Dijet azimuthal decorrelations for $\Delta \phi_{\text{dijet}} < 2\pi/3$ in perturbative QCD

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ABSTRACT: We point out an inconsistency in perturbative QCD predictions previously used for dijet azimuthal decorrelations for azimuthal angles of $\Delta \phi_{\text{dijet}} < 2\pi/3$ between the two jets. We show how the inconsistency arises and how the calculations can be modified to provide more accurate results that exhibit a smaller scale dependence and give a better description of the data than the inconsistent results. We also explain how the quality of the predictions strongly depends on a perceivedly minor detail in the definition of the dijet phase space and give recommendations for future measurements.

KEYWORDS: Jets, Hadronic Colliders
1 Introduction

Measurements of dijet azimuthal decorrelations in hadron-hadron collisions provide a unique testing ground for the predictions of perturbative quantum chromodynamics (pQCD). The dijet azimuthal decorrelation studies the production rates of dijet events as a function of the azimuthal angular separation between the two jets in an event that define the dijet system, $\Delta \phi_{dijet} = |\phi_{jet1} - \phi_{jet2}|$. The measured quantity, labeled $P$ in this article and originally proposed by the DØ collaboration [1], is the dijet differential cross section, $d\sigma_{dijet}/d\Delta \phi_{dijet}$, normalized by the inclusive dijet cross section, $\sigma_{dijet}$, integrated over $\Delta \phi_{dijet}$:

$$P = \frac{1}{\sigma_{dijet}} \cdot \frac{d\sigma_{dijet}}{d\Delta \phi_{dijet}}. \quad (1.1)$$

The range of kinematically accessible values in $\Delta \phi_{dijet}$ is indicated in figure 1 for processes with final states of different jet multiplicities. In $2 \to 2$ processes $\Delta \phi_{dijet}$ has always the largest possible value of $\Delta \phi_{dijet} = \pi$ (figure 1 a). If $\Delta \phi_{dijet}$ is significantly below $\pi$, then the quantity $P$ is probing hard $2 \to 3$ and $2 \to 4$ processes, i.e. three-jet and four-jet production. Following the DØ measurement, the quantity $P$ was also measured by the CMS and ATLAS collaborations [2, 3]. In all measurements the data are fairly well described by the theory predictions at next-to-leading order (NLO) pQCD for $3\pi/4 \lesssim \Delta \phi_{dijet} < \pi$. For smaller $\Delta \phi_{dijet}$, in particular for $\Delta \phi_{dijet} < 2\pi/3$, the theory predictions exhibit a large renormalization scale dependence and lie significantly below the data.

In this article, we focus on the comparison of fixed-order pQCD predictions and data in the kinematic region of $\Delta \phi_{dijet} < 2\pi/3$. In section 2 we introduce and compare the phase space definitions in the different analyses and discuss their effects on the kinematic constraints in $2 \to 3$ processes. In section 3 we show that the pQCD calculations by two of the experimental collaborations [1, 2] for the region of $\Delta \phi_{dijet} < 2\pi/3$ are inconsistent, and demonstrate how a correct treatment provides pQCD predictions with a reduced scale...
Table 1. Summary of the parameters defining the dijet phase space in the DØ, CMS, and ATLAS measurements of dijet azimuthal decorrelations [1–3]. Variables are defined in the text.

| Parameter | DØ \((pp, 1.96 \text{ TeV})\) | CMS \((pp, 7 \text{ TeV})\) | ATLAS \((pp, 7 \text{ TeV})\) |
|-----------|---------------------------|---------------------------|---------------------------|
| jet algorithm | Run II cone | anti-\(k_t\) | anti-\(k_t\) |
| jet radius | \(R_{\text{cone}} = 0.7\) | \(R = 0.5\) | \(R = 0.6\) |
| \(y_{\text{initial}}\) | \(\infty\) | 5.0 | 2.8 |
| \(y_{\text{final}}\) | 0.5 | 1.1 | 0.8 |
| \(p_{T\text{min}}\) | 40 GeV | 30 GeV | 100 GeV |
| \(p_{T\text{max}}\) ranges | 75–100 GeV | 80–110 GeV | 110–160 GeV |
| | 100–130 GeV | 110–140 GeV | 160–210 GeV |
| | 130–180 GeV | 140–200 GeV | 210–260 GeV |
| | \(> 180 \text{ GeV}\) | 200–300 GeV | 260–310 GeV |
| | | \(> 300 \text{ GeV}\) | 310–400 GeV |
| | | \(> 400 \text{ GeV}\) | 400–500 GeV |
| | | \(> 500 \text{ GeV}\) | 500–600 GeV |
| | | \(> 600 \text{ GeV}\) | 600–800 GeV |
| | | | \(> 800 \text{ GeV}\) |

