Efficient Fourier Transforms for Transverse Momentum Dependent Distributions

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Abstract

Hadron production at low transverse momenta in semi-inclusive deep inelastic scattering can be described by transverse momentum dependent (TMD) factorization . This formalism has also been widely used to study the Drell-Yan process and back-to-back hadron pair production in e^+e^- collisions. These processes are the main ones for extractions of TMD parton distribution functions and TMD fragmentation functions, which encode important information about nucleon structure and hadronization. One of the most widely used TMD factorization formalism in phenomenology formulates TMD observables in coordinate b_{\perp} -space, the conjugate space of the transverse momentum. The Fourier transform from b_{\perp} -space back into transverse momentum space is sufficiently complicated due to oscillatory integrands and requires a careful and computationally intensive numerical treatment in order to avoid potentially large numerical errors. In this paper we develop a fast two-dimensional numerical Fourier transform algorithm that can potentially improve the numerical accuracy of TMD calculations and boost the numerical performance to carry out global QCD analysis of TMDs.

1. Introduction

The transverse momentum dependent (TMD) parton distribution functions (PDFs) and fragmentation functions (FFs) have received great attention from both theoretical and experimental communities in recent years. These TMD PDFs and FFs, or in short called TMDs, provide new information on hadron structure: the three-dimensional imaging of hadrons in both longitudinal and transverse momentum space [1–4]. Significant progress has been made in the last few years in terms of measuring transverse momentum dependent unpolarized and polarized cross sections in experiments, as well as extracting the associated spin-independent and spin-dependent TMDs in phenomenology, see Refs. [5, 6] and references therein.

TMDs are non-perturbative objects in Quantum Chromodynamics (QCD) and thus they have to be either computed on the lattice, or extracted from experimental data. For recent developments on lattice computation of TMDs, see Ref. [7]. On the other hand, in order to extract TMDs from the experimental data, one relies on proper QCD factorization theorems [8]. TMD factorization [9–12] describes cross sections in scattering events where the relevant transverse momentum q_{\perp} of the observed final state is much smaller than the hard scale $Q: q_{\perp} \ll Q$. In such a regime, the cross section can be factorized in terms of TMD PDFs and/or FFs and perturbatively calculable short distance hard coefficients. The relevant processes that have been extensively studied include semi-inclusive deep inelastic scattering (SIDIS) [13, 14], Drell-Yan process in proton-proton collisions [15, 16], and back-to-back dihadron production in e^+e^- collisions [17, 18]. There are also other new opportunities in studying TMDs which are proposed recently in e.g. Refs. [19–28], and usually involve jet measurements.

Within the TMD factorization formalism, the cross section is written as a convolution of the relevant transverse momentum dependent functions. To motivate our discussion and thus make the case more concrete, let us take SIDIS

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as an example. The differential cross section for the unpolarized scattering process of $e(\ell) + p(P) \rightarrow e(\ell') + h(P_h) + X$ can be written as [29]

$$\frac{d\sigma^{h}}{dx_{\rm bj}\,dy\,dz\,d^{2}q_{\perp}} = \frac{2\pi\alpha_{\rm EM}^{2}}{Q^{2}}\frac{1+(1-y)^{2}}{y}\,F_{UU}(x_{\rm bj},z,q_{\perp},Q^{2}),\tag{1}$$

where the standard SIDIS variables are defined as

$$q = \ell - \ell', \qquad Q^2 = -q^2, \qquad x_{\rm bj} = \frac{Q^2}{2P \cdot q}, \qquad y = \frac{P \cdot q}{P \cdot \ell}, \qquad z = \frac{P \cdot P_h}{P \cdot q}.$$
 (2)

The unpolarized structure functions F_{UU} in Eq. (1) can be factorized as follows

$$F_{UU}(x_{\rm bj}, z, q_{\perp}, Q) = H(Q, \mu) \sum_{q} e_{q}^{2} \int d^{2}\mathbf{k}_{\perp} d^{2}\mathbf{p}_{\perp} f_{q/p}(x_{\rm bj}, k_{\perp}^{2}) D_{h/q}(z, p_{\perp}^{2}) \,\delta^{(2)}\left(\mathbf{k}_{\perp} + \mathbf{p}_{\perp}/z - \mathbf{q}_{\perp}\right),\tag{3}$$

where $\mathbf{q}_{\perp} = \mathbf{P}_{h\perp}/z$, e_q is the fractional electric charge for the quarks, and $H(Q,\mu)$ is the hard function to be given by Eq. (33) in Sec. 4. On the other hand, $f_{q/p}(x_{bj}, k_{\perp}^2)$ and $D_{h/q}(z, p_{\perp}^2)$ are the unpolarized quark TMD PDF and FF, respectively. Here we have suppressed the additional scale parameters in the TMDs, which are associated with QCD evolution of the TMDs [30–34]. In general, the convolution and integration of TMDs over the momenta \mathbf{k}_{\perp} and \mathbf{p}_{\perp} are quite involved. Thus in the original Collins-Soper-Sterman (CSS) approach [35], one takes a Fourier transformation from the momentum space to the coordinate \mathbf{b}_{\perp} space, ¹

