On the $g \to Q\overline{Q}$ Rate

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1 The DGLAP splitting kernel

The standard expression for $g \to q\overline{q}$, with q a massless quark is the DGLAP splitting expression

$$\mathrm{d}P_{g\to q\overline{q}} = \frac{\alpha_s}{2\pi}\,\frac{\mathrm{d}m^2}{m^2}\,\frac{1}{2}\left(z^2+(1-z)^2\right)\,\mathrm{d}z\ . \tag{1}$$

The z dependence can be related e.g. to the $e^+e^- \to \gamma^* \to q\overline{q}$ angular distribution,

$$\frac{\mathrm{d}\sigma_{e^+e^-\to\gamma^*\to q\overline{q}}}{\mathrm{d}\cos\theta} \propto 1+\cos^2\theta \propto (1+\cos\theta)^2+(1-\cos\theta)^2 \propto z^2+(1-z)^2 \tag{2}$$

for

$$z = \frac{1+\cos\theta}{2} = \frac{(E+p_z)_q}{(E+p_z)_{\gamma^*}}\ . \tag{3}$$

The last equality refers to a lightcone definition of the energy–momentum sharing in the branching.

Now instead consider $g \to Q\overline{Q}$, where Q is a massive quark, in reality c or b, with mass m_Q. Introducing the notation

$$r_Q = \frac{m_Q^2}{m_{\gamma^*}^2}\ , \tag{4}$$

$$\beta_Q = \sqrt{1-\frac{4m_Q^2}{m_{\gamma^*}^2}} = \sqrt{1-4r_Q}\ , \tag{5}$$

the γ^* decay rate is changed to

$$\frac{\mathrm{d}\sigma_{e^+e^-\to\gamma^*\to q\overline{q}}}{\mathrm{d}\cos\theta} \propto \beta_Q\left(1+\cos^2\theta+4r_Q\sin^2\theta\right) \propto \beta_Q\left(z^2+(1-z)^2+8r_Q z(1-z)\right)\ . \tag{6}$$

The last expression here is valid for z defined in terms of angles, but no longer for the alternative lightcone definition. Thus the same applies for the DGLAP rate

$$\mathrm{d}P_{g\to Q\overline{Q}} = \frac{\alpha_s}{2\pi}\,\frac{\mathrm{d}m^2}{m^2}\,\frac{\beta_Q}{2}\left(z^2+(1-z)^2+8r_Q z(1-z)\right)\,\mathrm{d}z\ , \tag{7}$$

whereas the z-integrated rate

$$\frac{\mathrm{d}P_{g\to Q\overline{Q}}}{\mathrm{d}m^2} = \frac{\alpha_s}{2\pi}\,\frac{1}{m^2}\,\frac{1}{3}\beta_Q(1+2r_Q) \tag{8}$$

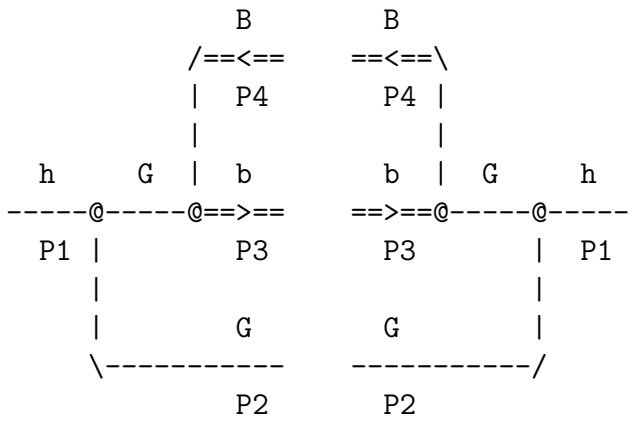
is unambiguous. For ease of plotting we will often use

$$\frac{\mathrm{d}P_{\mathrm{g}\to\mathrm{Q}\overline{\mathrm{Q}}}}{\mathrm{d}m} = 2m\,\frac{\mathrm{d}P_{\mathrm{g}\to\mathrm{Q}\overline{\mathrm{Q}}}}{\mathrm{d}m^2} = \frac{\alpha_\mathrm{s}}{2\pi}\,\frac{1}{m}\,\frac{2}{3}\beta_\mathrm{Q}(1+2r_\mathrm{Q}) \tag{9}$$

as reference for the DGLAP answer.