For a given process (e.g. \(pp\) or \(p\bar{p}\) collisions) and center-of-mass energy, the measured quantity \(P\), defined in equation (1.1), depends on additional choices, including the jet algorithm with its parameters, and the requirements on the jet rapidities \(y\) and the transverse jet momenta \(p_T\) with respect to the beam direction. The initial jet selection may be carried out in a limited \(y\) region, with \(|y| < y_{\text{initial}}\) (where \(y_{\text{initial}}\) can be adapted to the detector acceptance). The dijet system is then defined by the two jets with the highest \(p_T\) inside this region; here, these are labeled “jet1” and “jet2”. The final phase space for the rapidities \(y_{1,2}\) of jet1 and jet2 is then further constrained by \(|y_{1,2}| < y_{\text{final}}\). Furthermore, the \(p_T\) of jet2 is required to be above a given threshold, \(p_{T\text{min}}\), and the analysis results are presented in different regions of the \(p_T\) of jet1, \(p_{T\text{max}}\). An overview of the choices for these parameters in the analyses by the DØ, CMS, and ATLAS experiments is given in table 1. The main difference between the three scenarios regarding the scope of this article is the choice of \(y_{\text{initial}}\). In the DØ scenario, the \(y\) region for the initial jet selection is unlimited \((y_{\text{initial}} = \infty)\), while the ATLAS and CMS scenarios are limited to \(y_{\text{initial}} = 2.8\) and 5.0,
Figure 1. Sketches of the azimuthal angular separation $\Delta \phi_{\text{dijet}}$ between the two jets leading in $p_T$ in an event for $2 \rightarrow 2$, $2 \rightarrow 3$, and $2 \rightarrow 4$ processes. Also indicated is the kinematically accessible range in $\Delta \phi_{\text{dijet}}$ for the three configurations.

respectively \cite{3,4}. As a consequence of the choices for $y_{\text{initial}}$ and $p_{T\text{min}}$, the three scenarios then have different kinematic constraints for $2 \rightarrow 3$ processes as explained below:

- **Kinematic constraints for an unlimited $y$ region, $y_{\text{initial}} = \infty$**
  For $y_{\text{initial}} = \infty$, the selected jets, jet1 and jet2, are always the two jets leading in $p_T$ of the entire event. This selection criterion results in the kinematic constraint that the smallest possible $\Delta \phi_{\text{dijet}}$ value in a $2 \rightarrow 3$ process (i.e. in a three-jet final state) is $\Delta \phi_{\text{dijet}} = \frac{2\pi}{3}$ (cf. figure 1 b), while angles of $\Delta \phi_{\text{dijet}} < \frac{2\pi}{3}$ are only accessible in final states with four or more jets (cf. figure 1 c). Therefore, for $y_{\text{initial}} = \infty$, the dijet cross section for $\Delta \phi_{\text{dijet}} < \frac{2\pi}{3}$ is a four-jet quantity, meaning that the lowest order pQCD contributions are from the four-jet tree-level matrix elements.

- **Kinematic constraints for a limited $y$ region, $y_{\text{initial}} < \infty$**
  If the $y$ region for the initial jet selection is limited, it is possible that the two jets, selected for the dijet system, are not the two jets leading in $p_T$ of the whole event. Table 2 gives an example for the ATLAS scenario, in which the leading jet in the event has $|y| > y_{\text{initial}}$. In this case, the dijet system is made of the second and third leading jets, which are the two highest $p_T$ jets inside the limited $y$ region. Since there is no kinematic constraint for the azimuthal angular separation between the second and third leading jets, the region $\Delta \phi_{\text{dijet}} < \frac{2\pi}{3}$ is also populated by three-jet final states. If such configurations are not prohibited by other phase space constraints, the dijet cross section for $\Delta \phi_{\text{dijet}} < \frac{2\pi}{3}$ is a three-jet quantity.