$$F_{UU}(b_{\perp}, Q) = \int d^2 \mathbf{q}_{\perp} \ e^{-i\mathbf{q}_{\perp} \cdot \mathbf{b}_{\perp}} \ F_{UU}(q_{\perp}, Q), \tag{4}$$

and thus one can write

$$F_{UU}(q_{\perp}, Q) = H(Q, \mu) \sum_{q} e_{q}^{2} \int \frac{d^{2} \mathbf{b}_{\perp}}{(2\pi)^{2}} e^{i\mathbf{q}_{\perp}\cdot\mathbf{b}_{\perp}} f_{q/p}(x_{\rm bj}, b_{\perp}) D_{h/q}(z, b_{\perp}) ,$$

= $H(Q, \mu) \sum_{q} e_{q}^{2} \frac{1}{2\pi} \int_{0}^{\infty} db_{\perp} b_{\perp} J_{0}(q_{\perp}b_{\perp}) f_{q/p}(x_{\rm bj}, b_{\perp}) D_{h/q}(z, b_{\perp}) ,$ (5)

where $b_{\perp} = |\mathbf{b}_{\perp}|$ is the magnitude of the vector \mathbf{b}_{\perp} , J_0 is the Bessel function of the first kind of order 0, and $f_{q/p}(x_{bj}, b_{\perp})$, $D_{h/q}(z, b_{\perp})$ are the Fourier transform of the TMD PDF and FF, respectively.

For the polarized scattering, the generic structure of the cross sections can be written as [10, 29]

$$\boldsymbol{q}_{\perp}^{\alpha} F(\boldsymbol{q}_{\perp}^{2},\cdots), \qquad \boldsymbol{q}_{\perp}^{\alpha} \boldsymbol{q}_{\perp}^{\beta} F(\boldsymbol{q}_{\perp}^{2},\cdots)$$
(6)

with $F(q_{\perp}^2)$ representing a generic function of q_{\perp}^2 and " \cdots " denoting the other kinematic variables. The Fourier transform of such functions will lead to Bessel functions of order 1 and 2. In fact, as shown in [38], all the spin-dependent structure functions at leading-power can be expressed in terms of a integration over b_{\perp} multiplied by the Bessel functions of J_0 , J_1 , or J_2 .

Without loss of generality the integration form stemming from the Fourier transform encountered in TMD observables can be written as

$$\int_0^\infty dx \ f(x) \ J_n(x),\tag{7}$$

where $x = b_{\perp}q_{\perp}$, $J_n(x)$ is the Bessel function of order *n*, and f(x) is usually a smooth function of *x* that slowly decay as $x \to \infty$. Such an integration can be extremely computationally intensive and time consuming with standard

¹There are also other approaches in the literature that do not work in the \mathbf{b}_{\perp} space, see e.g. Refs. [36, 37]. Notice that we drop explicit dependence on x_{bj} and z for the rest of this paper.

integration routines based on adaptive Gaussian quadratures or Monte Carlo integration methods due to the oscillation nature of the Bessel functions. In the context of TMD global analysis, one has to compute the above integration many times, and for different kinematic regions, in order to find the best fit for the non-perturbative TMDs. This has become a huge hurdle for TMD phenomenology in the past for carrying out the global QCD analysis on TMDs using the data from HERMES, COMPASS, JLAB 6 GeV, Relativistic Heavy Ion Collider (RHIC) and BELLE experiments and it will become even more challenging for the large amount data that is expected from the JLab 12 GeV program and the future Electron Ion Collider (EIC). Because of this, and because of the complexity of the TMD evolution improving the efficiency and the speed of the numerical integration of Eq. (7) is extremely desirable.

Ogata has introduced a quadrature formula in Ref. [39] that is optimized for integrands with Bessel functions for exactly the same integral as in Eq. (7). In this paper, we further optimize the Ogata's quadrature method for the numerical Fourier transform in Eq. (7), to obtain a high efficient algorithm. We demonstrate that the optimized Ogata's quadrature is more efficient than the traditional adaptive Gaussian quadrature method and Monte Carlo method in terms of convergence, and also leads to smaller errors. The rest of this paper is organized as follows. In Sec. 2, we summarize the relevant formalism for the Ogata quadrature method and describe our optimized numerical algorithm in detail. In Sec. 3, we give a demonstration of the optimized Ogata quadrature and benchmark the algorithm against adaptive Gaussian quadrature using an exponential function which has an analytic Fourier transform. In Sec. 4, we apply our numerical method to an example of a phenomenological form of TMDs. We conclude our paper in Sec. 5.

