Study on the azimuthal angle correlation between two jets in the top quark pair plus multi-jet process

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\textbf{Abstract}

An azimuthal angle correlation between two jets is studied in the top quark pair plus multi-jet process at the 14 TeV LHC. The event samples are generated by merging the $t\bar{t}$ plus up to 3 partons matrix elements with parton showers. The generated event samples exhibit a strong azimuthal angle correlation between the two highest $p_T$ jets with large rapidity separation, when the $t\bar{t}$ plus up to 2 or 3 partons matrix elements are properly merged. The distribution of the azimuthal angle correlation differs non-negligibly from the prediction of the matrix element level, mainly because of the strong Sudakov suppression of events with relatively low $p_T$ jets. The impacts of including the $t\bar{t}$ plus 3 partons matrix elements in the merging are studied in detail, and they are found to improve significantly the prediction of the azimuthal angle correlation.

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1 Introduction

Since the discovery of the Higgs boson was announced in the summer of 2012, the LHC measurements of its properties have so far been supporting the standard model (SM) predictions [1, 2, 3, 4]. The Higgs sector of the SM respects the charge-conjugation and parity (CP) symmetry and the Higgs boson should be CP even. Therefore if an admixture of the CP odd component is observed, it will be a direct evidence of CP violation in the Higgs sector and thus physics beyond the SM.

From the analyses on the tree level matrix elements (MEs), it has been shown that the azimuthal angle difference between two partons (gluon, quarks or antiquarks) produced in association with the Higgs boson produced by gluon fusion is very sensitive to the CP property of the Higgs boson [5, 6, 7, 8]. Several analyses including effects of higher order corrections show that the correlation found at the tree level MEs can be observed as the azimuthal angle difference between the two hardest jets despite smearing, see e.g. refs. [9, 10, 11, 12, 13]. However the attempts to observe the CP odd admixture precisely in this approach are expected to be difficult due to large theoretical uncertainties in the Monte Carlo event simulation, particularly in our use of the parton shower (PS) which can simulate the QCD radiation only in the soft and/or collinear limit.

It has been pointed out in ref. [14] that two partons produced in association with a top quark pair has a large azimuthal angle correlation near the threshold \( m_{t\bar{t}} \sim 2m_t \) and it is similar to that of two partons produced together with the CP odd Higgs boson via gluon fusion. The claim of ref. [14] is that the experimental technique to measure such an angular correlation between jets can be established first by using these SM processes which have large cross sections. More precisely, we measure the azimuthal angle difference between two jets produced in association with a top quark pair and tune the Monte Carlo event generator to reproduce the data quantitatively. If an event generator tuned in this way is used, the theoretical uncertainty of the prediction of the azimuthal angle correlation between two jets produced in association with the Higgs boson can be reduced significantly. This will help achieve precise measurements of the CP property of the Higgs boson.

In the present paper we attempt to create a bridge between the proposal of ref. [14] and actual experimental measurements, by studying our present capability and limitation of simulating the top quark pair plus multi-jet production process, so that experimentalists can use the real data to improve our simulation tools to be used to probe more fundamental physics such as the CP property of the Higgs boson. The simplest method to include leading higher order corrections to the top quark pair production is to apply PS evolution to the exclusive top quark pair events, where the top quark pair plus multi-jet process is described by PS evolution from top quark pair production scales down to hadronization scales. The event samples generated in this method are expected to reproduce qualitatively the multi-jet event rates and the jet \( p_T \) and rapidity distributions, since the successive emission of the PS follows the QCD prediction in the soft and/or collinear region and the overall jet rates have been fitted to the data in \( e^+e^- \) and hadronic collisions. Those events, however, do not have correct correlations among jets since the PS emits azimuthally symmetric
radiation about a parent momentum direction. To reproduce azimuthal angle correlations between two jets, at least the \( t\bar{t} + 2\)-parton MEs should be embedded. In order to combine event samples for different parton multiplicity generated by the leading order MEs with PS evolution and to produce a realistic overall description of event structures without double counting or missed phase space, the so-called merging of the MEs with PS evolution is required \[15, 16, 17\]. Given a merging scheme, in general, the merging scale and the maximal number of partons provided by MEs should be fixed. A more precise description of multi-jet events is expected for larger values of the maximal number of partons provided by MEs. Since large computational power is required for generating MEs event samples with higher parton multiplicity, it is desirable to choose the merging scale as high as possible. If the merging algorithm is properly performed, event structures such as \( p_T \) of jets, jet rates and \( p_T \) of heavy objects accompanied with jets should not depend too much on the merging scale, and it is indeed confirmed in refs. \[17, 18\] for the top quark pair production. However, this will not be the case for angular correlations between jets. If the merging scale is chosen to be higher than a defined jet scale, angular correlations between two jets will depend strongly on the merging scale, because one or both of the two jets can be a jet which has its origin in a parton generated by the PS. Obviously angular correlations between two jets are complicated observables and special care is required for producing a reliable simulation which accommodates them correctly. Our objective in the present paper is, therefore, to clarify these issues which are theoretically important when simulating the top quark pair plus multi-jet process at the LHC that gives the azimuthal angle correlation between two jets. We believe that this work helps experimentalists tune their event generators for simulating multi-jet processes to probe more fundamental physics, following the proposal of ref. \[14\].

The CKKW-L merging scheme \[15, 16, 19, 20\] is implemented in the merging algorithm used in this work. We show that, when the two highest \( p_T \) jets are selected for studying the azimuthal angle correlation between jets, a non-negligible amount of the correlation is lost by accidentally selecting a jet which has its origin in a parton generated by the PS, if the maximal number of partons provided by the MEs is set to two. We find that the loss of the correlation can be avoided by including the \( t\bar{t} + 3\)-parton MEs in the merging algorithm, thus the prediction of the azimuthal angle correlation can be improved significantly. Our results are also compared to the result of a naive approach in which PS evolution is applied to the MEs event samples of only the \( pp \rightarrow t\bar{t} + 2\)-parton process. We find a non-negligible difference in the distribution of the azimuthal angle correlation, which is induced by the strong Sudakov suppression of events with relatively low \( p_T \) jets.

