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Mass effects in the PYTHIA generator

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Abstract

The role of the different b-quark mass parameters which are used in the PYTHIA generator and their relation with the mass definitions used in fixed order matrix element calculations is described. As an example, we have compared the generator prediction with preliminary DELPHI data. The results are relevant to the measurement of the b-quark mass at the scale of the Z boson mass, done in DELPHI by comparing the 3-jet rates in b-quark enriched and depleted samples of events. They can be applied in analyses based on the $R_3^{b\ell}$ observable which is used in this measurement.

1 Introduction

$R_3^{b\ell}$, the normalized three jet rate of b-quarks with respect to ℓ-quarks is one of the observables used by DELPHI to probe b-quark mass effects at the Z boson mass scale. The PYTHIA and HERWIG generators[1] are used to compute hadronization corrections enabling to translate the hadron level observables into parton level ones suitable for comparison with fixed-order analytical Leading-Order (LO) or Next-to-leading (NLO) results.

This note describes our present understanding of how the b-quark mass enters in the parton shower and hadronization processes as implemented in the PYTHIA generator. Both treatments have been found critical in the prediction of the hadronization corrections. Particular concerns are the determination of the value of the b-quark mass which should be used and the corresponding uncertainty. The quantitative conclusions reached are expected to apply directly for the observable studied ($R_3^{b\ell}$). This note is intended to present the conclusions reached after many discussions among the people interested that came out right after the first measurement of the b quark mass at the M_Z scale was done [1]. The issues presented in this note become essential when the other sources of uncertainties affecting $m_b(M_Z)$ are reduced.

2 b-quark mass parameters in PYTHIA

The PYTHIA generator uses three kinds of masses to describe the parton shower and hadronization of b-quarks:

- The kinematical mass[2], M_b, entering in the parton shower and in the LO matrix element (ME) expressions used to correct the probability of gluon emission of the first branching of the parton shower (PMAS(5,1) = 5 GeV/c^2).
- The constituent mass, M_b^{const}, used to derive not yet found B hadron masses and entering also in the string hadronization process (PARF(105) = 5 GeV/c^2).
- The set of already known B hadron masses.

It is essential to stress that, although not completely arbitrary, these three kinds of masses are not connected to each other in the generator and are set independently. An exception is the connection made between the constituent mass and B hadron masses in cases of B hadrons not yet found experimentally. The expression used to derive these masses in PYTHIA is the hadron mass formula [2, 3],

$$m_B = m_0 + \sum_i M_i^{const} + k(M_d^{const})^2 \sum_{i<j} \frac{<\sigma_i \cdot \sigma_j>}{M_i^{const} M_j^{const}} \qquad (1)$$

where we have a constant term, a sum over constituent masses and a spin-spin interaction term for each quark pair in the hadron. The constants m_0 and k are fitted from known masses, treating mesons and baryons separately, and M_d^{const} is the constituent d quark mass. For mesons with orbital angular momentum $L = 1$ the spin-spin coupling is assumed

[1]The versions of PYTHIA and HERWIG used throughout this note are 6.131 and 6.1, respectively, each with their corresponding DELPHI tuned sets of parameters.

[2]This mass, although called kinematical, can be considered as an effective mass.

to vanish. This formula is based on a constituent quark model and though remarkably successful [4] it is not derived from the QCD Lagrangian. Hence the constituent b-quark masses extracted from this expression do not have a well-defined relationship to the quark mass appearing in the QCD Lagrangian.

3 Sensitivity to variations of the M_b parameter in PYTHIA

It has been observed in various studies [1, 5, 6] that when the kinematical mass parameter M_b is varied, the $R_3^{b\ell}$ observable changes accordingly at parton level, but remains almost constant at hadron level. Therefore, the hadronization correction automatically shifts by as much as $R_3^{b\ell}$ does at parton level (see figure 1). This situation has led to lot of discussion among experimentalists and theorists.

3.1 Discussion in the context of the b-quark mass measurement at LEP

The consequence of this behaviour of the generator for the b-quark mass measurements at LEP is that the results obtained could become arbitrary or affected by a quite large systematic uncertainty, because they strongly depend on the choice made for the input parameter M_b in the generator.

However such a dependence of the hadronization correction with M_b cannot be considered physical. Different arguments have been given in different studies to show why and to get around what appears to be a contradiction:

- Turn *on* and *off* mass effects in the generator (MSTJ(47) = 3 or 1). This means that the massive or massless ME calculations are used in the matching of the first branching of the parton shower [1, 5].
- Consider the variations of the M_b input parameter only in the LO ME expression used for the just mentioned matching [6], and not in the parton shower process.
- The mass parameter can also be understood in the QCD Lagrangian as a coupling constant at the quark-gluon vertex. Hence, one can modify α_s^b rather than M_b in order to change the amount of gluon radiation off b-quarks. This is equivalent to varying $\Lambda_{\rm QCD}$ in PYTHIA only for $b\bar{b}$ events[3].