2 A matrix element expression

The above expression does not put the $\mathrm{g}\to\mathrm{Q}\overline{\mathrm{Q}}$ branching into the context of a real process. The most convenient choice for such an exercise is the Higgs decay $\mathrm{H}\to\mathrm{gg}\to\mathrm{Q}\overline{\mathrm{Q}}\mathrm{g}$. Using CalcHep the one contributing graph is



with Q = b here. This gives a numerator expression

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8*p1.p3^2*p1.p2-4*p1.p3^2*Mh^2+8*p1.p3*p1.p2^2-12*p1.p3*p1.p2*Mh^2
+4*p1.p3*Mh^4+4*p1.p2^3-4*p1.p2^2*Mbp^2-6*p1.p2^2*Mh^2+4*p1.p2*Mh^4-Mh^6
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For convenience it is converted to the energy fractions

$$x_i = \frac{2E_i}{M} = \frac{2p_0p_i}{M^2} \tag{10}$$

using the more standard labels $\mathrm{H}(0)\to\mathrm{Q}(1)\,\overline{\mathrm{Q}}(2)\,\mathrm{g}(3)$, and with $M = m_\mathrm{H}$. Also introduce $r = m_\mathrm{Q}^2/M^2$, not to be confused with $r_\mathrm{Q} = m_\mathrm{Q}^2/m_{\mathrm{g}^*}^2$ by analogy with the γ^* case above. Multiplied by $-2/M^6$ the numerator turns into

$$\begin{aligned} & -2x_1^2x_3 + 2x_1^2 - 2x_1x_3^2 + 6x_1x_3 - 4x_1 - x_3^3 + 3x_3^2 - 4x_3 + 2 + 2rx_3^2 \\ = \;& x_1^3 + x_1^2x_2 + x_1x_2^2 + x_2^2 - 3x_1^2 - 4x_1x_2 - 3x_2^2 + 4x_1 + 4x_2 - 2 + 2rx_3^2 \end{aligned} \tag{11}$$

using the relationship $x_1 + x_2 + x_3 = 2$ to derive the second line.

The denominator is $((p_0-p_3)^2)^2 = M^4(1-x_3)^2 = M^4(x_1+x_2-1)^2$, giving the ratio

$$\begin{aligned} & \frac{x_1^3 + x_1^2x_2 + x_1x_2^2 + x_2^2 - 3x_1^2 - 4x_1x_2 - 3x_2^2 + 4x_1 + 4x_2 - 2 + 2rx_3^2}{(x_1+x_2-1)^2} \\ = \;& \frac{x_1^2+x_2^2}{1-x_3} - 2 + 2r\frac{x_3^2}{(1-x_3)^2}\ . \end{aligned} \tag{12}$$

The prefactor to the matrix element is $-128 g_s^2 \lambda_{\rm Hgg}^2$, to be compared with the H $\to$ gg matrix element $32 \lambda_{\rm Hgg}^2 M^4$. Combining this with the omitted numerator and denominator prefactors gives altogether

$$\frac{-128 g_s^2 \lambda_{\rm Hgg}^2}{32 \lambda_{\rm Hgg}^2 M^4} \frac{M^6}{-2} \frac{1}{M^4} = \frac{2 g_s^2}{M^2} = \frac{8 \pi \alpha_{\rm s}}{M^2} \; . \tag{13}$$