It depends on the requirements on $y_{\text{initial}}$, ($p_{T\text{max}}/\sqrt{s}$), and ($p_{T\text{min}}/\sqrt{s}$), whether a leading jet is kinematically allowed outside the region $|y| < y_{\text{initial}}$ and, as a consequence, three-jet configurations can populate the region of $\Delta \phi_{\text{dijet}} < \frac{2\pi}{3}$. This can be tested.

\footnote{An event with exactly three jets can have $\Delta \phi_{\text{dijet}} = \frac{2\pi}{3}$ only in a “Mercedes Star” configuration, where the jets have $p_{T1} = p_{T2} = p_{T3}$ and $\Delta \phi_{1,2} = \Delta \phi_{1,3} = \Delta \phi_{2,3} = \frac{2\pi}{3}$. If the two jets leading in $p_T$ in a three-jet event (with $p_{T1} \geq p_{T2} \geq p_{T3}$) had $\Delta \phi_{\text{dijet}} < \frac{2\pi}{3}$, the vector sum of their transverse momenta could only be balanced, if the third jet had $p_{T3} > p_{T2}$, which would, however, contradict the assumption that $p_{T2} \geq p_{T3}$.}
Table 2. The topology of an exclusive three-jet event, with the jet variables \( p_T \), \( y \), and \( \phi \) (left) and the event quantities \( \Delta \phi_{2,3} \), three-jet invariant mass \( M_{3\text{-jet}} \), and the momentum fractions \( x_1 \) and \( x_2 \) for a center-of-mass energy of \( \sqrt{s} = 7 \text{ TeV} \). In this event, the highest \( p_T \) jet is produced at large rapidity. If the dijet selection is restricted to jets with \( |y| < y_{\text{initial}} = 2.8 \) (as in the ATLAS scenario, see text), the selected dijet system does not include the highest \( p_T \) jet. This enables the azimuthal angular separation of the jets in the dijet system (here, \( \Delta \phi_{\text{dijet}} \) is determined by the azimuthal angle between the second and the third jet, \( \Delta \phi_{2,3} \)) to fall below the limit of \( \Delta \phi_{\text{dijet}} = 2\pi/3 \).

| \( p_T \) (GeV) | \( y \) | \( \phi \) (radians) | \( \Delta \phi_{2,3} \) (radians) | \( M_{3\text{-jet}} \) (TeV) |
|----------------|-----|----------------|-------------------|----------------|
| 405            | 2.805 | 0.000 \( \cdot \pi \) | 0.528 \( \cdot \pi \) | 2.745 |
| 401            | -0.75 | 0.920 \( \cdot \pi \) | 0.990 |
| 101            | -0.75 | 1.448 \( \cdot \pi \) | 0.155 |

We summarize our findings as follows:

- The denominator of \( P \), \( \sigma_{\text{dijet}} \), is the inclusive dijet cross section, which is a two-jet quantity in all scenarios.

- For \( \Delta \phi_{\text{dijet}} \geq 2\pi/3 \), the numerator of \( P \), \( d\sigma_{\text{dijet}}/d\Delta \phi_{\text{dijet}} \), is a three-jet quantity in all scenarios.

- For \( \Delta \phi_{\text{dijet}} < 2\pi/3 \), the numerator of \( P \) is a four-jet quantity, if the initial \( y \) region is unlimited (\( y_{\text{initial}} = \infty \)) as in the D\O\ scenario, or if the \( y_{\text{initial}} \) and \( p_T \) requirements prohibit the two jets with the highest \( p_T \)'s in an event from having \( |y| > y_{\text{initial}} \), as in the CMS scenario.

- If the \( y_{\text{initial}} \) and \( p_T \) requirements allow one of the two jets leading in \( p_T \) to have \( |y| > y_{\text{initial}} \), then the numerator of \( P \) is a three-jet quantity for all \( \Delta \phi_{\text{dijet}} \). This is the case in the ATLAS scenario for the \( p_T^{\text{max}} \) regions up to 400–500 GeV in \( p_T^{\text{max}} \).
Figure 2. The pQCD predictions of order $O(\alpha_s^3)$ for the dijet differential cross section $d\sigma/d\Delta\phi_{\text{dijet}}$, as a function of $\Delta\phi_{\text{dijet}}$ in different regions of $p_{T\text{max}}$ for all analysis bins of the ATLAS measurement. The figure demonstrates that the $O(\alpha_s^3)$ contributions to bins with $\Delta\phi_{\text{dijet}} < 2\pi/3$ and $p_{T\text{max}} < 500\text{ GeV}$ are small but non-zero.