2. Optimized Ogata Quadrature Formalism

In this section we first review the original Ogata quadrature formalism and then discuss our optimization scheme for performing high efficiency numerical integrals relevant to TMD analysis. The Ogata method, based on a quadrature formalism was first introduced in Ref. [40] by Frappier and Olivier. The quadrature formula for the integrand of the form $|x|^{2n+1}f(x)$ reads:

$$\int_{-\infty}^{\infty} dx |x|^{2n+1} f(x) = h \sum_{j=-\infty, j\neq 0}^{\infty} w_{nj} |x_{nj}|^{2n+1} f(x_{nj}) + O\left(e^{-c/h}\right) ,$$
(8)

where the function f(x) must be an integrable function for the sum to be finite. The nodes x_{nj} and the weights w_{nj} of the quadrature are given by

$$x_{nj} = h\xi_{nj} , \qquad w_{nj} = \frac{2}{\pi^2 \xi_{n|j|} J_{n+1}(\pi \xi_{n|j|})} , \qquad (9)$$

with $j = \pm 1, \pm 2, \cdots$, and ξ_{nj} the zeros of the Bessel function $J_n(\pi x)$ of order *n*, i.e. $J_n(\pi \xi_{nj}) = 0$, and the parameter 1/h represents the node density. The term $O(e^{-c/h})$ accounts for the error of the quadrature sum approximation at a finite *h* as described in equation (2.2) of Ref. [39], and *c* is a positive constant, whose precise value depends on the functional form of f(x). For the time being, we will be interested in the case of f(x) being an even function of *x* which results in the following quadrature formula

$$\int_0^\infty dx \, x^{2n+1} \, f(x) = h \sum_{j=1}^\infty w_{nj} \, x_{nj}^{2n+1} \, f(x_{nj}) + O\left(e^{-c/h}\right). \tag{10}$$

In practice the sum in Eq. (10) is truncated at a given j = N which introduces an error of

$$\mathcal{I}_{nN+1} = h \sum_{j=N+1}^{\infty} w_{nj} \, x_{nj}^{2n+1} \, f(x_{nj}). \tag{11}$$

and the quadrature formula becomes

$$\int_{0}^{\infty} dx \, x^{2n+1} f(x) = h \sum_{j=1}^{N} w_{nj} \, x_{nj}^{2n+1} f(x_{nj}) + \left[I_{nN+1} + O\left(e^{-c/h}\right) \right]. \tag{12}$$

The following change of variables, see Ref. [39], optimizes the convergence of integrals of the typical TMD functional form from Eq. (7):

$$x = \frac{\pi}{h}\psi(t) \qquad \text{with} \quad \psi(t) = t \tanh\left(\frac{\pi}{2}\sinh t\right) , \tag{13}$$

so that Eq. (7) becomes

$$\int_{0}^{\infty} dx f(x) J_{n}(x) = \frac{\pi}{h} \int_{0}^{\infty} dt \, \psi'(t) f\left(\frac{\pi}{h}\psi(t)\right) J_{n}\left(\frac{\pi}{h}\psi(t)\right) = \frac{\pi}{h} \int_{0}^{\infty} dt \, |t|^{2n+1} \frac{\psi'(t) f\left(\frac{\pi}{h}\psi(t)\right) J_{n}\left(\frac{\pi}{h}\psi(t)\right)}{t^{2n+1}} , \qquad (14)$$

where $\psi'(t) = d\psi(t)/dt$. At this point, it is important to realize that the part of the integrand beside the factor $|t|^{2n+1}$ is an even function of *t*, and thus we can apply Eq. (10) and obtain the following quadrature formula

$$\int_{0}^{\infty} dx f(x) J_{n}(x) = \pi \sum_{j=1}^{N} w_{nj} f\left(\frac{\pi}{h} \psi(x_{nj})\right) J_{n}\left(\frac{\pi}{h} \psi(x_{nj})\right) \psi'(x_{nj}) + \left[I'_{nN+1} + O\left(e^{-c/h}\right)\right],$$
(15)

where \mathcal{I}'_{nN+1} are the same truncation errors defined in Eq. (11) but with the transformed integrand,

$$I'_{nN+1} = \pi \sum_{j=N+1}^{\infty} w_{nj} f\left(\frac{\pi}{h}\psi(x_{nj})\right) J_n\left(\frac{\pi}{h}\psi(x_{nj})\right) \psi'(x_{nj}).$$
(16)

Eq. (15) is the aforementioned Ogata quadrature formula, which we advocate in our current paper. The variable substitution has the useful asymptotic behavior

$$\frac{\pi}{h}\psi(x_{nj}) \approx \pi\xi_{nj} \left[1 - 2\exp\left(-\frac{\pi}{2}e^{x_{nj}}\right)\right],\tag{17}$$

such that the asymptotic behavior for the Bessel function becomes

$$J_n\left(\frac{\pi}{h}\psi(x_{nj})\right) \approx 2\pi\xi_{nj}J_{n+1}(\pi\xi_{nj})\exp\left(-\frac{\pi}{2}e^{x_{nj}}\right).$$
(18)

This variable substitution then enforces the double exponential convergence of the quadrature sum in j.

