 + N + N^2}{N(N+1)(N+2)} \left( \frac{1}{M-1} - \frac{1}{M} \right) - S_1(M) - S_1(N) \right] + \frac{1}{N^2},
\end{align}

and

\begin{align}
C^{(1)}_{L,qq}(N, M, Q^2) &= 4 C_F \frac{4}{(M+1)(N+1)}, \\
C^{(1)}_{L,qg}(N, M, Q^2) &= 4 C_F \frac{4}{M(M+1)(N+1)}, \\
C^{(1)}_{L,gq}(N, M, Q^2) &= T_R \frac{8}{(N+1)(N+2)}.
\end{align}

In single-inclusive $e^+e^-$ annihilation, the quark scattering coefficient in Eq. (2.20) at NLO is [196]

\begin{align}
H_q^{(1)}(N, Q^2) &= 2 C_F \left[ 5 S_2(N) + S_1^2(N) + S_1(N) \left( \frac{3}{2} - \frac{1}{N(N+1)} \right) - \frac{2}{N^2} \\
&\quad + \frac{3}{(N+1)^2} - \frac{3}{2} \frac{1}{(N+1)} - \frac{9}{2} + \frac{1}{N} \right],
\end{align}

while for the gluon it is

\begin{align}
H_g^{(1)}(N, Q^2) &= 4 C_F \left[ - S_1(N) \frac{N^2 + N + 2}{(N-1)N(N+1)} - \frac{4}{(N-1)^2} + \frac{4}{N^2} \\
&\quad - \frac{3}{(N+1)^2} + \frac{4}{(N-1)N} \right].
\end{align}
APPENDIX B

Splitting Functions in Mellin Space

In this appendix, the \( N \)-th moments of the splitting functions in both the spacelike and timelike regions are given up to \( \mathcal{O}(\alpha_s^3 \equiv \alpha_s^3/(4\pi)^3) \) corrections \[38\],

\[
P_{ij}^{S,T}(N, Q^2) \approx \alpha_s(Q^2) P_{ij}^{S,T(0)}(N) + \alpha_s^2(Q^2) P_{ij}^{S,T(1)}(N),
\]

which are necessary to evolve the PDFs and FFs, respectively, at NLO in the QCD formalism. The well-known expressions for spacelike and timelike splitting functions at leading order (\( \alpha_s \)) accuracy are given by \[197, 198\]

\[
P_{NS \pm}^{S,T(0)} = -C_F \left[ 4S_1(N) - 3 - \frac{2}{N(N+1)} \right], \tag{B.2a}
\]

\[
P_{qq}^{S(T(0))} = 2n_f P_{gg}^{T(0)} = 2n_f \frac{N^2 + N + 2}{N(N+1)(N+2)}, \tag{B.2b}
\]

\[
P_{gg}^{S(T(0))} = 2C_F \frac{N^2 + N + 2}{N(N-1)(N+1)}, \tag{B.2c}
\]

\[
P_{gg}^{S,T(0)} = -C_A \left[ 4S_1(N) - \frac{11}{3} - \frac{4}{N(N-1)} - \frac{4}{(N+1)(N+2)} \right] - \frac{2n_f}{3}, \tag{B.2d}
\]
where $C_A = 3$. Note that the off-diagonal timelike splitting functions $P^{(0)}_{qq}$ and $P^{(0)}_{gq}$ are opposite to that in Ref. [199].

At NLO ($\alpha_s^2$), the spacelike and timelike splitting functions in Mellin space are given by [197, 199, 200]

$$P^{S(1)}_{NS\pm} = P^{T(1)}_{NS\pm} - \Delta^{(1)}_{NS}$$

$$= -C_F^2 \left[ 8S_1(N)\frac{(2N+1)}{N^2(N+1)^2} + 8 \left( 2S_1(N) - \frac{1}{N(N+1)} \right) \left( S_2(N) - S_{2\pm}'(\frac{N}{2}) \right) \right]$$

$$+ 12S_2(N) + 32S_{2\pm}(N) - 4S_{3\pm}'(\frac{N}{2})$$

$$- \frac{3}{2} - 4 \left( \frac{3N^2 + N^2 - 1}{N^3(N+1)^2} \right) \pm 8 \left( \frac{2N^2 + 2N+1}{N^3(N+1)^3} \right)$$