In all three cases the hadronization correction remains constant, i.e. the effects observed at parton level are also present at hadron level. However these checks don't explain why PYTHIA behaves in this way when M_b is modified. Moreover, they don't help to specify which value of M_b should be used in the generator.

[3]It is for this reason that the measurement of $R_3^{b\ell}$ can be interpreted both as a determination of the b-quark mass at the Z boson mass scale or as a test of the flavour independence of α_s.

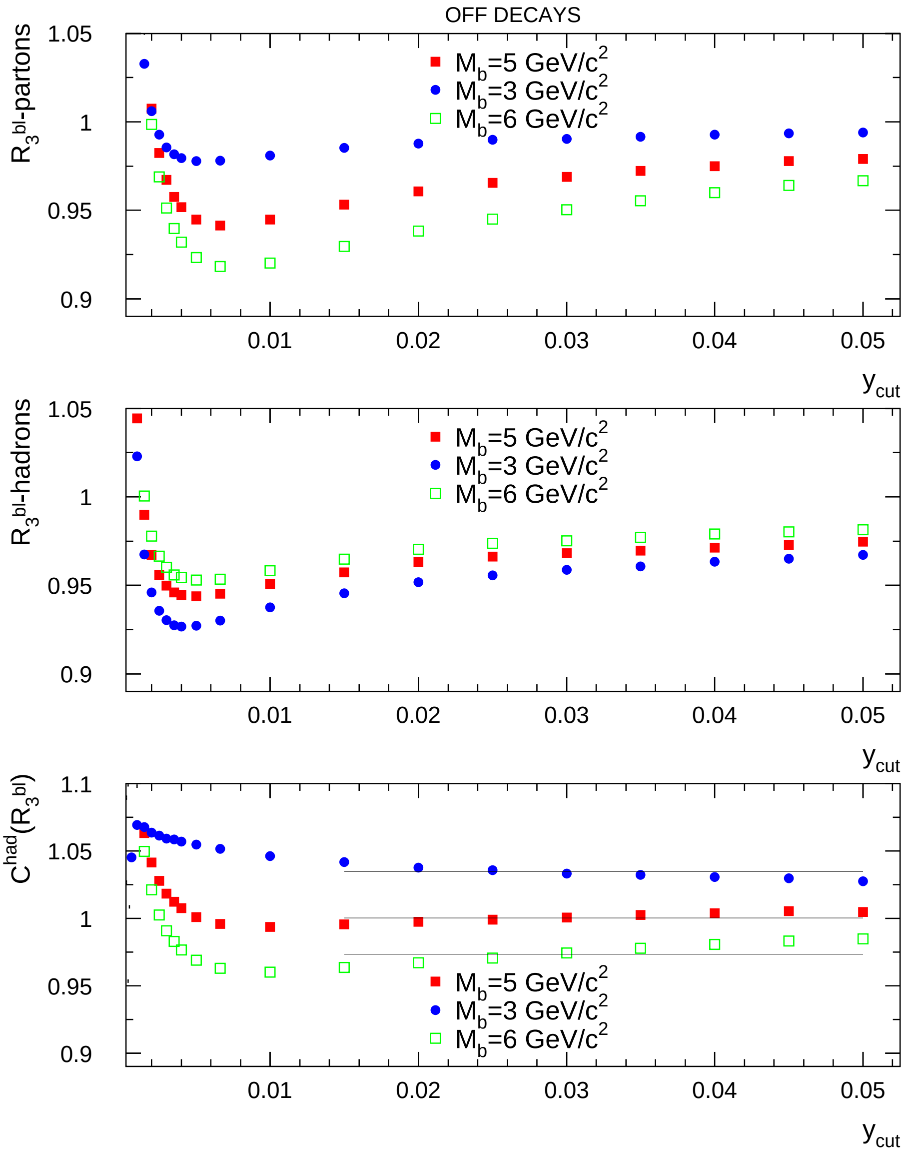

Figure 1: $R_3^{b\ell}$ at parton and hadron level and its hadronization correction as a function of y_c for three different values of the kinematical mass of PYTHIA. DURHAM is used to reconstruct jets.