We note in passing that this is not the first attempt to estimate higher order corrections to the azimuthal angle correlation between two partons produced in association with a top quark pair. The azimuthal angle difference between two jets in the top quark pair plus multi-jet process has been studied with the aim of the scalar top quark search in ref. \[21\], of the gluino search in ref. \[22\] and of investigating top quark mass effects in the effective Higgs-gluon coupling in refs. \[23\] and \[24\].

In the next section, details of the merging algorithm are described. Section 3.1 provides a setup for simulating the top quark pair plus multi-jet process and analyzing the azimuthal
angle correlation. A discussion on the merging scale and the jet definition is presented in Section 3.2. In Section 3.3 the impacts of including the $t\bar{t} + 3$-parton MEs in the merging algorithm are studied. The comparison with the naive approach is performed in Section 3.4. Section 4 summarizes our findings.

2 Implementation of the merging algorithm

In order to combine the event samples for different parton multiplicity obtained by the leading order matrix elements (MEs) with additional partons generated by the parton shower (PS), the ideas proposed by Catani, Krauss, Kuhn, Webber [15,16] and Lonnblad [19,20] are introduced. This is known as the CKKW-L merging scheme. The reason for using the CKKW-L scheme is that the PS model [25,26] in PYTHIA8 [27,28] used throughout the present work is ideal for this scheme. The merging algorithm is described in this section. The theoretical details of the merging scheme are not introduced, and for these refer to the original publications [15,16,19,20] or the other publications [29,30,31] in which several merging schemes are studied.

2.1 The merging algorithm

The merging algorithm proceeds as follows.

1. Generate the unweighted event samples for the $pp \rightarrow t\bar{t} + 0, 1, \ldots, N$-parton processes at $\sqrt{s} = 14$ TeV according to the exact leading order MEs. $N$ is the maximal number of partons provided by the MEs. We use MadGraph5_aMC@NLO [32] version 5.2.2.1 for this purpose. The soft and collinear singularities in the $pp \rightarrow t\bar{t} + 1, \ldots, N$-parton processes are regularized by a cutoff on the longitudinal-boost invariant $k_\perp$ variable [33], which is also used as the merging scale definition.

\[
k_{\perp iB} = p_{Ti},
\]

\[
k_{\perp ij} = \min(p_{Ti}, p_{Tj}) \sqrt{(y_i - y_j)^2 + (\phi_i - \phi_j)^2} / R,
\]

where $p_{Ti}$, $y_i$ and $\phi_i$ are the transverse momentum with respect to the beam, rapidity and azimuthal angle of particle $i$. $R$ is the radius parameter and $R = 1$ is used if not otherwise specified. No phase space constraint is imposed on the top and anti-top quarks. A fixed value is used for the scales in $\alpha_s$ and in parton distribution functions (PDFs) at this step.

2. Select an event sample for the $pp \rightarrow t\bar{t} + n$-parton process with a probability proportional to its integrated cross section obtained in step 1,

\[
P_n = \frac{\sigma(pp \rightarrow t\bar{t} + n)}{\sum_{i=0}^{N} \sigma(pp \rightarrow t\bar{t} + i)}.
\]
3. In order to calculate extra weight on the event sample, a PS history of the event sample is constructed by successively clustering two partons into one parton. This procedure yields a set of the sequential intermediate processes $pp \rightarrow t \bar{t}$, $pp \rightarrow t \bar{t} + 1$-parton, $pp \rightarrow t \bar{t} + (n-1)$-parton together with the corresponding clustering scales $p_{1} > p_{2} > \cdots > p_{n}$, which are ordered. Since we calculate weight of Sudakov form factors by making trial emission with PYTHIA8, the evolution variable in PYTHIA8 is used for the clustering scale variable. The detailed clustering procedure and the definition of the clustering scale variable are presented in Section 2.2. The other relevant issues in step 3 are

- A clustering pair which has the lowest clustering scale is always chosen.
- Only clusterings which correspond to the QCD $1 \rightarrow 2$ vertices are allowed.
- Sequential clustering scales are required to be ordered. However, this is not always true in MEs event samples. In some samples we end up with no possibility of finding pairs whose clustering scales are higher than scales obtained at previous clustering steps. In such a case we restart the clustering procedure again from the generated $pp \rightarrow t \bar{t} + n$-parton process, but this time a clustering pair whose clustering scale is a next-higher scale is chosen at the first clustering step. The restarting will be repeated until a set of ordered clustering scales is obtained. If the restarting strategy still does not help, the construction of a PS history for the event sample is abandoned.
- We do not include the top and anti-top quarks in the clustering procedure, and only light quarks and gluons in the initial and final states are clustered. This should be reasonable, since collinear radiation from a top quark is highly suppressed by its large mass.

4. Weight the event sample by $\alpha_s$ and PDF factors which are calculated based on the PS history obtained in step 3. The $\alpha_s$ factor is determined from the clustering scales $p_{1} > p_{2} > \cdots > p_{n}$,

$$\frac{\alpha_s^2(\mu_R)\alpha_s(p_{1})\cdots\alpha_s(p_{n})}{\alpha_s^{2+n}_{\text{fixed}}},$$

$$\mu^2_R = E_T^2(t) + E_T^2(\bar{t}) + \sum_{i=1}^{n} p_{i}^2,$$  

where $\alpha_{s,\text{fixed}}$ is the one used in step 1 and $E_T^2 = m^2 + p_T^2$. $\mu_R$ is chosen to be the highest scale in the event sample, because this is the scale of the core process $pp \rightarrow t \bar{t}$. If the construction of a PS history fails in step 3, the $\alpha_s$ factor is

$$\frac{\alpha_s^{2+n}(\mu_R)}{\alpha_s^{2+n}_{\text{fixed}}},$$

$$\mu^2_R = E_T^2(t) + E_T^2(\bar{t}) + \sum_{i=1}^{n} p_{T_i}^2.$$
The procedure to calculate the PDF weight factor is described in Section 2.3. If the event sample is rejected, select a new event sample according to step 2.