So far we only considered the (squared) matrix elements. Now we need to consider the phase space factors as well. Using e.g. the Review of Particle Physics we get

$$\Gamma_2 = \frac{|M_2|^2}{16 \pi M} \tag{14}$$

$$\begin{aligned} {\rm d}\Gamma_3 &= \frac{1}{(2\pi)^5} \frac{|M_3|^2}{16 \pi M} \, {\rm d}E_1 \, {\rm d}E_2 \, {\rm d}\varphi \, {\rm d}(\cos\theta) \, {\rm d}\chi \\ &= \frac{1}{(2\pi)^5} \frac{|M_3|^2}{16 \pi M} \frac{M}{2} {\rm d}x_1 \frac{M}{2} {\rm d}x_2 \, 8\pi^2 = \frac{|M_3|^2}{256 \pi^3} M \, {\rm d}x_1 \, {\rm d}x_2 \; , \end{aligned} \tag{15}$$

since decays are isotropic in angles for a spin 0 particle. The ratio is

$$\begin{aligned} \frac{{\rm d}\Gamma_3}{\Gamma_2} &= \frac{|M_3|^2}{|M_2|^2} \frac{M^2}{16\pi^2} \, {\rm d}x_1 \, {\rm d}x_2 = \frac{8 \pi \alpha_{\rm s}}{M^2} \frac{M^2}{16 \pi^2} \left(\frac{x_1^2 + x_2^2}{1 - x_3} - 2 + 2r \frac{x_3^2}{(1-x_3)^2} \right) {\rm d}x_1 \, {\rm d}x_2 \\ &= \frac{\alpha_{\rm s}}{2\pi} \left(\frac{x_1^2 + x_2^2}{1 - x_3} - 2 + 2r \frac{x_3^2}{(1-x_3)^2} \right) {\rm d}x_1 \, {\rm d}x_2 \; . \end{aligned} \tag{16}$$

This will be the standard fully differential matrix element expression.

As an alternative form, note that ${\rm d}x_1 \, {\rm d}x_2 = {\rm d}x_1 \, {\rm d}x_3$ and that $x_3 = 1 - m^2/M^2$ so that ${\rm d}x_3/(1-x_3) = {\rm d}m^2/m^2$. Thus

$${\rm d}P = \frac{{\rm d}\Gamma_3}{\Gamma_2} = \frac{\alpha_{\rm s}}{2\pi} \frac{{\rm d}m^2}{m^2} \left(x_1^2 + x_2^2 - 2(1-x_3) + 2r \frac{x_3^2}{(1-x_3)} \right) {\rm d}x_1 \tag{17}$$

For massless quarks and in the limit $m^2 \to 0$ we may choose $x_1 \approx z, x_2 \approx 1 - z$, so that the standard DGLAP expression is recovered, with an extra factor of 2 since we have two gluons that can branch.

The allowed phase space for the complete expression is compactly given by

$$\frac{(1-x_1)(1-x_2)(1-x_3)}{x_3^2} > r \; , \tag{18}$$

which is not so convenient for integration.

An alternative setup is to relate $x_{1,2}$ to the $\cos\theta$ angle in the rest frame of the g*, similarly to what was done for γ^* previously:

$$p_{\rm Q,\overline{Q}} = \frac{m}{2} \left(1; \pm \beta_{\rm Q} \sin\theta, 0, \pm \beta_{\rm Q} \cos\theta \right) \; . \tag{19}$$

Introducing the ratio $\delta = m^2/M^2$, the boost along the z axis is $\beta_z = (1-\delta)/(1+\delta)$, and the boosted momenta give

$$x_{1,2} = \frac{1}{2} \left(1 + \delta \pm (1 - \delta) \, \beta_{\rm Q} \, \cos\theta \right) \; , \tag{20}$$

$$x_3 = 1 - \delta \; . \tag{21}$$

Then, using that $r/\delta = (m_{\mathrm{Q}}^2/M^2)/(m^2/M^2) = m_{\mathrm{Q}}^2/m^2 = r_{\mathrm{Q}}$, the integration becomes