3 Perturbative QCD calculations for cross section ratios

The pQCD prediction for a ratio $R$ of two cross sections $\sigma_A$ and $\sigma_B$ in a given relative order of $\alpha_s$ (e.g. LO or NLO) can be computed from the ratio of the pQCD predictions for $\sigma_A$ and $\sigma_B$. For this purpose, both must be computed at the same relative order, which is not necessarily the same absolute order in $\alpha_s$. A LO result is then given by $R_{\text{LO}} = \sigma_A^{\text{LO}}/\sigma_B^{\text{LO}}$ and a NLO result by $R_{\text{NLO}} = \sigma_A^{\text{NLO}}/\sigma_B^{\text{NLO}}$. If numerator and denominator are calculated in different relative orders, cancellation effects between theoretical uncertainties can be compromised leading to an artificially increased renormalization scale dependence of the results as discussed with respect to jet shapes in sections 3.1 and 4 of reference [7].

For two-jet quantities, the LO and NLO pQCD predictions are given by calculations to order $O(\alpha_s^2)$ and $O(\alpha_s^3)$, respectively. For each additional jet required for the final state, the respective powers of $\alpha_s$ increase by one, so that for example the LO (NLO) predictions for three-jet quantities are given by pQCD calculations to order $O(\alpha_s^3)$ ($O(\alpha_s^4)$). Combined with the findings from section 2, we obtain the rules for the calculation of the LO and NLO results for the quantity $P$ in the three scenarios and in the different regions of $\Delta\phi_{\text{dijet}}$. These rules are listed in table 3 and compared to the computational procedures applied in the experimental publications [1–3]. The theory results published by DØ and CMS for $\Delta\phi_{\text{dijet}} < 2\pi/3$ and labeled “NLO” in references [1, 2] are inconsistent, because they mix relative orders for the numerator (LO) and denominator (NLO). Replacing the NLO result for the denominator (in $O(\alpha_s^3)$) by the corresponding LO ($O(\alpha_s^2)$) provides
the correct LO result for \( P \) below \( \Delta \phi_{\text{dijet}} = 2\pi/3 \). Alternatively, the correct NLO results at \( \Delta \phi_{\text{dijet}} < 2\pi/3 \) can be obtained by replacing the four-jet LO \( (O(\alpha_s^4)) \) results by results based on the four-jet matrix elements at NLO pQCD \( (O(\alpha_s^5)) \), which have become available in the last years [8, 9].

### 4 Results

Following the prescriptions in table 3 we have computed the LO and NLO pQCD predictions for \( P \) in the DØ, CMS, and ATLAS scenarios in the different \( \Delta \phi_{\text{dijet}} \) regions. For comparison, we also derive the inconsistent “mixed-order” results for \( P \) as published by DØ and CMS.

All calculations are made in the \( \overline{\text{MS}} \)-scheme [10] and for five massless quark flavors, using NLOJET++ [5, 6] interfaced to fastNLO [11, 12]. The results are obtained for renormalization and factorization scales of \( \mu_R = \mu_F = p_{\text{Tmax}} \), with the MSTW2008NLO [13] parameterization of the parton distribution functions of the proton, and with \( \alpha_s \) evolved from a value of \( \alpha_s(M_Z) = 0.120 \) according to the two-loop solution of the renormalization group equation. The uncertainty due to the scale dependence is computed from the variations of the ratio \( P \) for correlated variations of the scales in the numerator and denominator of \( \mu_R = \mu_F = p_{\text{Tmax}}/2 \) and \( \mu_R = \mu_F = 2p_{\text{Tmax}} \). The ATLAS collaboration has published non-perturbative corrections [14, 15], which are applied to the pQCD results to get the final theory prediction. These corrections are typically below 1% and never larger than 3%. The DØ and CMS collaborations have not provided non-perturbative corrections. In these cases, the pQCD results are directly compared to the data. The theoretical calculations in this study differ slightly from the calculations used in the CMS and DØ publications due to different choices of the parton distribution functions and \( \alpha_s(M_Z) \). Furthermore, the DØ collaboration chose different renormalization and factorization scales

\[\text{in reference [16] non-perturbative corrections for the DØ results are shown to be typically below 2% and never larger than 4%. In the CMS publication [2] the non-perturbative corrections are quoted to vary between } -13\text{% at } \Delta \phi_{\text{dijet}} = \pi/2 \text{ and } +4\text{% at } \Delta \phi_{\text{dijet}} = \pi.\]