5. Calculate the weight of the Sudakov form factors by making trial emission with PYTHIA8 on the set of the sequential intermediate processes $pp \rightarrow t\bar{t}$, $pp \rightarrow t\bar{t} + 1$-parton, ... $pp \rightarrow t\bar{t} + (n - 1)$-parton and on the generated process $pp \rightarrow t\bar{t} + n$-parton. The general procedure to calculate the Sudakov form factors of an intermediate process $pp \rightarrow t\bar{t} + m(<n)$-parton is as follows,

(a) Perform the PS on the intermediate process $pp \rightarrow t\bar{t} + m$-parton. The starting scale of the evolution variable is set to $p_{\perp m}$. (More precisely, we veto any emission whose evolution scale is higher than $p_{\perp m}$. If emission is vetoed, the event set remains the same as if the emission had never occurred. The evolution will be continued downwards from the vetoed value.) Look at the evolution scale of the first emission $p_{\perp \text{evol 1st}}$. If $p_{\perp \text{evol 1st}} > p_{\perp m} + 1$, the Sudakov weight for the intermediate process is zero, thus reject the event sample.

The procedure to calculate the Sudakov form factors of the generated process $pp \rightarrow t\bar{t} + n$-parton is different for $n < N$ and $n = N$,

(b) Perform the PS on the generated process $pp \rightarrow t\bar{t} + n$-parton. The starting scale of the evolution variable is set to $p_{\perp n}$. If $n = N$, the event sample is accepted and all partons are allowed to shower further. If $n < N$, look at all particles in the final state after the first emission, namely $n + 1$ partons. If they all are above the cutoff defined in step 1, reject the event sample. If any of them is inside the cutoff, the event sample is accepted and all partons are allowed to shower further. Note that this procedure is allowed, only when a PS model constructs a preliminary kinematics after each emission, which is the case in PYTHIA8.

If the event sample is rejected, select a new event sample according to step 2. The other relevant issues in step 5 are

- For the $pp \rightarrow t\bar{t} + 0$-parton process, no matter whether it is the intermediate process ($m = 0$) or the generated process ($n = 0$), the starting scale of the evolution variable is the center-of-mass energy of the proton-proton system, 14 TeV.

- When the construction of a PS history fails in step 3, the Sudakov weight for the event sample is always set to 1, namely the event sample is never rejected in step 5. It is still needed to control the PS evolution from the generated process $pp \rightarrow t\bar{t} + n$-parton. For the starting scale of the evolution variable, the smallest clustering scale in step 3 is used when $n = N$, and the value of the merging scale is used when $n < N$.

- In this study any emission from top and anti-top quarks is vetoed. This should be reasonable, because phase space constraints are not imposed between the top or anti-top quark and light partons when generating the MEs event samples in step 1.
Figure 1: Illustrating that an incoming parton $a$ and an outgoing parton $c$ in a process $a \rightarrow Xc$ are clustered into an incoming parton $b$ and hence a new process $b\rightarrow X$ is produced (from left to right), and that a process $a\rightarrow Xc$ is induced by ISR $a\rightarrow bc$ from a process $b\rightarrow X$ in the backwards evolution (from right to left).

6. Repeat the algorithm from step 2 until a large number of the accepted event samples is accumulated.

2.2 Construction of a parton shower history

In step 3 of the merging algorithm, a PS history is constructed by successively clustering two partons into one parton. A PS history consists of a set of the sequential intermediate processes together with the corresponding clustering scales which are ordered. A PS history is used to calculate the weight factors on a MEs event sample which would have been taken into account if the PS model in PYTHIA8 had generated the same event configuration, namely the Sudakov, $\alpha_s$ and PDF factors. As a result, the clustering procedure should be as close to the inverse of the PS generation in PYTHIA8 as possible. Because the detailed definition of the evolution variable and the kinematics construction are different for the initial state radiation (ISR) and the final state radiation (FSR) in PYTHIA8, the clustering procedure is also different for the clustering of incoming and outgoing partons and that of two outgoing partons. The former procedure is described in Section 2.2.1 and the latter in Section 2.2.2. The full understanding of the kinematics construction of the PS [25, 26] in PYTHIA8 is necessary. In the following sections we use the knowledge and notation in the original publications [25, 26].

2.2.1 Reconstruction of initial state radiation

Suppose that an incoming parton $a$ and an outgoing parton $c$ in a process $a \rightarrow Xc$ are clustered into a parton $b$ and hence an intermediate process $b\rightarrow X$ together with a clustering scale $p_{\perp\text{clus}}$ is produced as illustrated in Figure 1 (from left to right). The clustering has to proceed as if the process $a\rightarrow Xc$ had been induced by the ISR $a\rightarrow bc$ from the hard process $b\rightarrow X$ in the backwards evolution [34] with the evolution scale $p_{\perp\text{evol}} = p_{\perp\text{clus}}$. Once a pair of the incoming parton $a$ and the outgoing parton $c$ is determined, the incoming parton from another side is uniquely selected as a recoiling parton $r$. The clustering scale
$p_{\perp \text{clus}}$ is derived from

$$p_b = p_a - p_c,$$  \hspace{1cm} (5a)

$$z = \frac{m_{br}^2}{m_{ar}^2} = \frac{(p_b + p_r)^2}{(p_a + p_r)^2},$$  \hspace{1cm} (5b)

$$p_{\perp \text{clus}}^2 = -(1 - z)(p_b)^2.$$  \hspace{1cm} (5c)

Here $z$ can be interpreted as the energy fraction $E_b/E_a$ in the $a + r$ rest frame. The new incoming parton $b$ after the clustering is not moving along the $z$-axis and it is a spacelike particle. We need to make the $b$ on-shell (massless) and moving along the $z$-axis. The algorithm is as follows. Note that $X$ expresses all the other particles in the final state, hence in our case $X = t\bar{t} + g$ for instance.

1. Read the azimuthal angle $\phi_c$ of $c$.
2. Rotate $c$ and $X$ in azimuth by $-\phi_c$.
3. Calculate the 4-momentum of $b$ from $p_b = p_a - p_c$.
4. Boost $b$, $r$ and $X$ to the $b + r$ rest frame, and then rotate them in polar angle to have $b$ and $r$ moving along the $z$-axis.
5. Rotate $X$ in azimuth by $+\phi_c$.
6. Construct the 4-momenta of the massless incoming partons $b$ and $r$ in the $b + r$ rest frame, $p_b = (m_{br}/2, 0, 0, m_{br}/2)$ and $p_r = (m_{br}/2, 0, 0, -m_{br}/2)$.
7. Boost $b$, $r$ and $X$ along the $z$-axis to have $r$ having its original momentum.