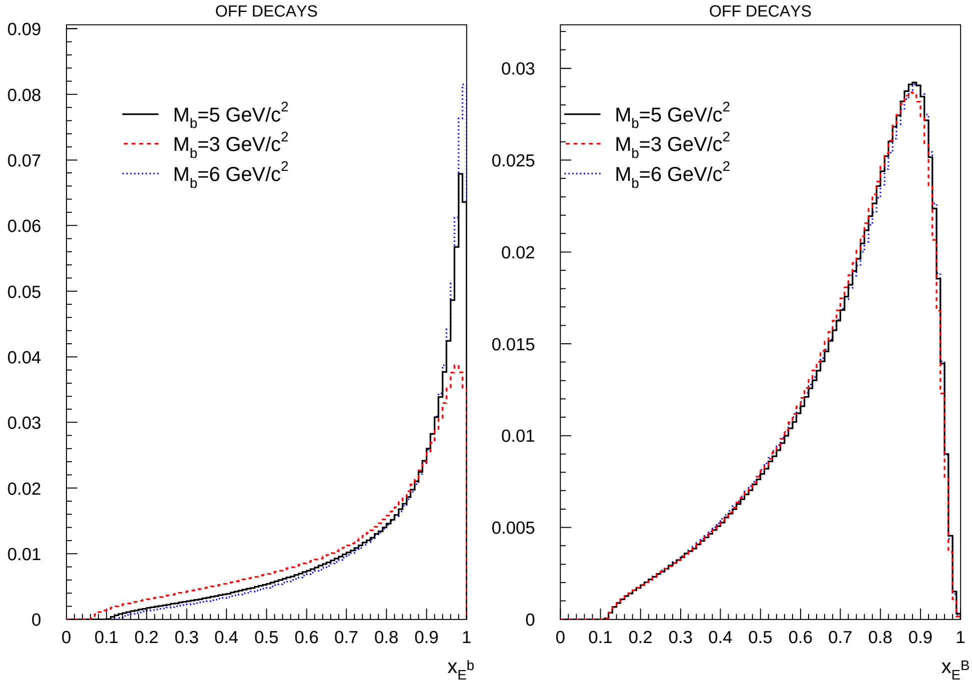

Figure 2: b-quark scaled energy distribution (left) and B hadron scaled energy distribution (right) for M_b = 3, 5 and 6 in PYTHIA.

3.2 Interpretation of the observed behaviour

In this section the reason why in PYTHIA the effects observed at parton level when M_b is changed do not propagate to the hadron level is explained. This lack of sensitivity was shown in figure 1 for the $R_3^{b\ell}$ observable. A similar insensitivity is observed for the b-quark scaled energy distribution (see figure 2). This behaviour can be explained taking into account the following features of the generator:

- M_b and M_b^{const} are not connected,
- B hadron masses are hardcoded,
- the Peterson fragmentation function depends on the ϵ_b parameter, which is fixed to the tuned value.

When M_b is changed in PYTHIA the constituent mass remains constant and so do hadron masses and energies. Therefore, if M_b changes, decreased or increased, the number of jets at parton level increases or decreases but, as hadron masses remain constant, the particles/jets/energy needed to form B hadrons are the same, so these particles/jets/energy are recombined to form the same number of jets at hadron level. This situation however is unphysical in the sense that if M_b changes B hadron masses should also change accordingly.

3.3 Modified PYTHIA setup for technical investigations

It was found that when all b-mass parameters used in the generator (see Section 2) are physically connected the above described behaviour disappears. To prove this, the following modifications of the PYTHIA generator have been made in order to connect the three kinds of masses:

- Connect the two b-quark masses (kinematical and constituent) by the simplest assumption of $M_b = M_b^{const}$,
- make all B hadron masses (including already known ones) depend on M_b^{const} through the mass formula of Eq. (1),
- make the Peterson fragmentation function depend on M_b^{const} through $\epsilon_b \propto 1/(M_b^{const})^2$.

Figures 3 and 4 show that now, when M_b is changed, the effects produced at parton level are also observed - almost identically - at hadron level. In such a setup of the generator, the hadronization corrections to be applied to the $R_3^{b\ell}$ observable would remain basically constant[4].

From this exercise we conclude that a coherent picture within the generator is obtained when the mass parameter values are connected. The next step is to find the value to be used for the b quark mass M_b in the standard generator (where the mass parameters are not connected) and the uncertainty associated to it. In the following sections we describe our best guesses.

4 Identifying the kinematical mass M_b in PYTHIA with the pole mass in NLO ME calculations

The NLO analytical calculations [7, 8] used to interpret the $R_3^{b\ell}$ measurements in terms of a b-quark mass at the scale of M_Z are not expressed in terms of the mass parameters described in Section 2 for PYTHIA. They use instead either running or pole mass definitions which are directly derived from the QCD Lagrangian. The first step is to find out how precisely M_b, the kinematical b-quark mass parameter used in the perturbative part of the PYTHIA treatment, can be identified, in a quantitative sense (for the $R_3^{b\ell}$ observable), with one of these two definitions: the pole mass, which is a priori more closely related to the kinematical mass parameter in PYTHIA than the running mass.

To check this identification we should use the theoretically most precise ME calculations [7, 8] to compute $R_3^{b\ell}$ and compare with the PYTHIA prediction. If there is consistency, then the values of the mass parameter used in PYTHIA and of that used in the ME calculation should be very close (i.e. within the theoretical uncertainty of the ME calculation used). The NLO ME calculations [7, 8] are available for $R_3^{b\ell}$ using both the running and pole mass definitions. This means that we can fit the prediction from PYTHIA (using its default value $M_b = 5$ GeV/c^2) with the NLO prediction to extract a value for both the pole mass and the running mass $m_b(M_Z)$ (as it was done in [1] for the measured $R_3^{b\ell}$). We believe that the theoretical uncertainties for the extracted $m_b(M_Z)$ are better estimated than those associated with the obtained pole mass. Therefore we use the extracted $m_b(M_Z)$ to do the comparison which can be done in two equivalent ways:

[4]Particle decays have been turned off for this exercise since, for small values of M_b, the computed B hadron masses are too low and problems appear in the decay processes. It has been checked that the same behaviour is observed when particles are allowed to decay for variations of M_b above 4 GeV/c^2.