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Table 3. Correspondence between absolute orders in \( \alpha_s \) in the calculations of numerator and denominator and the relative order in the quantity \( P \). The right column comments on the calculations used in the experimental publications.
Figure 3. Measurements of dijet azimuthal decorrelations at hadron colliders from the DØ, CMS, and ATLAS experiments (from left to right) are displayed as a function of the azimuthal opening angle $\Delta \phi_{\text{dijet}}$ of the dijet system for different requirements of the leading jet $p_T$ (different markers). The measurements are compared to theoretical predictions based on NLO (solid lines) or LO pQCD (dashed lines), depending on whether the measured quantity is a three-jet or four-jet variable, respectively. The scale dependence of the pQCD calculation is indicated by the shaded areas.

The experimental results from the DØ, CMS, and ATLAS measurements are displayed in figure 3 over the entire $\Delta \phi_{\text{dijet}}$ range. The data are compared to theory at NLO or LO, depending on the $\Delta \phi_{\text{dijet}}$ range and the scenario. Over the whole range of $p_T$ and $\Delta \phi_{\text{dijet}}$, the theoretical predictions are in agreement with the data, except for the ATLAS data at small $\Delta \phi_{\text{dijet}}$. 

of $\mu_R = \mu_F = p_T_{\text{max}}/2$, and the CMS collaboration applied non-perturbative corrections. For the purpose of the following discussion, these differences are negligible.
The region of small $\Delta\phi_{\text{dijet}}$, including the transition at $\Delta\phi_{\text{dijet}} = 2\pi/3$ and the effects of the inconsistent mixed-order predictions, are further investigated in the following. Figure 4 shows the ratios of data over the different theory predictions for $\Delta\phi_{\text{dijet}} \lesssim 3\pi/4$. The ratios are computed for the NLO results, the LO results, and the inconsistent results from mixed relative orders. Also shown are the uncertainty bands due to the scale dependence of the different theoretical calculations. For $\Delta\phi_{\text{dijet}} > 2\pi/3$, in all scenarios the NLO pQCD predictions are compared to the data. For $\Delta\phi_{\text{dijet}} > 3\pi/4$, these give a good description of the data within scale uncertainties, which are below 5–10%. In the range $2\pi/3 < \Delta\phi_{\text{dijet}} < 3\pi/4$, the $O(\alpha_s^3)$ (i.e. three-jet NLO) calculation for the numerator is running out of phase space for three-jet final states as $\Delta\phi_{\text{dijet}} \to 2\pi/3$. This causes the $O(\alpha_s^3)$ calculation to effectively become a four-jet LO calculation. In this $\Delta\phi_{\text{dijet}}$ range the NLO prediction still describes the data, but with an increasing scale dependence of up to
30% as $\Delta \phi_{\text{dijet}} \rightarrow 2\pi/3$.

For the CMS and DØ scenarios at $\Delta \phi_{\text{dijet}} < 2\pi/3$, we first focus on the inconsistent mixed-order calculations as published by the experiments. Figure 4 shows that over most of the range (and in particular towards lower $\Delta \phi_{\text{dijet}}$) these predictions are significantly below the data even outside their large scale dependence, and they do not describe the $\Delta \phi_{\text{dijet}}$ dependence of the data. Compared to the inconsistent mixed-order calculations, the correct LO predictions have a significantly reduced scale dependence, and they give a much better description of the data. While they still do not reproduce the $\Delta \phi_{\text{dijet}}$ dependence, almost all individual data points agree with the LO prediction within the reduced scale uncertainty.

Although, for the ATLAS scenario the pQCD predictions for $\Delta \phi_{\text{dijet}} < 2\pi/3$ are technically still of NLO, their scale dependence is as large as that of the mixed-order predictions for the CMS scenario, and the description of the data by both are equally poor.