With the algorithm, the transverse momentum of the clustered parton $b$ is translated into the kinematics of $X$. As required, $b$ is put on mass shell (massless) and it moves along the $z$-axis. The kinematics of $r$ does not change. The algorithm is tested as follows. We apply the algorithm to a process $ar \rightarrow Xc$ which was induced by ISR $a \rightarrow bc$ of PYTHIA8 from a hard process $br \rightarrow X$ and then we confirm that the algorithm correctly reproduces the process $br \rightarrow X$.

### 2.2.2 Reconstruction of final state radiation

Suppose that two outgoing partons $b$ and $c$ are clustered into an outgoing parton $a$ and hence a set of partons $a$ and $r$ together with a clustering scale $p_{\perp \text{clus}}$ is produced as illustrated in Figure 2 (from left to right). The parton $r$ is either incoming or outgoing. The clustering has to proceed as if the set of the partons $b, c$ and $r$ had been induced by the FSR $a \rightarrow bc$ from the set of the partons $a$ and $r$ with the evolution scale $p_{\perp \text{evol}} = p_{\perp \text{clus}}$. Unlike the reconstruction of the ISR, the recoiling parton $r$ will not be uniquely determined. Once $r$ is
determined, the clustering scale $p_{\perp \text{clus}}$ is derived from

\begin{equation}
    p_a = p_b + p_c,
\end{equation}

\begin{equation}
    z = \frac{(p_a + p_r) \cdot p_b}{(p_a + p_r) \cdot p_a},
\end{equation}

\begin{equation}
    p_{\perp \text{clus}}^2 = z(1-z)(p_a)^2.
\end{equation}

Again $z$ can be interpreted as the energy fraction $E_b/E_a$ in the $a+r$ rest frame. The new outgoing parton $a$ after the clustering is off mass shell. We need to make $a$ on mass shell. There are two approaches depending on whether the recoiling parton $r$ is outgoing or incoming.

When $r$ is an outgoing parton, the parton $a$ is put on mass shell by giving energy and momentum of the parton $a$ to the parton $r$, while the 4-momentum of $a+r$ is kept unchanged. The kinematics of all the other partons indicated by $X$ in Figure 2 will not be affected. The algorithm is as follows.

1. Boost $a$ and $r$ to the $a+r$ rest frame, $p_{a,0}$ and $p_{r,0}$.

2. Construct the energy and absolute value of momentum of the partons $a$ and $r$ which are put on mass shell with the on-shell mass $m_a$ and $m_r$ in the $a+r$ rest frame,

\begin{equation}
    m_{ar}^2 = (p_{a,0} + p_{r,0})^2,
\end{equation}

\begin{equation}
    E_{a,\text{new}} = \frac{m_{ar}^2 + m_a^2 - m_r^2}{2m_{ar}},
\end{equation}

\begin{equation}
    E_{r,\text{new}} = \frac{m_a^2 - m_{ar}^2 + m_r^2}{2m_{ar}},
\end{equation}

\begin{equation}
    |\vec{p}_{a,\text{new}}| = |\vec{p}_{r,\text{new}}| = \sqrt{E_{a,\text{new}}^2 - m_a^2}.
\end{equation}

\footnote{When $r$ is incoming parton, the following derivation of $p_{\perp \text{clus}}$ is not exactly correct, since the 4-momentum of $a+r$ is not conserved during the FSR. However, because no significant deviation from a correct value is numerically found, the following derivation is always used here for simplicity.}
3. Modify the magnitude of the momentum of a and r to $|\vec{p}_{a,\text{new}}|$ and $|\vec{p}_{r,\text{new}}|$ respectively, while the direction of the momentum is kept unchanged,

$$p_{a}^{i} = \frac{p_{a,0}^{i}}{|\vec{p}_{a,\text{new}}|}, \quad p_{r}^{i} = \frac{p_{r,0}^{i}}{|\vec{p}_{r,\text{new}}|}, \quad (i = 1, 2, 3) \tag{8}$$

4. Boost these back to the original $a + r$ frame.

When $r$ is an incoming parton, the parton $a$ is put on mass shell by reducing the 4-momentum of both $a$ and $r$, while the 4-momentum $p_{r} - p_{a}$ is kept unchanged. The 4-momentum of the partons $a$ and $r$ which are both massless is derived from,

$$\alpha = \frac{p_{r}^{3}}{E_{r}} = 1 \text{ or } -1, \tag{9a}$$

$$p_{r,\text{after}}^{\mu} = \left(E_{r} - \frac{(p_{a}^{2})}{2(E_{a} - \alpha p_{a}^{3})}, 0, 0, \alpha \left(E_{r} - \frac{(p_{a}^{2})}{2(E_{a} - \alpha p_{a}^{3})}\right)\right), \tag{9b}$$

$$p_{a,\text{after}}^{\mu} = \left(E_{a} + E_{r,\text{after}} - E_{r}, p_{a}^{1}, p_{a}^{2}, p_{a}^{3} + p_{r,\text{after}}^{3} - p_{r}^{3}\right). \tag{9c}$$

Our algorithm is tested as follows. We apply the algorithm to a process which was induced by FSR of PYTHIA8 from a hard process and then we confirm that the algorithm correctly reproduces the hard process before the FSR occurs.

### 2.3 PDF weight

When an incoming parton and an outgoing parton are clustered in step 3 of the merging algorithm as described in Section 2.2.1, it is needed to weight the event sample by a PDF factor in step 4. The PDF weight factor originates from a probability of ISR in the backwards evolution approach [34]. The probability of the ISR $a \rightarrow bc$ in PYTHIA8 is given by [25, 26]

$$dP_{a\rightarrow bc} = \frac{dp_{a}^{2} \alpha_{s}(p_{a}^{2}) f_{a}(x/z, p_{a}^{2}) dz}{2\pi} \frac{P_{a\rightarrow bc}(z)}{f_{b}(x, \pi^{2})} \tag{10}$$