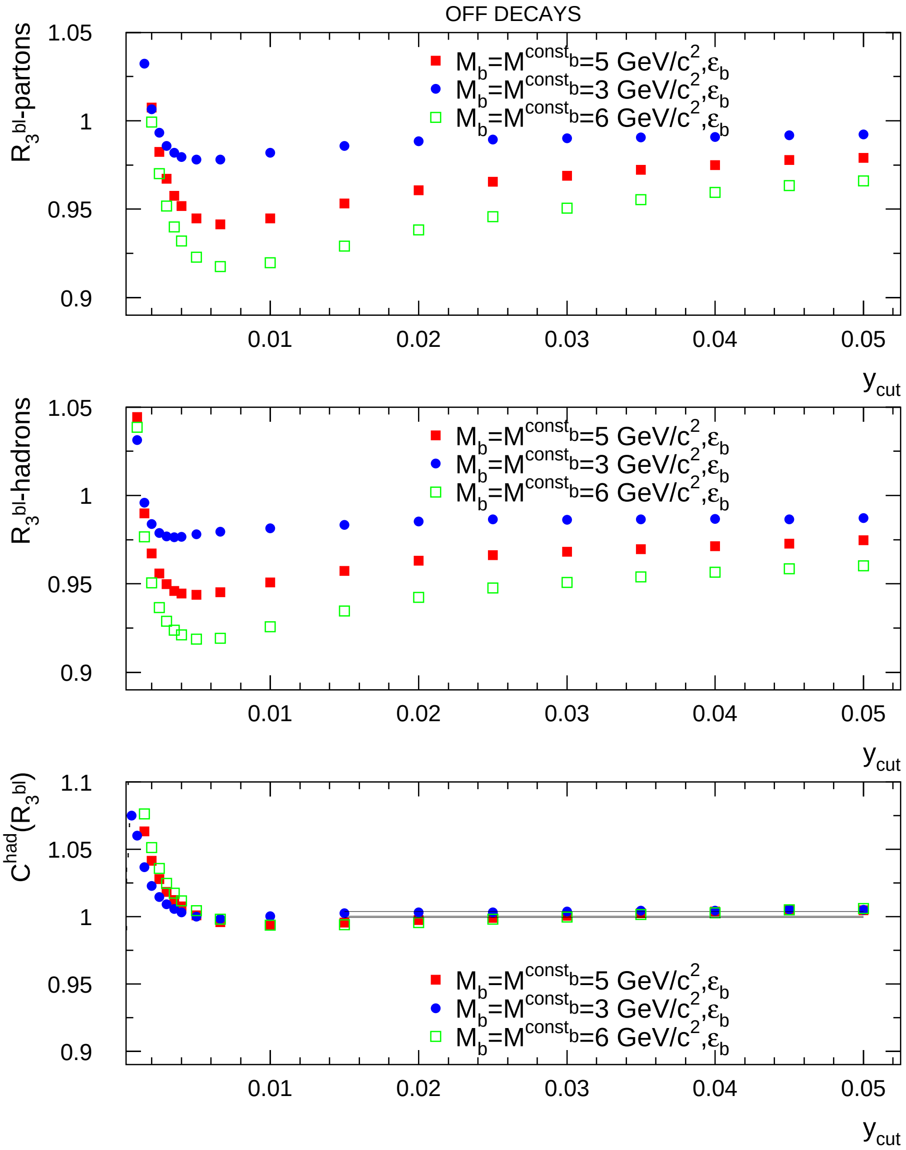

Figure 3: $R_3^{b\ell}$ at parton and hadron level and its hadronization correction as a function of y_c for three different values of M_b, when $M_b = M_b^{const}$, B hadron masses are constructed from M_b^{const} and $\epsilon_b \propto 1/(M_b^{const})^2$.