The quadrature sum has two parameters, h and N, which control the efficiency and the magnitude of the error terms. To generate a high efficiency algorithm, the numerical integration must be performed with a small N while at the same time the error terms must also be small, to ensure reliable results. By inspecting Eqs. (16) and (18) one notes that for a small number of function calls the truncation errors will be large if h is too small. At the same time for larger values of h the quadrature error grows as $\sim e^{-c/h}$, see Eq. (8). These observations indicate the need to find optimal values for h and N that keep the error term in Eq. (15) as small as possible. We found that such optimal values can be obtained by enforcing the largest contribution to the quadrature to be the first term in the truncated sum of Eq. (10) which can be achieved by maximizing the contribution of the first node, i.e.

$$\frac{\partial}{\partial h} \left(h(h\xi_{n1})^{2n+1} f(h\xi_{n1}) \right) = 0.$$
⁽¹⁹⁾

By solving numerically Eq. (19) for *h* one finds the optimal value of *h* for the quadrature method in Eq. (10). We will refer to this optimal value as h_u .

It is now worth noting that h_u will tend to be a large value. This makes intuitive sense since minimizing truncation errors can be achieved by using a large spacing parameter. However, taking a large value of h introduces quadrature errors which behave like $e^{-c/h}$ and tend to be large for $h = h_u$. This issues can be mitigated by using the following scheme. We first use the condition in Eq. (19) to minimize truncation errors in Eq. (10). We then impose the condition that the final nodes of Eq. (10) and Eq. (15) are placed at the same location by enforcing that

$$h_{\rm u}\xi_{nN} = \frac{\pi}{h}\psi(h\xi_{nN}) \ . \tag{20}$$

This ensures that the quadrature in Eq. (15) has the same truncation errors as Eq. (10) with h_u . The solution for h in the above equality is given by

$$h = \frac{1}{\pi \xi_{nN}} \sinh^{-1} \left(\frac{2}{\pi} \tanh^{-1} \left(\frac{h_{\rm u}}{\pi} \right) \right) \,. \tag{21}$$

This value, labeled as h_t is the optimal value for h to be used in Eq. (15). Note that h_t is suppressed by a large factor of $\pi \xi_{nN}$ so that $h_t \ll h_u$. In Fig. 1 we plot the ratio h_t/h_u as a function of h_u for N = 10, 20, and 40. We find that in all cases $\frac{h_t}{h_u} \ll 1$ which avoids large errors in Eq. (19).



Figure 1: The solution of Eq. (21) as a function of h_u at several values of N. The solution is written as h_t/h_u to demonstrate that for $h_u < \pi$, that $h_t \ll h_u$.

In summary, for a given choice of number of integrand evaluations N, our procedure minimizes the error contribution in h as well as truncation errors by applying the conditions Eq. (20) and Eq. (19). The application of these conditions determines an optimal choice for h in implementing the quadrature formula of Eq. (15). We shall refer to this procedure as "the optimized Ogata quadrature formula." We will demonstrate below the efficiency of our formalism, first through the use of toy TMDs, and then through QCD based TMDs.

3. Benchmarking the Numerical Precision

In this section, we demonstrate the efficiency of the optimized Ogata quadrature method using toy TMDs for which the exact Bessel transform is known. We will compare the numerical efficiency of the optimized Ogata quadrature against the adaptive Gaussian quadrature, which is available in QUADPACK integration routine in Ref. [41]. It is important to emphasize that even though we mainly demonstrate the method for the integration involving Bessel function $J_0(x)$, we have checked that it works equally well for integration involving either $J_1(x)$ or $J_2(x)$, relevant for TMD studies in polarized scattering.