$$\begin{aligned}
& \int_{x_{1,\min}}^{x_{1,\max}} \left(x_1^2 + x_2^2 - 2(1-x_3) + 2r \frac{x_3^2}{(1-x_3)} \right) \mathrm{d}x_1 \\
= & \int_{-1}^{1} \frac{1}{2} \left((1+\delta)^2 + (1-\delta)^2 \, \beta_{\mathrm{Q}}^2 \, \cos^2\theta - 4\delta + 4 \, \frac{r}{\delta} \, (1-\delta)^2 \right) \frac{1}{2} \, (1-\delta) \, \beta_{\mathrm{Q}} \, \mathrm{d}(\cos\theta) \\
= & \frac{1}{2} \, \beta_{\mathrm{Q}} \, (1-\delta)^3 \int_{-1}^{1} \left(1 + \beta_{\mathrm{Q}}^2 \, \cos^2\theta + 4 r_{\mathrm{Q}} \right) \frac{1}{2} \, \mathrm{d}(\cos\theta) \\
= & \frac{1}{2} \, \beta_{\mathrm{Q}} \, (1-\delta)^3 \int_{-1}^{1} \left(1 + \cos^2\theta + 4 r_{\mathrm{Q}} \, \sin^2\theta \right) \frac{1}{2} \, \mathrm{d}(\cos\theta) \\
= & \frac{2}{3} \, \beta_{\mathrm{Q}} \, (1 + 2 r_{\mathrm{Q}}) \, (1-\delta)^3 \, , \qquad (22)
\end{aligned}$$

i.e. again we recover the DGLAP rate, but with the additional $(1-\delta)^3$ suppression of large g^* masses m, and a trivial factor of two from having two gluon ends. We will refer to this expression as the ME rate.

There is no guarantee that the $(1-\delta)^3$ factor is universal, but it is as plausible a suppression near the kinematical limit as any. The quark mass dependence and the g^* angular decay distribution are identical with the $\mathrm{e}^+\mathrm{e}^- \to \gamma^* \to \mathrm{q}\overline{\mathrm{q}}$ process, and here the universal character is more convincing.

3 The PYTHIA algorithm

The main points of the PYTHIA algorithm, as it impacts the $\mathrm{g} \to \mathrm{Q}\overline{\mathrm{Q}}$ rate, are as follows.

- Evolution is ordered in terms of a decreasing $\mathrm{p}_{\perp\mathrm{evol}}^2$. This is so hardcoded that no attempt will be made to change on that.
- The allowed z range is related to the $\mathrm{p}_{\perp\mathrm{evol}}$ evolution variable

$$z_{\max,\min}(\mathrm{p}_{\perp\mathrm{evol}}^2) = \frac{1}{2} \pm \sqrt{\frac{1}{4} - \frac{\mathrm{p}_{\perp\mathrm{evol}}^2}{M^2}} \qquad (23)$$

  where now M is the full dipole mass. If the same z definition is to be used as for $\mathrm{g} \to \mathrm{gg}$ then it isimportant that z stays away from the singularities at $z = 0, 1$. Here, technically, one could imagine to have a different z definition for $\mathrm{g} \to \mathrm{q}\overline{\mathrm{q}}$ and $\mathrm{g} \to \mathrm{gg}$, but again we will not go down that path.
- Initially, the lower cutoff of the $\mathrm{p}_{\perp\mathrm{evol}}^2$ evolution variable provides the maximally allowed z range. The splitting kernel is overestimated by noting that $z^2 + (1-z)^2 < 1$, so that the evolution rate can be overestimated by the length of the maximally allowed z range, times a half for each allowed quark flavour. An z is picked flat in this overestimated range.
- As the downwards evolution in $\mathrm{p}_{\perp\mathrm{evol}}^2$ proceeds, a potential branching is rejected if the chosen z value lies outside the allowed z range for that particular $\mathrm{p}_{\perp\mathrm{evol}}^2$ scale. By the veto algorithm this means that the proper z range is accounted for at each $\mathrm{p}_{\perp\mathrm{evol}}^2$ scale.