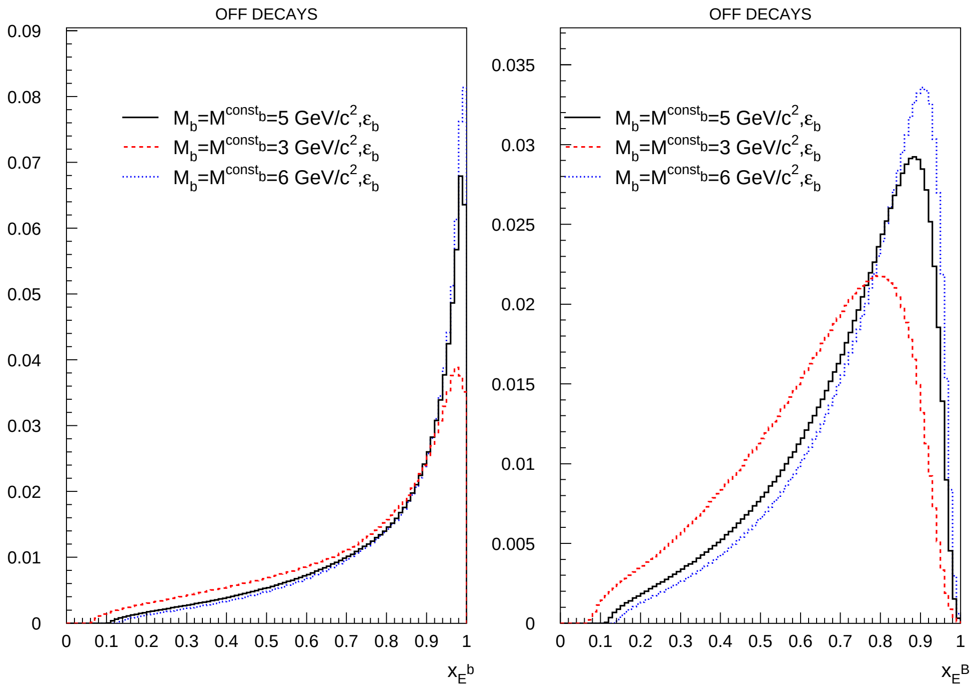

Figure 4: b-quark scaled energy distribution (left) and B hadron scaled energy distribution (right) for M_b = 3, 5 and 6 in PYTHIA.

- The value of $m_b(M_Z)$ obtained can be re-expressed in terms of a pole mass using perturbative QCD, and compared directly to $M_b = 5$ GeV/c^2 used in PYTHIA.
- Or else the reverse: the value $M_b = 5$ GeV/c^2 used in PYTHIA, assumed to be the pole mass, can be re-expressed in terms of a running mass using perturbative QCD. One obtains $m_b(M_Z) = 3.08$ GeV/c^2, for a value of $\alpha_s(M_Z) = 0.1183 \pm 0.0027$ from [9], using in two steps a 2-loop expression (pole mass to $m_b(M_b)$) and 3-loop renormalization group equations (RGE) (from $m_b(M_b)$ to $m_b(M_Z)$). Then this value can be compared directly to the value extracted by fitting the NLO ME calculations to the prediction from PYTHIA.

The results from this comparison (following the second prescription) are shown in table 1 for different values of y_c, using DURHAM and CAMBRIDGE jet clustering algorithms. The differences between the PYTHIA and NLO predictions are in all cases well within the estimated theoretical errors, which are estimated as the magnitude of the contribution from higher order terms not considered in the calculation of $R_3^{b\ell}$. This mass difference could in principle be added up as additional source of uncertainty or else considered already included in the theoretical part of the error in the analysis, since the differences are well within this error.

We conclude from this comparison that for the $R_3^{b\ell}$ observable the kinematical mass parameter M_b in PYTHIA can be identified with the pole mass used in fixed order NLO calculations within the precision of the NLO calculations expressed in terms of the running mass.

y_c (DURHAM)	$R_3^{b\ell}$	$m_b(M_Z)$ (GeV/c^2)	$\Delta_{m_b(M_Z)}$ (GeV/c^2)
0.015	0.9539 ± 0.0004	3.28 ± 0.27	0.20 ± 0.27
0.02	0.9611 ± 0.0005	3.13 ± 0.29	0.05 ± 0.29
0.025	0.9667 ± 0.0005	3.00 ± 0.29	-0.08 ± 0.29
0.03	0.9711 ± 0.0006	2.89 ± 0.29	-0.19 ± 0.29
y_c (CAMBRIDGE)	$R_3^{b\ell}$	$m_b(M_Z)$ (GeV/c^2)	$\Delta_{m_b(M_Z)}$ (GeV/c^2)
0.005	0.9578 ± 0.0004	3.00 ± 0.13	-0.08 ± 0.13
0.007	0.9567 ± 0.0004	3.10 ± 0.04	0.02 ± 0.04
0.01	0.9601 ± 0.0004	3.12 ± 0.09	0.04 ± 0.09
0.015	0.9667 ± 0.0005	3.01 ± 0.16	-0.07 ± 0.16

Table 1: Extracted values of $m_b(M_Z)$ obtained for DURHAM and CAMBRIDGE at different values of y_c taking the $R_3^{b\ell}$ predicted by PYTHIA as input. The differences between the values obtained and the mass set in PYTHIA, which corresponds to $m_b(M_Z) = 3.08$ GeV/c^2, are also written. The quoted uncertainties on $m_b(M_Z)$ account for the statistical uncertainty of the Monte Carlo predicted $R_3^{b\ell}$ (which has a negligible contribution) and the theoretical uncertainty of the NLO prediction for this observable.

5 Determining the value of the kinematical mass M_b in PYTHIA

As was shown in the previous section the kinematical mass M_b in PYTHIA can be identified with the pole mass used in NLO calculations of $R_3^{b\ell}$. Hence one could consider to use directly the pole mass value determined from the low energy data.