To assess the efficacy of our quadrature method we will map the error of the integration relative to the exact known result as a function of number of integrand calls. As discussed before we are interested in performing integrals of the form

$$W(q_{\perp}) = \int_0^\infty db_{\perp} b_{\perp} \ \widetilde{W}(b_{\perp}) \ J_0(b_{\perp} q_{\perp}) \ , \tag{22}$$

where the function $\widetilde{W}(b_{\perp})$ contains the b_{\perp} space TMD physics. Therefore we will use a toy $\widetilde{W}(b_{\perp})$ which mimics the b_{\perp} space behavior of realistic unpolarized TMDs that has an exact analytic Fourier-Bessel transform. Specifically we

choose the gamma distributions which are given in terms of the distribution's mean, β , and variance, σ , as

$$\widetilde{W}(b_{\perp};\beta,\sigma) = \frac{1}{b_{\perp}} \left(\frac{\beta b_{\perp}}{\sigma^2}\right)^{\beta^2/\sigma^2} \frac{e^{-\frac{\beta b_{\perp}}{\sigma^2}}}{\Gamma\left(\frac{\beta^2}{\sigma^2}\right)} \,.$$
(23)

This function has an exponential b_{\perp} -dependence, and has been used in the literature for TMD studies [42]. Its exact Fourier-Bessel transform is given by

$$W^{\text{exact}}(q_{\perp};\beta,\sigma) = \left(\frac{\sigma^2}{\beta}\right) \frac{\Gamma\left(\frac{\beta^2}{\sigma^2} + 1\right)}{\Gamma\left(\frac{\beta^2}{\sigma^2}\right)} {}_2\tilde{F}_1\left(\frac{1}{2}\left(\frac{\beta^2}{\sigma^2} + 1\right), \frac{1}{2}\left(\frac{\beta^2}{\sigma^2} + 2\right); 1; -\frac{q_{\perp}^2\sigma^4}{\beta^2}\right), \tag{24}$$

where $_{2}\tilde{F}_{1}(a, b; c, d)$ is the regularized Gaussian hyper-geometric function. The function $\widetilde{W}(b_{\perp}; \beta, \sigma)$ has a single peak



Figure 2: Left panel: The integrand of Eq. (22) with \widehat{W} from Eq. (23) as a function of b_{\perp} for small, moderate and large transverse momenta $q_{\perp} = 0.2$, 2, and 4 GeV. We choose Q = 2 GeV in Eq. (26). Right panel: The relative percent error Eq. (28) of the Ogata quadrature is plotted as a function of h for small, moderate and large transverse momentum q_{\perp} at N = 15, the number of nodes used in the integration.

in b_{\perp} space, which is given in terms of β and σ as

$$b_{\perp}^{\text{peak}} = \frac{\beta^2 - \sigma^2}{\beta}.$$
 (25)

We further introduce a parameter Q to our toy TMD model, which is the inverse of the b_{\perp}^{peak} , i.e.

$$Q = \frac{1}{b_{\perp}^{\text{peak}}} = \frac{\beta}{\beta^2 - \sigma^2}.$$
(26)

Such a Q-dependence mimics the hard scale Q encountered in QCD based TMDs such as the photon virtuality in SIDIS reactions. [35, 43]. Notice that it is the quantity q_{\perp}/Q that controls how oscillating the toy TMD is. The larger q_{\perp}/Q is, the more oscillating the integrand is in b_{\perp} space and the more numerically intensive the integration becomes.

For our demonstration, we take Q = 2 (GeV) and $\sigma = 1$ (GeV⁻¹) similar to the usual JLab kinematics. We choose $q_{\perp} = 0.2, 2$, and 4 (GeV), and plot the integrands on the left hand side of Fig. 2. As one can see clearly, the integrands do become more oscillating as q_{\perp}/Q increases. To test the precision of our formalism, we take N = 15 in our optimized Ogata formula in Eq. (15),

$$W^{\text{Ogata}}(q_{\perp};\beta,\sigma) = \pi \sum_{j=1}^{15} w_{nj} f\left(\frac{\pi}{h}\psi(h\xi_{nj})\right) J_n\left(\frac{\pi}{h}\psi(h\xi_{nj})\right) \psi'(h\xi_{nj}).$$
(27)

The relative percent error is defined as

rel. error(%) =
$$\left| \frac{W^{\text{exact}}(q_{\perp};\beta,\sigma) - W^{\text{Ogata}}(q_{\perp};\beta,\sigma)}{W^{\text{exact}}(q_{\perp};\beta,\sigma)} \right| \times 100$$
, (28)

where the exact result $W^{\text{exact}}(q_{\perp};\beta,\sigma)$ is given in Eq. (24). On the right panel of Fig. 2, we plot the relative percent error of the numerical integration as a function of the parameter *h* for $q_{\perp} = 0.2$, 2, and 4 GeV, respectively. One can see that in each case, there is an optimal value of the parameter *h*, which minimizes the measured error.