- Once a consistent candidate $(\mathrm{p}^2_{\perp\mathrm{evol}}, z)$ pair has been found, the $\mathrm{q\overline{q}}$ pair mass is calculated as
$$m^2 = \frac{\mathrm{p}^2_{\perp\mathrm{evol}}}{z(1-z)} \tag{24}$$
Note that the Jacobian has the convenient property that
$$\frac{\mathrm{d}\mathrm{p}^2_{\perp\mathrm{evol}}}{\mathrm{p}^2_{\perp\mathrm{evol}}}\,\mathrm{d}z = \frac{\mathrm{d}m^2}{m^2}\,\mathrm{d}z \tag{25}$$
so the two evolution measures populate the phase space equally, just traced in a different "time" order, which has indirect consequences via the Sudakov.
- A q flavour is chosen at random among the possibilities. Its mass is found and its β_q value is calculated. Below the threshold $\beta_\mathrm{q} = 0$.
- A weight $W = \beta_\mathrm{q}\,(z^2 + (1-z)^2)$ is assigned and gives the survival probability for the trial branching.
- The kinematics of the $\mathrm{g} \to \mathrm{q\overline{q}}$ branching is first constructed identically with the $\mathrm{g} \to \mathrm{gg}$ one, i.e. assuming the quark massless, and using an energy-sharing interpretation of the z variable.
- Masses are introduced by shrinking the three-momenta in the $\mathrm{q\overline{q}}$ rest frame while keeping the "decay" angles fixed, notably the $\cos\theta$ one.

This has been the only existing implementation up until now. From now on we will refer to it as option 1.

An obvious shortcoming is that the branching kernel is only $z^2 + (1-z)^2$ rather than the full $z^2 + (1-z)^2 + 8r_\mathrm{Q}z(1-z)$ one. This means that Pythia falls below the DGLAP and ME expressions in the threshold regions. Since also the full kernel is bounded from above by unity, it is straightforward to add the mass-dependent term to the weight W. The thus modified code is denoted option 2. It has the same low-mass behaviour as the DGLAP and ME expressions, up to corrections from the finite gg dipole mass.

In the high-m^2 region, $m^2 \to M^2$, the Pythia rate falls faster than the DGLAP one, but not as fast as the ME one. One could argue that this is as good an answer as any, given that the $(1-\delta)^3$ factor need not be universal. Nevertheless, let us investigate how to recover the DGLAP and ME expressions.

A key observation is that a given m^2 value can be reached from a curve of points in the $(\mathrm{p}^2_{\perp\mathrm{evol}}, z)$ plane. These $\mathrm{p}^2_{\perp\mathrm{evol}}$ values correspond to different allowed z ranges, so the z range open for the specific $\mathrm{p}^2_{\perp\mathrm{evol}}$ of a branching is not the same as the z range open for the m^2 reached. We can instead use the kinematics of eqs. (19) and (20). Here $\beta_\mathrm{Q} = 1$ since the starting point of the construction is massless quarks, which later are transformed to massive ones, with preserved $\cos\theta$. Since $z = x_1/(x_1+x_2)$ by the energy-sharing definition used in Pythia, the minimal z is obtained for $\cos\theta = -1$:
$$z_{\min}(m^2) = \frac{1+\delta-(1-\delta)}{2(1+\delta)} = \frac{\delta}{1+\delta} = \frac{m^2}{M^2+m^2}\ . \tag{26}$$
One point of the Jacobian in eq. (25) is that z is flat in the z range for a fixed m^2 if it was it for a fixed $\mathrm{p}^2_{\perp\mathrm{evol}}$. Introducing the shorthand
$$I_z(m^2) = \int_{z_{\min}(m^2)}^{1-z_{\min}(m^2)} \Big(z^2 + (1-z)^2 + 8r_\mathrm{Q}z(1-z)\Big)\,\mathrm{d}z \tag{27}$$

it therefore follows that the weight

$$W = \frac{2}{3}\,\beta_{\mathrm{Q}}\,(1+2r_{\mathrm{Q}})\,\frac{z^2+(1-z)^2+8r_{\mathrm{Q}}z(1-z)}{I_z(m^2)} \tag{28}$$

will average to $(2/3)\,\beta_{\mathrm{Q}}\,(1+2r_{\mathrm{Q}})$. Recalling that the initial overestimate provides a factor $1/2$, a Monte Carlo acceptance by W will reproduce the DGLAP rate in eq. (8).