However, one potential drawback is that the physics involved when considering mass effects in inclusive observables such as $R_3^{b\ell}$ is not the same as that relevant to the exclusive analyses of specific B hadrons which are used to extract values of the pole mass near the production threshold. In particular the detailed mix of bound hadrons and the fraction of excited states are different, and moreover not entirely known experimentally.

For this reason we have investigated an alternative method to determine the kinematical mass M_b in PYTHIA, based on the LEP data itself. As an example, we have applied this method to preliminary data collected by DELPHI. As was shown in Section 3, the only way to see effects at the hadron level which can be compared to data upon varying M_b is to use the modified setup of the generator described in Section 3.3, where a connection was established between M_b and the constituent mass M_b^{const}, and where the latter was used to compute all B hadron masses. This modified setup could be used to tune M_b based on the data and the result would be meaningful as long as the connection assumed could be justified. As a first approximation we have used $M_b = M_b^{const}$, although in principle a more complicated relation could also be considered.

As already mentioned, the constituent mass is not well defined in QCD. However, it does predict (phenomenologically) masses for all B hadrons. On the contrary, in Heavy Quark Effective Theory (HQET) mass parameters are well defined but, at present, it can describe only a subset of the B hadron masses. Having all this in mind, our strategy was the following:

1. establish the relation between the pole mass M_b used in HQET - which we can

identify with the kinematical mass parameter M_b in PYTHIA[5]- and the constituent mass M_b^{const}, such that both predict the same B hadron masses for the subset where this comparison can be done,

2. extract the value of M_b^{const} which describes our data best using observables which are independent of (or at least only weakly correlated with) $R_3^{b\ell}$,

3. consider the uncertainties inherent to the use of HQET and those derived from the fit as an extra contribution to the total error in our analysis.

In order to quantify the uncertainty from considering the pole mass as the constituent mass in the mass formula to determine all B hadron masses, we use HQET to relate the masses of the $B = \bar{b}q$ ($q = u, d, s$) mesons, m_B, with the b-quark pole mass, M_b:

$$m_B = M_b + \overline{\Lambda} + \mathcal{O}(1/M_b) \tag{2}$$

where $\overline{\Lambda}$ is the binding energy at LO in the $1/M_b$ expansion. This binding energy was found to be [10]:

$$\overline{\Lambda} = 0.40 \pm 0.10 \text{ GeV}/c^2 \tag{3}$$

Compatible results were obtained by CLEO: $\overline{\Lambda} = 0.39 \pm 0.03$ (stat) $\pm$ 0.06 (syst) $\pm$ 0.12 (theo) GeV/c^2 [11].

If the measured mass of $B^{\pm}$ and B^0 mesons, $m_B = 5.279$ GeV/c^2, is used to derive the constituent and pole masses needed to describe the measured data through the mass formula of Eq. (1) and through the HQET relation of Eq. (2) respectively, the values found are:

$$\begin{aligned} M_b^{const} &= 4.99 \text{ GeV}/c^2 \\ M_b &= 4.88 \pm 0.10 \text{ GeV}/c^2 \end{aligned} \tag{4}$$

The difference between the two masses is 0.11$\pm$0.10 GeV/c^2, so $\pm$0.11 GeV/c^2 can be considered as the error made when the assumption of $M_b = M_b^{const}$ is applied and the mass formula is used to derive B hadron masses instead of HQET.

Next we need to find an observable sensitive to the variation of M_b in the modified setup of the generator so that by fitting to the measured data the M_b parameter of PYTHIA can be determined. As shown in figures 3 and 4 the $R_3^{b\ell}$ and the x_E^b observables are examples of such observables. For this tuning, we use instead the y_{32} distribution of b over ℓ events normalized to the total number of b and ℓ events, $R^{b\ell}(y_{32})$, where y_{32} is the y_c transition value in which a 3-jet event becomes a 2-jet one:

$$R^{b\ell}(y_{32}) = \frac{N^b(y_{32})/N^b}{N^\ell(y_{32})/N^\ell} \tag{5}$$

Two jet clustering algorithms, DURHAM and CAMBRIDGE, were used to form jets.

The $R^{b\ell}(y_{32})$ distribution was then measured at hadron level for both jet algorithms by correcting for detector effects bin by bin the ratio distribution (12 bins were taken between 0 and 0.06) [12]. The preliminary measured distributions for DURHAM and CAMBRIDGE can be seen in figure 5, where only statistical errors were considered. The