Intuitively having a small node spacing *h* should result in a small error, since the error in *h* is of the order $O(e^{-c/h})$ in Eq. (15). However, the truncation errors I'_{nN+1} in Eq. (15) will generate large errors in the numerical integration, due to the factors of $f\left(\frac{\pi}{h}\psi(h\xi_{nj})\right) J_n\left(\frac{\pi}{h}\psi(h\xi_{nj})\right)$, unless one increases *N* significantly. Therefore, for a small and fixed number of nodes *N*, there is an optimized *h* that minimizes the errors as argued in Sec. 2. On the right panel of Fig. 2, we indicate with stars the values of *h* which are determined by the optimization conditions Eqs. (19) and (20). We find that within this range of kinematics, our optimization conditions indeed determine suitable values of *h* for our quadrature method which is key to achieve high efficiency in the numerical integration.



Figure 3: From left to right, the relative percent error of optimized Ogata and adaptive Gaussian quadrature as a function of total number of calls N_{tot} to the integrand at small, moderator and large transverse momentum: $q_{\perp}/Q = 0.1$ (left), $q_{\perp}/Q = 1$ (middle), and $q_{\perp}/Q = 2$ (right).

We now compare the efficiency of the optimized Ogata quadrature against adaptive Gaussian quadrature. Note that the optimized Ogata quadrature first samples the integrand to determine the optimal value of *h* using Eq. (19), then the integration routine samples the integrand at *N* nodes to perform the sum. This results in a total number of integrand calls N_{tot} . Likewise, we measure the total number of function calls of adaptive Gaussian quadrature requested by the numerical routine. In Fig. 3 we plot the relative error as a function of N_{tot} for small, intermediate and large values of q_{\perp}/Q . As is evident, the optimized Ogata quadrature method is more efficient than adaptive Gaussian quadrature, for all three probed regions of q_{\perp}/Q with relative errors that go below 0.1% with fairly less number of function calls than the adaptive Gaussian quadrature.

4. Application to TMDs

In this section we use the optimized Ogata quadrature to calculate the SIDIS q_{\perp} -differential cross sections in QCD TMD factorization framework. We then use these calculations to describe COMPASS charged hadron multiplicity data [14]. In addition, we use adaptive Gaussian quadrature and Vegas Monte Carlo algorithm for the same calculations to benchmark the performance.

Let's first summarize the basic ingredients for the implementation of the unpolarized SIDIS structure function F_{UU} in Eq. (5) in the CSS TMD framework [9, 32]. In such context the TMD PDFs and TMD FFs can be expressed

as

$$f_{q/p}(x_{\rm bj}, b_{\perp}; \mu, \zeta) = \sum_{j} \int_{x_{\rm bj}}^{1} \frac{d\hat{x}}{\hat{x}} C_{q/j}^{pdf} \left(x_{\rm bj}/\hat{x}, b_{*}, \mu_{b_{*}} \right) f_{j/p} \left(\hat{x}, \mu_{b_{*}} \right) \exp\left(S_{\rm pert} - g_A(x_{\rm bj}, b_{\perp}, b_{max}) - \frac{1}{2} g_K(b_{\perp}, b_{max}) \ln\left(\frac{\zeta}{Q_0^2}\right) \right)$$
(29)

$$D_{h/q}(z,b_{\perp};\mu,\zeta) = \sum_{j} \int_{z}^{1} \frac{d\hat{z}}{\hat{z}^{3}} C_{j/q}^{ff}(z/\hat{z},b_{*},\mu_{b_{*}}) d_{h/j}(\hat{z},\mu_{b_{*}}) \exp\left(S_{\text{pert}} - g_{B}(z,b_{\perp},b_{max}) - \frac{1}{2}g_{K}(b_{\perp},b_{max}) \ln\left(\frac{\zeta}{Q_{0}^{2}}\right)\right),$$
(30)

where μ is the renormalization scale, ζ is the rapidity scale, $C_{q/j}^{pdf}$ and $C_{j/q}^{ff}$ are perturbatively calculable coefficient functions (see Ref. [32]), and $f_{j/p}(\hat{x}, \mu_{b*})$ and $d_{h/j}(\hat{z}, \mu_{b*})$ are the standard collinear PDFs and FFs, respectively. We will use the initial scale $Q_0^2 = 2.4 \text{ GeV}^2$. We follow the usual b_* -prescription [9] to avoid the Landau pole of α_s , with

$$b_* = \frac{b_\perp}{\sqrt{1 + b_\perp^2 / b_{max}^2}}.$$
 (31)