$$- \frac{2}{3} S_2(N) - \alpha_s - 16S_{2\pm}(N) + 2S_{3\pm}'(\frac{N}{2})$$

$$- \frac{2}{9} \left( 151N^4 + 236N^3 + 88N^2 + 3N + 18 \right) \pm 4 \left( \frac{N^2 + 2N + 1}{N^3(N+1)^3} \right)$$

$$- \frac{1}{2} n_f C_F \left[ -\frac{80}{9} S_1(N) + \frac{16}{3} S_2(N) + \frac{2}{3} + \frac{8}{9} \left( \frac{11N^2 + 5N - 3}{N^2(N+1)^2} \right) \right], \quad \text{(B.3a)}$$

$$P^{S(1)}_{qq} = P^{T(1)}_{qq} - \Delta^{(1)}_{qq}$$

$$= P^{(1)}_{NS\pm} + 2n_f C_F \left[ \frac{(5N^5 + 32N^4 + 49N^3 + 38N^2 + 28N + 8)}{(N-1)N^3(N+1)^3(N+2)^2} \right], \quad \text{(B.3b)}$$
\[ P^{S(1)}_{gg} = P^{T(1)}_{gg} - \Delta^{(1)}_{gg} \]
\[ = -\frac{1}{2} n_f C_A \left[ -\frac{80}{9} S_1(N) + \frac{16}{3} + \frac{8 (38N^4 + 76N^3 + 94N^2 + 56N + 12)}{(N - 1)N^2(N + 1)^2(N + 2)} \right] \]
\[ - \frac{1}{2} n_f C_F \left[ 4 + 8 \frac{(2N^6 + 4N^5 + N^4 - 10N^3 - 5N^2 - 4N - 4)}{(N - 1)N^3(N + 1)^3(N + 2)} \right] \]
\[ - C_A^2 \left[ \frac{268}{9} S_1(N) + 32 S_1(N) \frac{(2N^5 + 5N^4 + 8N^3 + 7N^2 - 2N - 2)}{(N - 1)^2N^2(N + 1)^2(N + 2)^2} - \frac{32}{3} \right. \]
\[ + 16 S_{2+}^I \left( \frac{N}{2} \right) \frac{(N^2 + N + 1)}{(N - 1)N(N + 1)(N + 2)} \]
\[ - 8S_1(N) S_{2+}^I \left( \frac{N}{2} \right) - 16 S_{3+}^I \left( \frac{N}{2} \right) \]
\[ - 8 \frac{(457N^9 + 2742N^8 + 6040N^7 + 6098N^6 + 1567N^5 - 2344N^4 - 1632N^3)}{(N - 1)^2N^3(N + 1)^3(N + 2)^3} \]
\[ - \frac{2}{9} \frac{(560N^2 + 1488N + 576)}{(N - 1)^2N^3(N + 1)^3(N + 2)^3} \] \hspace{1cm} (B.3c)
\[ P_{q\bar{q}}^{S(1)} = \frac{8}{3} n_f C_F \left[ \left( S_1(N) - \frac{8}{3} \right) \frac{(N^2 + N + 2)}{(N - 1)N(N + 1)} + \frac{1}{(N + 1)^2} \right] \]
\[ + 4C_F C_A \left[ \left( S_1^2(N) + S_2(N) - S_{2, \phi} \left( \frac{N}{2} \right) \right) \frac{(N^2 + N + 2)}{(N - 1)N(N + 1)} - S_1(N) - \frac{17N^4 + 41N^2 - 22N - 12}{3(N - 1)^2 N^2(N + 1)} \right] \]
\[ + \frac{109N^9 + 621N^8 + 1400N^7 + 1678N^6 + 695N^5 - 1031N^4}{9(N - 1)^2 N^3(N + 1)^3(N + 2)^2} \]
\[ - \frac{1304N^3 + 152N^2 - 432N - 144}{9(N - 1)^2 N^3(N + 1)^3(N + 2)^2} \]
\[ + 4C_F C_F \left[ (5S_1(N) - S_1^2(N) - S_2(N)) \frac{(N^2 + N + 2)}{(N - 1)N(N + 1)} - 2S_1(N) \right] \]
\[ - \frac{12N^6 + 30N^5 + 43N^4 + 28N^3 - N^2 - 12N - 4}{2(N - 1)N^3(N + 1)^3} \], \quad (B.3e) \]