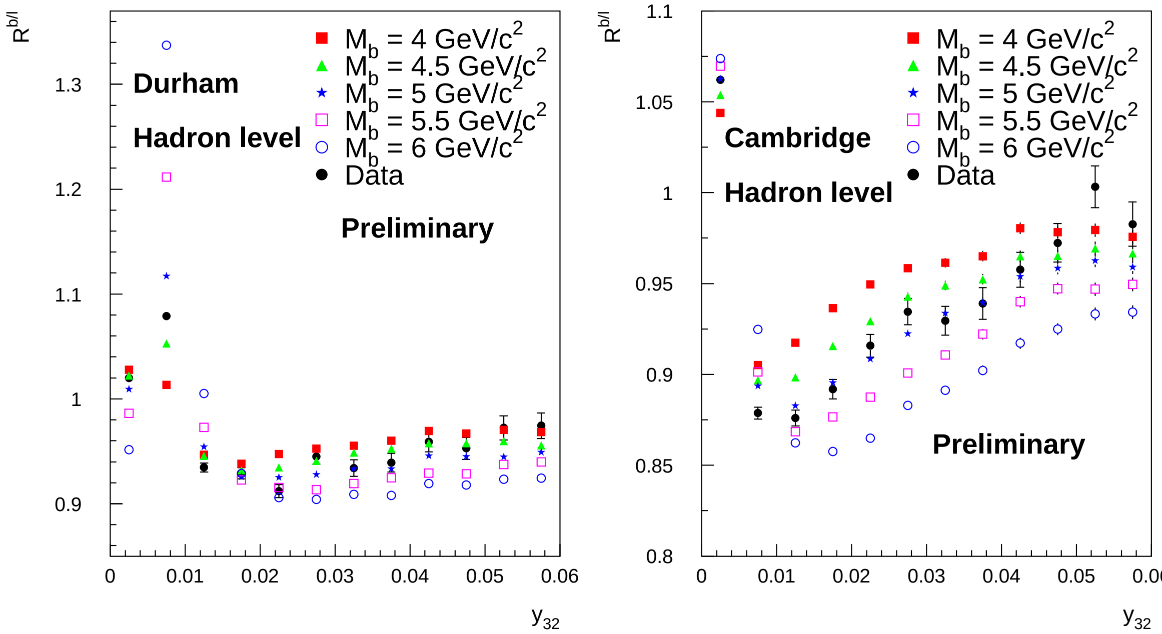

Figure 5: The $R^{b\ell}(y_{32})$ observable measured at hadron level and the PYTHIA prediction for different values of $M_b = 4, 4.5, 5, 5.5$ and 6 GeV$/c^2$ when DURHAM (left) and CAMBRIDGE (right) are used for jet reconstruction. The data results are preliminary.

PYTHIA prediction for this observable at hadron level[6] is also shown for different values of $M_b = 4, 4.5, 5, 5.5$ and 6 GeV$/c^2$.

For each jet algorithm, a polynomial interpolation was performed to obtain the value of M_b in PYTHIA that reproduces the data for each y_{32} bin, in the region $y_{32} \geq 0.02$ for DURHAM and $y_{32} \geq 0.01$ for CAMBRIDGE. In the low y_{32} region the distribution varies very rapidly and therefore the result obtained for M_b is more sensitive to the binning. For this reason it was decided not to use this region, although the sensitivity to M_b is larger on some of these bins. Figure 6 shows the M_b values obtained for DURHAM and CAMBRIDGE for each y_{32} bin.

The weighted mean of all bin results was found to be $M_b = 4.72 \pm 0.12$ (stat) GeV$/c^2$ for DURHAM and $M_b = 4.93 \pm 0.07$ (stat) GeV$/c^2$ for CAMBRIDGE.

Taking into account the uncertainty associated with the identification of the pole mass with the constituent mass in PYTHIA, the b mass parameter of PYTHIA is determined to be,

$$M_b = 4.93 \pm 0.07 \text{ (stat)} \pm 0.11 \text{ (theo) GeV}/c^2 \qquad (6)$$

which corresponds to the result obtained with CAMBRIDGE, due to its higher precision.

[5] This requires that the pole masses used in HQET and in the NLO ME calculations be consistent.

[6] Here hadron level means including the decays of all particles since the Monte Carlo is compared with the measured data.