5 Recommendations for future measurements

In section 3 we pointed out that for the numerator of $P$ in the ATLAS scenario the three-jet NLO cross section calculations formally are of NLO also for $\Delta \phi_{\text{dijet}} < 2\pi/3$. The results presented in section 4, however, demonstrate that these NLO predictions exhibit a larger scale dependence and that they give a worse description of the data than the LO predictions for the DØ and CMS results. The difference between the ATLAS and the DØ and CMS scenarios was traced back to the choice of $y_{\text{initial}}$ in the dijet selection as explained in section 2. In contrast to the DØ and CMS scenarios, the kinematic constraints in the ATLAS scenario do allow $2 \rightarrow 3$ processes to give small, but non-zero contributions to the dijet cross section for $\Delta \phi_{\text{dijet}} < 2\pi/3$. Therefore, in this $\Delta \phi_{\text{dijet}}$ range, while formally being a NLO pQCD prediction, the $\mathcal{O}(\alpha_s^4)$ calculation for the numerator effectively is only a LO prediction, since the $\mathcal{O}(\alpha_s^3)$ terms contribute less than one percent. This “formally NLO but effectively LO” calculation for the numerator exhibits the typical large scale dependence of a LO calculation while the NLO predictions for the denominator have a reduced scale dependence, as typical for NLO calculations. As a consequence, the NLO prediction for the ratio $P$ has a scale dependence, which is similar to that of the mixed-order calculations and larger than that of the LO predictions for the DØ and CMS scenarios.

Therefore, we strongly recommend that future measurements of dijet azimuthal decorrelations use values of $y_{\text{initial}}$ that, together with the $p_T\text{min}$ and $p_T\text{max}$ requirements, do not leave any phase space for $2 \rightarrow 3$ processes below $\Delta \phi_{\text{dijet}} = 2\pi/3$. Technically, this can be investigated by using a phase space generator or a three-jet pQCD LO calculation for the numerator of $P$.

6 Summary and conclusion

Measurements of dijet azimuthal decorrelations at hadron colliders continue to be a testing ground for pQCD predictions at higher orders, beyond what is probed in inclusive jet and inclusive dijet production. In particular in the phase space region of $\Delta \phi_{\text{dijet}} < 2\pi/3$,
dijet azimuthal correlations are sensitive to the dynamics of final states with four or more jets. In all previous publications of azimuthal decorrelations, based on the quantity \( P = (1/\sigma_{\text{dijet}}) \cdot (d\sigma_{\text{dijet}}/d\Delta\phi_{\text{dijet}}) \), this region was poorly described by theoretical predictions. In this article we have identified two reasons for this shortcoming.

In the publications by DØ [1] and CMS [2], the poor theoretical description of the data is related to the inconsistent mixing of different relative orders in \( \alpha_s \) in the predictions for the ratio \( P \). We have performed a consistent LO calculation by computing both, numerator and denominator, at LO. This correct LO pQCD prediction not only exhibits a smaller scale dependence, but also gives a better description of the experimental data for \( \Delta\phi_{\text{dijet}} < 2\pi/3 \).

The improvement due to the consistent LO calculation can, however, only be achieved for definitions of the dijet phase space that ensure the two jets of the dijet system to be also the two leading \( p_T \) jets in the events. We strongly recommend for future measurements of dijet azimuthal decorrelations at small \( \Delta\phi_{\text{dijet}} \) to perform the initial dijet selection accordingly.

If this is taken into account, the future usage of four-jet NLO calculations will provide NLO pQCD predictions for the whole \( \Delta\phi_{\text{dijet}} \) range, extending precision phenomenology for dijet azimuthal decorrelations to the region \( \Delta\phi_{\text{dijet}} < 2\pi/3 \). Since in this \( \Delta\phi_{\text{dijet}} \) region the quantity \( P \) is proportional to \( \alpha_s^2 \), future measurements with higher statistical precision can also be used for novel \( \alpha_s \) determinations. This recommendation also applies to measurements of dijet azimuthal decorrelations based on the quantity \( R_{\Delta\phi} \) [17, 18] when this is measured for \( \Delta\phi_{\text{max}} \leq 2\pi/3 \).

Acknowledgments

We thank our colleagues in the ATLAS, CMS, and D0 collaborations for many fruitful discussions. The work of M.W. is supported by grants DE-FG02-10ER46723 and DE-SC0009859 from the U.S. Department of Energy. M.W. also wishes to thank the Louisiana Board of Regents Support Fund for the support through the Eva J. Cunningham Endowed Professorship.

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