The perturbative Sudakov factor S_{pert} is given by

$$S_{\text{pert}} = \frac{1}{2} \int_{\mu_{b_*}}^{\mu} \frac{d\mu'}{\mu'} \left[2\gamma(\mu') - \ln\left(\frac{\zeta}{{\mu'}^2}\right) \gamma_K(\mu') \right] + \frac{1}{2} \widetilde{K}(b_{\perp}, \mu_{b_*}) \ln\left(\frac{\zeta}{\mu_{b_*}^2}\right), \tag{32}$$

i.e., the evolution is done from the auxiliary scale $\mu_{b_*} = 2e^{-\gamma_E}/b_*$ to the scale μ . In the actual phenomenology, we set the rapidity scale $\zeta = Q^2$ and set the renormalization scale $\mu = Q$. We will implement the TMD evolution at next-to-leading-logarithmic (NLL) accuracy, and use the coefficient functions *C* at next-to-leading order (NLO). All the relevant NLO coefficients and NLL anomalous dimensions can be found in Refs. [9, 32]. In addition, we use NLO expression for hard function $H(Q, \mu)$ in Eq. (5) from Ref. [32] reads

$$H(Q,\mu) = 1 + \frac{\alpha_s}{\pi} C_F \left[\frac{3}{2} \ln\left(\frac{Q^2}{\mu^2}\right) - \frac{1}{2} \ln^2\left(\frac{Q^2}{\mu^2}\right) - 4 \right],$$
(33)

and we set $\mu = Q$ so that the logarithmic terms vanish. Finally, we choose the parametrizations for the non-perturbative factors used in Refs. [44, 45] which are given by

$$g_A(x_{\rm bj}, b_{\perp}, b_{max}) = g_q b_{\perp}^2, \qquad g_B(z, b_{\perp}, b_{max}) = \frac{g_h}{z^2} b_{\perp}^2, \qquad g_K(b_{\perp}, b_{max}) = g_2 \ln\left(\frac{b_{\perp}}{b_*}\right), \tag{34}$$

with $g_q = 0.106 \text{ GeV}^2$, $g_2 = 0.21$, and $g_h = 0.042 \text{ GeV}^2$.

Having established the QCD based TMD setups, let's examine the behavior of the SIDIS cross section in b_{\perp} space. In Fig. 4 the b_{\perp} space integrand given in Eq. (5) for the SIDIS differential cross section is plotted, for three different values of $q_{\perp}/Q = 0.1$, 1.0 and 2.0, respectively. We take the lepton-proton center-of-mass energy square $S_{\ell p} = 52.7$ (GeV²), $x_{bj} = 0.25$, z = 0.5, and $Q^2 = 2.5$ (GeV²). These kinematics are within the coverage of the pion production in unpolarized lepton-proton SIDIS data at the HERMES experiment [13]. Just like in the case of the toy TMDs in Sec. 3, the integrand becomes more oscillating as q_{\perp}/Q increases. As a consequence, the numerical estimation of the Fourier-Bessel transform from b_{\perp} -space to q_{\perp} -space becomes increasingly more challenging for larger values of q_{\perp}/Q .

We next analyze the performance of our optimized Ogata quadrature to get the q_{\perp} -space cross sections against the adaptive Gaussian quadrature and the Vegas Monte Carlo integration routines. For that we consider a related experimental observable so-called hadron multiplicity which has been measured by both HERMES [13] and COMPASS [14] experiments. Such hadron multiplicity is defined as [14]

$$M^{h}(q_{\perp}; x_{\rm bj}, z, Q) = \frac{\pi}{z^2} \left. \frac{d\sigma^{h}}{dx_{\rm bj} dy dz d^2 q_{\perp}} \right| \left. \frac{d\sigma^{DIS}}{dx_{\rm bj} dy} \right.$$
(35)



Figure 4: SIDIS b_{\perp} space integrand from Eq. (5) for the differential cross section at NLO+NLL for π^+ production for three different values of transverse momenta: $q_{\perp}/Q = 0.1$, 1, and 2, respectively. For the rest of the external kinematics we select $S_{\ell p} = 52.7$ (GeV²), $x_{bj} = 0.25$, z = 0.5, and $Q^2 = 2.5$ (GeV²) within the coverage of the HERMES experiment [13].



Figure 5: The theoretical prediction for the hadron multiplicity, $|M^{h^+}(q_{\perp}; x_{bj}, z, Q)|$, as a function of q_{\perp}/Q , using three different integration algorithms: the optimized Ogata quadrature ("Ogata", left panel), the adaptive Gaussian quadrature ("Quad", middle panel), and the Vegas Monte Carlo algorithm ("Vegas", right panel). For illustration, we choose the kinematics to be consistent with the COMPASS experiment: $0.055 < x_{bj} < 0.1, z = 0.2$, and $3 \text{ GeV}^2 < Q^2 < 7 \text{ GeV}^2$. The experimental data from COMPASS [14] are also shown for comparison (red solid points).