\[ P_{q\bar{q}}^{T(1)} = 2n_f C_F^2 \left[ \left( S_1^2(N) - 3S_2(N) - \frac{2\pi^2}{3} \right) \frac{(N^2 + N + 2)}{(N - 1)N(N + 1)} \right] \]
\[ + 2S_1(N) \left( \frac{4}{(N - 1)^2} - \frac{2}{(N - 1)N} - \frac{4}{N^2} + \frac{3}{(N + 1)^2} - \frac{1}{(N + 1)} \right) \]
\[ - \frac{8}{(N - 1)^2 N} + \frac{8}{(N - 1)N^2} + \frac{2}{N^3} + \frac{8}{N^2} - \frac{1}{2N} \]
\[ + \frac{1}{(N + 1)^3} - \frac{5}{2(N + 1)^2} + \frac{9}{2(N + 1)} \]
\[ + 2n_f C_F C_A \left[ \left( -S_1^2(N) + 5S_2(N) - G^{(1)}(N) + \frac{\pi^2}{6} \right) \frac{(N^2 + N + 2)}{(N - 1)N(N + 1)} \right] \]
\[ + 2S_1(N) \left( -\frac{2}{(N - 1)^2} + \frac{2}{(N - 1)N} + \frac{2}{N^2} - \frac{2}{(N + 1)^2} + \frac{1}{N + 1} \right) \]
\[ - \frac{8}{(N - 1)^3} + \frac{6}{(N - 1)^2} + \frac{17}{9(N - 1)} + \frac{4}{N^2} - \frac{1}{12} \]
\[ - \frac{8}{N^2} + \frac{2}{N} - \frac{2}{N^2(N + 1)} - \frac{2}{(N + 1)^3} - \frac{7}{(N + 1)^2} \]
\[ - \frac{1}{N + 1} - \frac{8}{3(N + 2)^2} + \frac{44}{9(N + 2)} \], \quad (B.3f) \]
\[
\mathbf{P}_{gT}^{(1)} = \frac{1}{3} n_f \left[ S_1(N + 1) \frac{(N^2 + N + 2)}{N(N + 1)(N + 2)} + \frac{1}{N^2} - \frac{5}{3N} - \frac{1}{N(N + 1)} - \frac{2}{(N + 1)^2}
\right.
\]
\[
+ \frac{4}{3(N + 1)} + \frac{4}{(N + 2)^2} - \frac{4}{3(N + 2)} \right] 
\]
\[
+ \frac{1}{4} C_F \left[ \left( -2S_1^2(N + 1) + 2S_1(N + 1) + 10S_2(N + 1) \right) \frac{(N^2 + N + 2)}{N(N + 1)(N + 2)} 
\right.
\]
\[
+ 4S_1(N + 1) \left( -\frac{1}{N^2} + \frac{1}{N} + \frac{1}{N(N + 1)} + \frac{2}{(N + 1)^2} - \frac{4}{(N + 2)^2} \right)
\]
\[
- \frac{2N^3}{N^2} + \frac{5}{12} - \frac{1}{N} + \frac{4}{N^2(N + 1)} - \frac{2N(N + 1)^2}{N(N + 1)} - \frac{6}{N(N + 1)}
\]
\[
+ \frac{4}{N + 1} - \frac{23}{N + 1} - \frac{20}{N + 2} \left\right]
\]
\[
+ \frac{1}{4} C_A \left[ \left( 2S_1^2(N + 1) - \frac{10}{3} S_1(N + 1) - 6S_2(N + 1) + 2G^{(1)}(N + 1) - \pi^2 \right)
\right.
\]
\[
\times \frac{(N^2 + N + 2)}{N(N + 1)(N + 2)} 
\]
\[
- 4S_1(N + 1) \left( -\frac{2}{N^2} + \frac{1}{N} + \frac{1}{N(N + 1)} + \frac{4}{(N + 1)^2} - \frac{6}{(N + 2)^2} \right)
\]
\[
- \frac{40}{9(N - 1)} + \frac{4}{N^3} + \frac{8}{3N^2} + \frac{26}{9N} - \frac{8}{N^2(N + 1)^2}
\]
\[
+ \frac{22}{3N(N + 1)} + \frac{16}{(N + 1)^3} + \frac{68}{3(N + 1)^2} - \frac{190}{9(N + 1)}
\]
\[
+ \frac{8}{(N + 1)^2(N + 2)} - \frac{4}{(N + 2)^2} + \frac{356}{9(N + 2)} \right], \quad (B.3g)
\]
where the terms