In order to find the PDF weight factor, suppose the ISR $a \rightarrow bc$ with an evolution scale $p_{1,1}^{2}$ from a hard process $br \rightarrow X$ and hence a new process $ar \rightarrow Xc$ is produced as illustrated in Figure [1] (from right to left). Apart from Sudakov form factors, the differential probability of the process $ar \rightarrow Xc$ in proton-proton collisions is

$$f_{b}(x_{b}, p_{1,0}^{2}) f_{r}(x_{r}, p_{r}^{2}) d\hat{s} (br \rightarrow X, \hat{s} = s x_{b} x_{r}) \frac{dp_{1,1}^{2} \alpha_{s}(p_{1,1}^{2}) f_{a}(x, p_{1,1}^{2}) dz P_{a\rightarrow bc}(z)}{2\pi f_{b}(x_{b}, p_{1,1}^{2})} \tag{11a}$$

$$= f_{a}(x_{a}, p_{1,1}^{2}) f_{r}(x_{r}, p_{r}^{2}) d\hat{s} (br \rightarrow X, \hat{s} = s x_{b} x_{r}) \frac{dp_{1,1}^{2} \alpha_{s}(p_{1,1}^{2}) f_{a}(x, p_{1,1}^{2}) dz P_{a\rightarrow bc}(z)}{2\pi f_{b}(x_{b}, p_{1,1}^{2})} \tag{11b}$$

$$\sim f_{a}(x_{a}, p_{1,1}^{2}) f_{r}(x_{r}, p_{r}^{2}) d\hat{s} (ar \rightarrow Xc, \hat{s} = s x_{a} x_{r}) \frac{f_{b}(x_{b}, p_{1,1}^{2})}{f_{b}(x_{b}, p_{1,1}^{2})}. \tag{11c}$$
Eq. (11c) indicates that the description of the ISR with $p_{\perp}^2$ is improved by using the MEs of the process $ar \rightarrow Xc$. The factor consisting of PDFs in the end of eq. (11c) is the factor by which the MEs event sample for the process $ar \rightarrow Xc$ should be weighted,

$$\frac{f_b(x_b, p_{\perp}^0)}{f_b(x_b, p_{\perp}^1)}.$$  (12)

A flavor of the parton $b$, the energy fraction $x_b$ of the parton $b$ in the proton-proton frame and the clustering scale $p_{\perp}^1$ are necessary information for a calculation of the PDF weight factor. They are obtained when a PS history is constructed in step 3 of the merging algorithm. Moreover the central scale $p_{\perp}^0$ must be determined. It is defined in the same way as $\mu_R^2$ in eq. (3),

$$p_{\perp}^0 = E_T^2(t) + E_T^2(\bar{t}) + \sum_{i=1}^n p_{\perp}^i.$$  (13)

When a fixed value $\mu_{\text{fixed}}^2$ is used for the PDF scale in step 1 of the merging algorithm, the actual weight is

$$\frac{f_a(x_a, p_{\perp}^2)}{f_a(x_a, \mu_{\text{fixed}}^2)} \frac{f_b(x_b, p_{\perp}^0)}{f_b(x_b, p_{\perp}^1)} \frac{f_r(x_r, p_{\perp}^2)}{f_r(x_r, \mu_{\text{fixed}}^2)}.$$  (14)

When the construction of a PS history fails in step 3 of the merging algorithm, it is not possible to calculate the PDF weight factor. In such a case, the PDF factor in eq. (12) is absent and instead a factor

$$\frac{f_a(x_a, p_{\perp}^0)}{f_a(x_a, \mu_{\text{fixed}}^2)} \frac{f_r(x_r, p_{\perp}^0)}{f_r(x_r, \mu_{\text{fixed}}^2)}.$$  (15a)

$$p_{\perp}^0 = E_T^2(t) + E_T^2(\bar{t}) + \sum_{i=1}^n p_{\perp}^i.$$  (15b)

is used. This choice is reasonable from the following reason. When it is difficult to construct a PS history, the clustering scale $p_{\perp}^1$ tends to be high $p_{\perp}^1 \rightarrow p_{\perp}^0$, which results in the reduction of eq. (14) to eq. (15a).

### 2.4 Consistency checks of the merging algorithm

To check the self-consistency of the merging algorithm, the dependence of the differential jet rates on the merging scale $k_{\perp \text{cut}}$ and on the maximal number of partons $N$ provided by the MEs is analyzed. The differential jet rates are calculated by using the longitudinal-boost invariant $k_\perp$ definition in eq. (1) with a radius parameter $R = 1$. In Figure 3 the differential jet rates for $1 \rightarrow 0$, $2 \rightarrow 1$ and $3 \rightarrow 2$ jets (left to right) in the top quark pair plus multi-jet process at the 14 TeV LHC are plotted. A vertical dashed line indicates the merging scale $k_{\perp \text{cut}}$, which is 20 GeV for the top three figures and 80 GeV for the bottom three figures.
Figure 3: The differential jet rates for $1 \rightarrow 0$, $2 \rightarrow 1$ and $3 \rightarrow 2$ jets (left to right). The black solid curve represents the result of the merging with $N = 3$, while the other colored solid curves represent the contributions of the MEs event samples for different parton multiplicity, $n = 0$ (red), $n = 1$ (blue), $n = 2$ (green) and $n = 3$ (orange). A vertical dashed line indicates the merging scale $k_{\perp \text{cut}}$, 20 GeV for top and 80 GeV for bottom. The black dashed curve represents the result of the merging with $N = 1$ and $k_{\perp \text{cut}} = 20$ GeV.

The important observations in Figure 3 are summarized as follows.

- The merging is smooth around the merging scale. This tells that the problem of double counting and missed phase space is avoided.
- From comparisons between the figures in top and those in bottom, it is clear that the results are stable under varying the merging scale $k_{\perp \text{cut}}$ from 20 to 80 GeV. This fact
indicates that the cancellation of $k_{\perp \text{cut}}$ dependence is satisfactory.

From these observations we conclude that our merging algorithm satisfies requirements for the merging of the MEs with the PS evolution. The event samples generated by the merging algorithm are analyzed from the next section.