where the numerator is the SIDIS cross section for the production of a hadron *h* that we have been discussing so far, and the denominator is the inclusive DIS cross section. In Fig. 5, we plot the absolute value of the theoretical prediction for the hadron multiplicity, $|M^{h^+}(q_{\perp}; x_{bj}, z, Q)|$, as a function of q_{\perp}/Q , using the above mentioned integration algorithms. For illustration, we choose the kinematics to be consistent with hadron multiplicity data from COMPASS experiment: $0.055 < x_{bj} < 0.1$, z = 0.2, and $3 \text{ GeV}^2 < Q^2 < 7 \text{ GeV}^2$. The three panels (from left to right) correspond to the optimized Ogata (labeled as Ogata), adaptive Gaussian quadrature (labeled as Quad), and the Vegas Monte Carlo (labeled as Vegas), respectively. We also show the COMPASS experimental data in the plots for comparison. ² Note that at relatively large hadron transverse momentum $q_{\perp}/Q \gtrsim 2$, the theoretical calculations in TMD factorization formalism would become negative. There, one has to include the so-called *Y*-term [9], or switch/match onto the usual

 $^{^{2}}$ In order to describe the data, the normalization issue with the COMPASS data must be resolved. We follow the work done in [46] to normalize the COMPASS multiplicities such that the data and theory are equal at the lowest values of the transverse momentum in each *z* bin.



Figure 6: Comparison of COMPASS hadron multiplicity data [14] and absolute value of the theoretical calculations using the optimized Ogata algorithm with a number of nodes N = 15. The computations are performed for $0.02 < x_{bj} < 0.032$, $1.7 \text{ GeV}^2 < Q^2 < 3 \text{ GeV}^2$, and for 4 different $\langle z \rangle$ values as shown in the figure. The black solid curves are the absolute values of the theoretical results.

collinear factorization formalism [35, 47]. It is important to realize that even in this large q_{\perp} region, computations with high precision for the TMD factorization formalism of Eq. (5) is extremely important, in order to estimate the *Y*-term with high precision [48].

In each plot the inversion is performed using a small number of calls to the integrand in blue, a moderate number of function calls to the integrand in orange, and a large number of function calls to the integrand in green. We also provide the average number of calls $\langle N_{tot} \rangle$ for each case. As one can not, in the limit of large sampling, all the numerical integrators converge to the same result. However, we observe that the optimized Ogata quadrature converges to this result more than an order of magnitude faster than adaptive Gaussian quadrature, and even more than two orders of magnitude faster than Vegas Monte Carlo integration. This result demonstrates that our optimized Ogata algorithm can improve significantly the numerical efficiency of the Fourier-Bessel integration encountered in the TMD analysis.

Finally in Fig. 6, we plot four multiplicity distributions at different values of $\langle z \rangle = 0.2, 0.3, 0.4, 0.6$, respectively for the bins $0.02 < x_{bj} < 0.032$ and $1.7 \text{ GeV}^2 < Q^2 < 3 \text{ GeV}^2$ using the optimized Ogata algorithm with the number of nodes N = 15. It is worthwhile to emphasize again that the theory predictions become extremely efficient, thanks to the optimized Ogata quadrature. This gives us a great confidence that the optimized Ogata method would be ideal in the future for performing efficient numerical calculations and/or for the global analysis of TMDs. ³

5. Conclusions

In this paper we have developed a high performance numerical algorithm for Fourier transforms for TMD factorization formalism from position b_{\perp} space to transverse momentum q_{\perp} space using the optimized Ogata quadrature method, which uses the zeros of Bessel functions as nodes. For a relatively small and fixed number N of functional calls to the integrand, we derived conditions to find the optimal parameter h, which controls the node density. Such an optimized Ogata quadrature ensures the small number of calls while achieving a high accuracy at the same time, and thus becomes extremely efficient in TMD studies. We use both toy TMDs, and parametrizations of QCD based

³Note that we are not presenting a new fit here. Rather we just display, using fixed parameters from Refs. [44, 45], that this numerical method can be used to perform efficient numerical calculations for describing TMD data.

TMDs to demonstrate the efficiency of our integration algorithm. We found that the optimized Ogata quadrature performs an order of magnitude faster than adaptive Gaussian quadrature, and even two orders of magnitude faster than Vegas Monte Carlo integration for all regions of transverse momentum in semi-inclusive deep inelastic scattering. Our algorithm thus can have wide application in the future TMD computations and/or TMD global analysis. The Python code which illustrates the optimized Ogata quadrature is available for download with an open source licence at https://ucla-tmd.github.io/Ogata/.

Acknowledgements

Z.K. is supported by the National Science Foundation under Grant No. PHY-1720486. A.P. is supported by the National Science Foundation under Grant No. PHY-1623454 and the DOE Contract No. DE- AC05-06OR23177, under which Jefferson Science Associates, LLC operates Jefferson Lab. N.S. was supported by the DOE contract DE-SC0018106. J.T. is supported by the NSF Graduate Research Fellowships Program. This work is also supported within the framework of the TMD Topical Collaboration.

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