\[
\begin{align*}
\Delta_{NS}^{(1)} &= \frac{C_F^2}{2} \left[ -4 S_1(N) + 3 + \frac{2}{N(N+1)} \right] \left[ 2 S_2(N) - \frac{\pi^2}{3} - \frac{2N+1}{N^2(N+1)^2} \right], \\
\Delta_{qq}^{(1)} &= \frac{1}{2} n_f C_F \left[ \frac{80}{9} \frac{1}{N-1} + \frac{8}{N^3} + \frac{12}{N^2} - \frac{12}{N} + \frac{8}{(N+1)^3} + \frac{28}{(N+1)^2} \right. \\
&\quad \left. - \frac{4}{N+1} + \frac{32}{3} \frac{1}{(N+2)^2} - \frac{224}{9} \frac{1}{N+2} \right], \\
\Delta_{gg}^{(1)} &= \frac{1}{2} n_f C_F \left[ -\frac{16}{3} \frac{1}{(N-1)^2} + \frac{8}{9} \frac{1}{N-1} + \frac{8}{N^3} + \frac{16}{N^2} + \frac{12}{N} + \frac{8}{(N+1)^3} \right. \\
&\quad \left. - \frac{24}{(N+1)^2} + \frac{4}{N+1} - \frac{16}{3} \frac{1}{(N+2)^2} - \frac{224}{9} \frac{1}{N+2} \right] \\
&\quad - \frac{4}{3} n_f C_A \left[ S_2(N) - \frac{1}{(N-1)^2} + \frac{1}{N^2} - \frac{1}{(N+1)^2} + \frac{1}{(N+2)^2} - \frac{\pi^2}{6} \right] \\
&\quad + C_A^2 \left[ -8 S_1(N) S_2(N) + 8 S_1(N) \left( \frac{1}{(N-1)^2} - \frac{1}{N^2} + \frac{1}{(N+1)^2} - \frac{1}{(N+2)^2} + \frac{\pi^2}{6} \right) \right. \\
&\quad \left. + \left( 8 S_2(N) - \frac{4 \pi^2}{3} \right) \left( \frac{1}{N-1} - \frac{1}{N} + \frac{1}{N+1} - \frac{1}{N+2} + \frac{11}{12} \right) \right. \\
&\quad \left. - \frac{8}{(N-1)^3} + \frac{22}{3} \frac{1}{(N-1)^2} - \frac{8}{(N-1)^2} N - \frac{8}{N^3} - \frac{8}{N^2} \frac{14}{3} \frac{1}{N} \right] \\
&\quad \left. - \frac{8}{(N+1)^3} + \frac{14}{3} \frac{1}{(N+1)^2} - \frac{8}{(N+1)^2} (N+2) - \frac{8}{(N+1)(N+2)^2} \right] \\
&\quad - \frac{8}{(N+2)^3} + \frac{22}{3} \frac{1}{(N+2)^2} \right], \\
\end{align*}
\]

(B.4a, B.4b, B.4c)

are present specifically for the timelike functions. In Eqs. (B.3) the sum

\[
S_{m,\pm}^{(N)} = 2^{m-1} \sum_{j=1}^{N} \frac{1 + (-1)^j}{j^m}
\]

(B.5a)
has the analytic continuation

\[ S'_{m+}(\frac{N}{2}) \rightarrow S_m(\frac{N}{2}), \]  
\[ S'_{m-}(\frac{N}{2}) \rightarrow S_m(\frac{N-1}{2}), \]  

(B.5b)

(B.5c)

with

\[ S_3(N) = \sum_{j=1}^{N} \frac{1}{j^3} \rightarrow \zeta(3) + \psi^{(2)}_{N+1}, \]  
(B.6)

\[ \tilde{S}_\pm(N) = -\frac{5}{8} \zeta(3) \pm \left[ \frac{S_1(N)}{N^2} - \frac{\zeta(2)}{2} (\psi^{(0)}_{(N+1)/2} - \psi^{(0)}_{N/2}) + \text{Li}(N) \right], \]  
(B.7)

\[ G^{(1)}(N) = \psi^{(1)}_{(N+1)/2} - \psi^{(1)}_{N/2}. \]  
(B.8)

The last term in Eq. (B.7) involves the \( N \)-th moment of the dilogarithm function,

\[ \text{Li}(N) \equiv \int_0^1 dx \, x^{N-1} \frac{\text{Li}_2(x)}{1+x}, \]  
(B.9a)

which can be approximated using the expansion [192]

\[ \text{Li}(N) \approx \frac{1.01}{N+1} - \frac{0.846}{N+2} + \frac{1.155}{N+3} - \frac{1.074}{N+4} + \frac{0.55}{N+5}. \]  
(B.9b)
BIBLIOGRAPHY