One imperfection to note is that the allowed z range shrinks towards $z = 1/2$ in the $m^2 \to M^2$ limit, such that W is almost constant. This means that the angular dependence flattens out, rather than obeying the expected $1+\cos^2\theta$ shape. A further improvement on the scheme above therefore is to introduce a

$$z_\theta = \frac{1+\cos\theta}{2} = \frac{(1+\delta)\,z-\delta}{1-\delta} \tag{29}$$

which thereby is stretched out to the range $0 < z_\theta < 1$. This means that the equivalent of $I_z(m^2)$ in eq. (27) becomes the familiar $(2/3)\,(1+2r_{\mathrm{Q}})$, times a Jacobian $\mathrm{d}z/\mathrm{d}z_\theta$. Thus eq. (28) simplifies to

$$W = \beta_{\mathrm{Q}}\,\left(z_\theta^2+(1-z_\theta)^2+8r_{\mathrm{Q}}z_\theta(1-z_\theta)\right)\,\frac{1+\delta}{1-\delta}\;. \tag{30}$$

This defines option 3.

A special aspect is that, as already noted, DGLAP falls off slower than Pythia options 1 and 2, essentially owing to the $1-\delta$ denominator, so W can become arbitrarily large in the limit $m^2 \to M^2$. This is resolved by enhancing the $\mathrm{g} \to \mathrm{q\overline{q}}$ trial rate by fixed factor that then is used to reduce W accordingly. This factor is hardcoded to be 20. It is not enough at the very extreme tail of m^2 values, where therefore Pythia falls below the DGLAP rate, but this is a very minor blemish for all practical purposes.

By multiplying the W weight above by $(1-\delta)^3$ instead the ME rate in eq. (22) is reproduced. This gives option 4. Here no extra enhancement factor is required.

Studies so far have been with a fixed α_{s}, to simplify comparisons with the DGLAP and ME expressions. It is then also possible to use a low $\mathrm{p}^2_{\perp\mathrm{evol}}$ cutoff. The normal choice is to have a running $\alpha_{\mathrm{s}}(\mathrm{p}^2_{\perp\mathrm{evol}})$, hardcoded into the evolution algorithm. An option would be to have a $\alpha_{\mathrm{s}}(m^2)$ instead. For simplicity the effect of mass thresholds and second-order running is neglected, so that only an additional factor $\log(\mathrm{p}^2_{\perp\mathrm{evol}}/\Lambda^2)/\log(m^2/\Lambda^2)$ need to be included in the z weighting factor. These variants of options $1-4$ are available as options $5-8$. The scale choice impacts both rates and angular dependencies, and could have more of an effect than switching between the kinematics options $1-4$ for a fixed α_{s}.

The different options described above can be accessed by setting the option value in `TimeShower:weightGluonToQuark`. To summarize, these are

1. The old behaviour, which misses a mass term and therefore is somewhat low in the threshold region. At high masses it is intermediate in rate to the DGAP and ME results, and also has a flatter $\cos\theta$ distribution than them.

2. A modest change, which adds the missing mass term and therefore behaves better in the threshold region. At high masses there is no change. Should maybe be made new default.

3. The DGLAP shape, which has a high tail out to large masses. Should mainly be viewed as an extreme upper limit, not particularly likely.

4. The ME shape, which has a very suppressed tail out to large masses. Reproduces the correct behaviour for one specific process, with no claim of universality. It is hard to imagine that any other process would give an even stronger suppression, however, so probably represents a lower bound.

Option $5 - 8$ are the same as $1 - 4$ above, but with $\alpha_s(m^2)$ instead of $\alpha_s(p^2_{\perp\mathrm{evol}})$.

4 Phenomenology

The options have been studied in [1]. All options tend to give a larger $g \to b\bar{b}$ rate than observed at LEP/SLC, but within the large experimental errors options 1, 4, 5 and 8 are acceptable, at almost the same rate. Options 3 and 7 are way too high, and thus cannot be regarded as realistic. Since the choice of α_s argument does not seem to make a large difference, options 1 and 4 should be the prime target for further comparisons, where the difference is visible mainly in the invariant mass spectra, with option 4 more biased towards lower $b\bar{b}$ masses than option 1.

References

[1] F. Jiménez, "Charm and bottom production at particle colliders", LU TP 14-15 (master thesis, Lund University, 2014), see `http://particle.thep.lu.se/publications/index.html`