3 Study of the azimuthal angle correlation

3.1 Setup

To start with, a setup for our analyses is introduced. The unweighted event samples of the top quark pair plus multi-jet process at the 14 TeV LHC are generated with the merging algorithm described in Section 2. The merging scale $k_{\perp \text{cut}}$ and the maximal number of partons $N$ obtained by the leading order matrix elements (MEs) are important parameters in the merging algorithm and they are subject to study in the following sections. The physical observable which we are interested in is the azimuthal angle difference between the two hardest jets, $\Delta \phi = \phi_1 - \phi_2$. An event sample with two or more jets is picked up and the following requirement which is often called vector boson fusion (VBF) cut is applied to the two hardest jets,

$$y_1 \times y_2 < 0, \quad |y_1 - y_2| > 4.$$

(16)

The transverse momentum $p_T$ with respect to the beam of an object describes the hardness of the object. Therefore a jet which has the highest $p_T$ is called the hardest jet and another jet which has the second highest $p_T$ is called the second hardest jet, and these jets are assigned to the two hardest jets. To enhance the azimuthal angle correlation, an additional cut is applied [14],

$$m_{t\bar{t}} < 500 \text{ GeV}.$$

(17)

No other cuts are applied to the top and anti-top quarks and they are left undecayed. All particles satisfying a rapidity cut $|y| < 4.9$ except the top and anti-top quarks are clustered to construct inclusive jets according to the anti-$k_T$ algorithm [35]. The radius parameter is $R = 0.4$ if not otherwise specified. Fastjet [36] version 3.1.0 is used for this purpose. All the unweighted event samples according to the leading order MEs are generated by MadGraph5_aMC@NLO [32] version 5.2.2.1 and the parton shower (PS) is performed by PYTHIA8 [27, 28] version 8186. The parton distribution function (PDF) set CTEQ6L1 [37] is used for all needs including the PDF factors for the initial state radiation (ISR) in PYTHIA8. The default tune of the version 8186 is basically used in PYTHIA8 while some functions are turned off. The hadronization after the PS is turned off because it is not intended to study detector effect. To simplify the analysis, the multiple interaction is turned off. The rapidity ordering in the ISR is turned off as suggested in ref. [38]. All functions inducing azimuthal asymmetry in the PS are turned off, since azimuthal angle information of hard partons is provided by exact MEs in our study.
| Jet $p_T$ cut (GeV) | 20 | 30 | 40 |
|--------------------|----|----|----|
| Jet radius $R = 0.4$ | 11.0 | 4.0 | 2.2 |
| Jet radius $R = 0.7$ | 16.4 | 5.3 | 2.7 |

Table 1: Contamination rate (%) with different jet definitions. The event samples are generated with the merging parameters $N = 3$ and $k_{\perp \text{cut}} = 20$ GeV. Only those which pass the cuts in eqs. (16) (17) are analyzed.

### 3.2 Merging scale and jet definition

In order for each of the two hardest jets to have the correct azimuthal angle information, each of them must have its origin in a parton obtained by the MEs. If one or both of them originate from a parton generated by the PS, angular correlations between them disappear. The minimum requirement on the merging parameters is therefore

1. $N \geq 2$.
2. $k_{\perp \text{cut}} < p^{\text{jet}}_{T \text{cut}}$.

The requirement on the maximal number of partons $N$ provided by the MEs is obvious, since the leading order prediction of $\Delta \phi$ is obtained from the MEs for the $pp \to t\bar{t} + 2$-parton process [14]. It is discussed how much the $\Delta \phi$ prediction can be improved for $N = 3$ in Section 3.3. The requirement on the merging scale $k_{\perp \text{cut}}$ is introduced to avoid that the two hardest jets have their origin in a parton generated by the PS. The $\Delta \phi$ distribution will not be stable if $k_{\perp \text{cut}} > p^{\text{jet}}_{T \text{cut}}$. However it is not obvious how smaller $k_{\perp \text{cut}}$ should be than $p^{\text{jet}}_{T \text{cut}}$ for a stable result. As it is shown in the differential jet rates of Figure 3, there is not a sharp division at the merging scale between the contributions of the MEs event samples for different parton multiplicity. A too small $k_{\perp \text{cut}}$ is undesirable at all, since it can significantly reduce the efficiency of event generation. We, therefore, at first explore a relationship between $k_{\perp \text{cut}}$ and $p^{\text{jet}}_{T \text{cut}}$ from which $\Delta \phi$ is expected to be stable.

The contamination rate, which is defined as a rate of the contributions of the MEs event samples for the $pp \to t\bar{t} + 0$, 1-parton processes, is calculated with different jet definitions and summarized in Table 1 in units of percentage. The merging parameters are set to $N = 3$ and $k_{\perp \text{cut}} = 20$ GeV. Note that the almost identical result is obtained when $N = 2$ and $k_{\perp \text{cut}} = 20$ GeV, as expected. Only those which pass the cuts in eqs. (16) (17) are considered. It is shown that more than 10% of the azimuthal angle correlation $\Delta \phi$ will be contaminated i.e. lost when $k_{\perp \text{cut}}$ is set equal to the jet $p_T$ cut ($= 20$ GeV). The rate decreases with a rise in the jet $p_T$ cut as expected. In order to suppress the contamination rate while avoiding too inefficient event generation, $k_{\perp \text{cut}} = 20$ GeV is chosen for the merging scale and a radius parameter $R = 0.4$ with $p^{\text{jet}}_{T \text{cut}} = 30$ GeV is used for the jet definition hereafter.
Figure 4: $p_T$ and rapidity of the three partons in the event samples of the $pp \rightarrow t\bar{t} + 3$-parton process generated in the two different approaches [18] [19]. The blue solid curves represent the approach [18] and the red dotted curves represent the approach [19].

3.3 Result of the merging and impacts of the 3-parton MEs

The requirement on the maximal number of partons $N$ provided by the MEs, $N \geq 2$ is briefly discussed in Section 3.2. In general a more precise description of multi-jet processes is expected for larger values of $N$. Thus $\Delta \phi$ is also expected to be more precise for $N = 3$ than for $N = 2$. However it is not obvious how and how much the $\Delta \phi$ prediction can be improved. In the present section this issue is clarified from a detailed study on the impacts of including the $t\bar{t} + 3$-parton MEs.

When the PS generates additional partons from the MEs event samples for the highest parton multiplicity $N$ in the merging algorithm, these additional partons are constrained to be softer than the $N$ partons provided by the MEs in terms of the PS evolution variable. More precisely, by using the words in the merging algorithm in Section 2.1, a starting scale of the PS evolution variable from the $pp \rightarrow t\bar{t} + N$-parton process is set to the smallest clustering scale, $p_{\perp N}$. In order to explicitly confirm that the PS is well controlled, the event samples of the $pp \rightarrow t\bar{t} + 3$-parton process are exclusively generated in the following two different approaches [18] [19] and $p_T$ and rapidity of the generated three partons are compared in Figure 4. The three partons satisfy $k_\perp > 30$ GeV defined in eq. (1).
Figure 5: Left: The horizontal axis represents $p_T$ of the second hardest parton generated by the MEs, the vertical axis represents $p_T$ of the parton added by the ISR, in the event samples of the $pp \to t\bar{t} + 3$-parton process generated in the approach (19). Right: The horizontal axis represents $p_T$ of the second hardest parton generated by the MEs, the vertical axis represents $p_T$ of the parton added by the ISR, in the event samples of the $pp \to t\bar{t} + 4$-parton process generated in the approach (20).