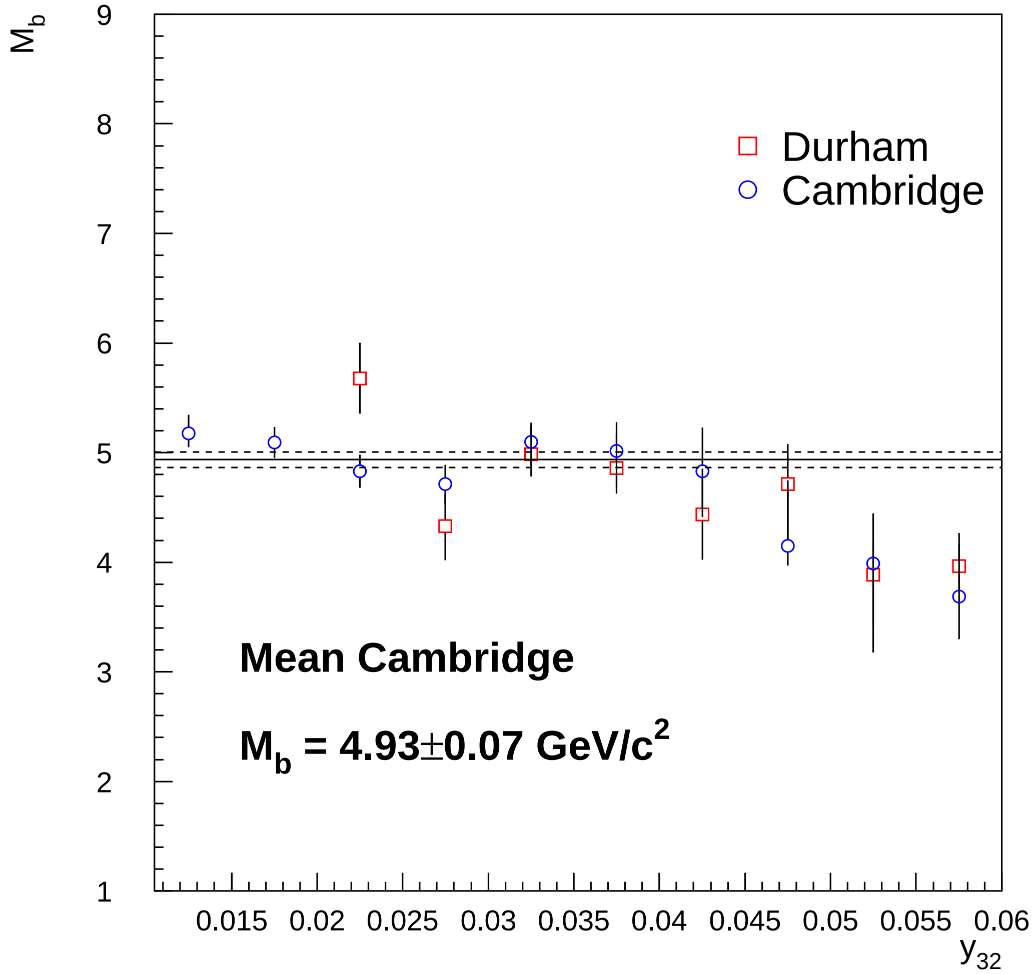

Figure 6: The fitted M_b values obtained for the DURHAM and CAMBRIDGE jet clustering algorithms for each bin y_{32}. The horizontal full line represents the mean of all bins for CAMBRIDGE and the dashed ones correspond to its statistical error.

6 Possibilities to set the kinematical mass M_b in PYTHIA

We would like to discuss the different possibilities one has to set the M_b parameter in the standard version of PYTHIA (in which B hadron masses are hardcoded and disconnected from M_b) to assure a reliable hadronization correction for the $R_3^{b\ell}$ observable. We consider them to be:

- As shown in Section 4, the M_b parameter can be identified with the pole mass within the uncertainty of the NLO matrix element calculations. Therefore, one possibility would be to take the value of M_b from measurements of the pole mass performed at threshold. We could then take the result obtained in [13]:

$$M_b = 4.98 \pm 0.13 \text{ GeV}/c^2 \tag{7}$$

  which, compared with other determinations, has a rather conservative error associated.

- Another possibility would be to take directly the pole mass extracted from our fit to the measured $R^{b\ell}(y_{32})$ at hadron level:

$$M_b = 4.93 \pm 0.13 \text{ GeV}/c^2 \tag{8}$$

- The last possibility is based on the fact that the mass extracted from our fit, i.e. 4.93 GeV/c^2, is 60 MeV smaller than the constituent mass reproducing the B meson masses through the mass formula (see Eq. 5), although both are compatible within errors. It could be justified to consider the range between these two masses as an uncertainty, since in each case the PYTHIA generator describes some aspect of the data better. Therefore, the mean between these masses could be used:

$$M_b = 4.96 \pm 0.13 \text{ GeV}/c^2 \tag{9}$$

The three possibilities listed above are compatible within the quoted errors.

7 Conclusions

The way in which the b-quark mass enters in the PYTHIA generator has been investigated and better understood. The three kinds of masses, the kinematical and constituent b-quark masses and the B hadron masses, should be connected when studying observables depending on the b-quark mass. When doing so and for the $R_3^{b\ell}$ observable it was shown that the hadronization process as implemented in the generators is independent of the b quark mass value.

In the context of the determination of $m_b(M_Z)$ via the measurement of $R_3^{b\ell}$ the kinematical b mass of PYTHIA was identified to be the pole mass used in the fixed-order theoretical calculations. A strategy to determine the value of this PYTHIA b pole mass from LEP data has been proposed using HQET and fitting the PYTHIA prediction to the preliminary measured $R^{b\ell}(y_{32})$ distribution at hadron level.

Different possibilities to set the M_b parameter in the standard version of PYTHIA, where B hadron masses are hardcoded, have been listed and discussed, all of them compatible within errors. In the context that motivated the study presented in this note, i.e. the determination of $m_b(M_Z)$ from the effect observed on $R_3^{b\ell}$, we consider advisable to set the kinematical b-quark mass in PYTHIA to the one obtained by a completely independent determination of the pole mass, as the one given in the first option, $M_b = 4.98 \pm 0.13$ GeV$/c^2$, in order to be safe of the possible correlation between $R_3^{b\ell}$ at the chosen y_c and $R^{b\ell}(y_{32})$.

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