- An event sample of the $pp \to t\bar{t} + 3$-parton process is generated by the MEs and weighted by the Sudakov factor. (blue solid) .

- An event sample of the $pp \to t\bar{t} + 2$-parton process is generated by the MEs and weighted by the Sudakov factor. Then 1 parton is added by the PS. (red dotted)

A good agreement between the two approaches is found. Note that when we mention that an event sample is weighted by the Sudakov factor, not only the Sudakov factor but also the $\alpha_s$ and PDF factors are included in the weight factor. The latter procedure (19) is actually performed in the merging algorithm with $N = 2$ (of course not only the 1 parton but more partons are generated by the PS until the evolution variable reaches a cutoff scale). An important finding in the latter approach (19) is that the 1 parton added by the PS does not necessarily have a lower $p_T$ than the 2 partons obtained by the MEs. In order to make it clearer, in the left graph of Figure 5 the horizontal axis represents $p_T$ of the second hardest parton generated by the MEs and the vertical axis represents $p_T$ of the parton added by the PS in the event samples of the $pp \to t\bar{t} + 3$-parton process generated in the approach (19). Only the samples which pass the cuts in eqs. (16) (17) and in which the additional parton is...
Figure 6: Left: $\Delta \phi$ distribution between the two hardest partons in the $pp \rightarrow t\bar{t}+3$-parton process generated in the three different approaches (18) (19) (21). Right: $\Delta \phi$ distribution. The blue solid curve represents the merging with $N = 3$, and the red dotted curve represents the merging with $N = 2$.

generated by the ISR are plotted. The graph shows that in the considerable fraction $\sim 21\%$ of the event samples indicated by the dots in the upper left of the graph, the parton added by the ISR has a higher $p_T$ than either or both of the 2 partons generated by the MEs. Note that about $82\%$ of the first PS from the $pp \rightarrow t\bar{t}+2$-parton process is ISR. This fact can cause a non-negligible loss of the correlation $\Delta \phi$ in the following way. A parton with the highest or second highest $p_T$ generated by the PS gives rise to the hardest or second hardest jet, which is thus selected for constructing $\Delta \phi$. We note that this problem exists, even though the merging scale is properly chosen.

The problem of generating the hardest or second hardest parton with the PS can be solved by including the $t\bar{t}+3$-parton MEs. The event samples of the $pp \rightarrow t\bar{t}+4$-parton process are exclusively generated in the following approach (20), which is actually performed in the merging algorithm with $N = 3$,

- An event sample of the $pp \rightarrow t\bar{t}+3$-parton process is generated by the MEs and weighted by the Sudakov factor. Then 1 parton is added by the PS.

The 1 parton added by the PS does not necessarily have a lower $p_T$ than the 3 partons generated by the MEs, which is the same as the procedure (19). An important difference from the procedure (19) is that the parton added by the PS seldom has a higher $p_T$ than the second hardest parton generated by the MEs. This fact is clearly shown in the right graph of Figure 5, where the horizontal axis represents $p_T$ of the second hardest parton generated by the MEs and the vertical axis represents $p_T$ of the parton added
by the ISR, in the event samples of the $pp \rightarrow t\bar{t} + 4$-parton process generated in the approach (20). Only the samples which pass the cuts in eqs. (16) (17) are plotted. This can effectively avoid that a jet which has its origin in a parton generated by the PS has the highest or second highest $p_T$, thus this jet is selected for a construction of $\Delta \phi$. Consequently, a loss of the correlation $\Delta \phi$ is reduced significantly in the merging with $N = 3$.

A loss of the correlation should be apparent when $\Delta \phi$ distributions are compared. At first, $\Delta \phi$ between the two hardest partons in the event samples of the $pp \rightarrow t\bar{t} + 3$-parton process exclusively generated in the above two approaches (18) (19) is plotted in the left graph of Figure 6, where the blue solid curve represents the approach (18) and the red dotted curve the approach (19). The green dashed curve represents the following approach,

- An event sample of the $pp \rightarrow t\bar{t} + 1$-parton process is generated by the MEs and weighted by the Sudakov factor. Then 2 partons are added by the PS. (green dashed)

In this approach (21) the correlation $\Delta \phi$ should be absent and only an enhancement at $|\Delta \phi| \sim \pi$ from kinematic reasons is shown in the graph. Note that, as is clear from the blue solid curve, the $t\bar{t} + 3$-parton MEs do exhibit the strong correlation $\Delta \phi$ between the two hardest partons with large rapidity separation, just like in the $t\bar{t} + 2$-parton MEs. When the blue solid curve and the red dotted curve are compared, a clear difference is found. The loss of about 20% of the correlation between the two hardest partons in the approach (19) can explain the difference. Note that it is clear from Figure 4 that the difference cannot be explained from the kinematic differences of the three partons.

Finally the $\Delta \phi$ distribution in the merging with $N = 3$ (blue solid curve) and that in the merging with $N = 2$ (red dotted curve) are shown in the right graph of Figure 6. A difference is clearly seen. This observation confirms the non-negligible loss of the correlation in the merging with $N = 2$ and the avoidance of a loss of the correlation in the merging with $N = 3$ which are expected from the above parton level analyses. Therefore it can be concluded that the prediction of $\Delta \phi$ can be improved significantly by extending the merging algorithm from $N = 2$ to $N = 3$, namely by including the $t\bar{t} + 3$-parton MEs in the merging.

3.4 Comparison with the non-merging

In this section a naive approach, which we call the non-merging approach, is introduced. In the non-merging approach, only the $t\bar{t} + 2$-parton MEs are used, and the PS evolution is applied to the MEs event samples of the $pp \rightarrow t\bar{t} + 2$-parton process. The two hardest jets can have their origin in a parton provided by the MEs and have a realistic representation of the internal jet structure generated by the PS, therefore the event samples should exhibit the correlation $\Delta \phi$. The Sudakov weight is absent, thus the $\Delta \phi$ prediction should be closer to the prediction of the leading order MEs. The result is compared to our best result obtained by the merging algorithm. A clear difference in the $\Delta \phi$ distribution is found,
Figure 7: Left: $\Delta \phi$ distribution. The blue solid curve represents the merging with $N = 2$, and the red dotted curve represents the non-merging. Right: $\Delta \phi$ distribution between the two partons in the $pp \rightarrow t\bar{t} + 2$-parton process obtained by the MEs including the Sudakov weight (blue solid curve) and by the MEs (red dotted curve).

which is induced by the large Sudakov suppression.

The setup for generating the event samples in the non-merging approach is summarized at first. When generating the MEs event samples of the $pp \rightarrow t\bar{t} + 2$-parton process, $\alpha_s$ values are determined from

$$\alpha_s^2(\mu_R)\alpha_s(p_{T1})\alpha_s(p_{T2}), \quad (22a)$$

$$\mu_R^2 = E^2_T(t) + E^2_T(\bar{t}) + p^2_{T1} + p^2_{T2}, \quad (22b)$$

and the scale in the PDFs is set to

$$\mu_{PDF}^2 = p^2_{T1} + p^2_{T2}, \quad (23)$$

where $p_{T1}$ and $p_{T2}$ represent $p_T$ of the two partons. The starting scale of the PS evolution variable is set to the lowest $p_T$ of the two partons obtained by the MEs on event by event basis.

In the left graph of Figure 7 the $\Delta \phi$ distribution in the merging (blue solid curve) and that in the non-merging (red dotted curve) are compared. For a fair comparison, the result of the merging with $N = 2$ is plotted. A clear difference is found. There are more events at $\Delta \phi \sim 0$ and less events at $|\Delta \phi| \sim \pi$ in the non-merged result. The origin of the difference can be apparent through a parton level analysis. In the right graph of Figure 7 $\Delta \phi$ between the two partons in the event samples of the $pp \rightarrow t\bar{t} + 2$-parton process exclusively generated by the MEs (red dotted curve) and by the MEs including the Sudakov weight (blue solid curve) are plotted, where the same difference is found. This tells that the difference is
Figure 8: $p_T$ of the two jets used in the left graph of Figure 7 is plotted in the left two graphs. $p_T$ of the two partons used in the right graph of Figure 7 is plotted in the right two graphs.

Sudakov effects should be more apparent in $p_T$ distributions of jets or partons. The $p_T$ distributions of the two jets used in the left graph of Figure 7 are shown in the left two graphs of Figure 8, likewise the $p_T$ distributions of the two partons used in the right graph of Figure 7 are shown in the right two graphs of Figure 8. Clearly there is strong Sudakov suppression of events with relatively low $p_T$ jets and partons. The kinematic differences of the jets induced by the Sudakov suppression can explain the difference between the merged and non-merged results in the left graph of Figure 7. The two jets in the non-merged result are less energetic, as a result there are less events with back to back jets in azimuth, $|\Delta \phi| \sim \pi$.

In addition to the clear difference in the $\Delta \phi$ distribution, the strong Sudakov suppression indicates that the non-merged result is not reliable. Therefore it can be concluded that the non-merging approach does not accommodate the correct prediction of $\Delta \phi$.

4 Conclusion

In this work the azimuthal angle correlation between the two highest $p_T$ jets, $\Delta \phi = \phi_1 - \phi_2$ in the top quark pair plus multi-jet process at the 14 TeV LHC has been studied. Our objective is to clarify theoretical issues which are important when producing a reliable simulation of the process which accommodates the correct $\Delta \phi$ distributions. The event samples are generated by a merging algorithm of the leading order matrix elements (MEs) with parton shower (PS) evolution. The CKKW-L merging scheme has been implemented in the merging algorithm, which has been validated by confirming the smooth merging at the merging scale and the cancellation of the merging scale dependence in the distributions of differential jet rates.

The generated event samples exhibit the strong correlation in $\Delta \phi$, when the maximal number of partons $N$ provided by the MEs in the merging is set to 2 or 3 and when the merging scale is properly chosen. The difference between the merging with $N = 3$ and that
with $N = 2$, namely the impacts of including the $t\bar{t} + 3$-parton MEs in the merging, has been studied carefully. From a parton level analysis using the exclusive $pp \to t\bar{t} + 3$-parton event samples, it is found that a parton generated by the PS has the second highest $p_T$ in a considerable fraction $\sim 20\%$ of the event samples of the merging with $N = 2$, even though the merging scale is properly chosen. This can cause a non-negligible loss of the correlation $\Delta \phi$ in the merging with $N = 2$, because a parton with the highest $p_T$ generated by the PS gives rise to the hardest or second hardest jet, which is thus selected for a construction of $\Delta \phi$. We have explicitly shown that a parton generated by the PS seldom has the largest or second highest $p_T$ if the $t\bar{t} + 3$-parton MEs are included in the merging, thus the loss of the correlation is significantly reduced in the merging with $N = 3$. It is worth noting here that the $t\bar{t} + 3$-parton MEs do exhibit the strong $\Delta \phi$ correlation between the two highest $p_T$ partons with large rapidity separation, just like in the $t\bar{t} + 2$-parton MEs. The non-negligible loss of the correlation in $N = 2$ and its avoidance in $N = 3$ which are estimated from the parton level analyses are observed as a clear difference in the $\Delta \phi$ distribution. We therefore conclude that the impact of including the $t\bar{t} + 3$-parton MEs is not negligible and the prediction of $\Delta \phi$ can be improved significantly by extending the merging algorithm from $N = 2$ to $N = 3$.

Our result has also been compared to the result of a naive approach in which PS evolution is applied to the MEs event samples of only the $pp \to t\bar{t} + 2$-parton process. The strong Sudakov suppression of events with low $p_T$ jets has been observed, which indicates that the naive approach is not reliable. Moreover, a clear difference in the $\Delta \phi$ distribution is found and this can be explained from the kinematic differences of the jets induced by the Sudakov suppression. Therefore, we conclude that the naive approach does not accommodate the correct prediction of the correlation $\Delta \phi$.

We note that our findings from the study on the top quark pair production should be applicable equally to other heavy particle production by gluon fusion. We hope that our findings help experimentalists perform the proposal of ref. [14] and hence achieve precise measurements of the CP property of the Higgs boson by using the azimuthal angle correlation between the two hardest jets at the LHC.

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