Mass distributions marginalized over per-event errors

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Abstract

We present generalizations of the Crystal Ball function to describe mass peaks in which the per-event mass resolution is unknown and marginalized over. The presented probability density functions are tested using a series of toy MC samples generated with Pythia and smeared with different amounts of multiple scattering and for different detector resolutions.

Keywords: statistics, invariant mass peaks

1. Introduction

A very common probability density function (p.d.f.) used to fit the mass peak of a resonance in experimental particle physics is the so-called Crystal Ball (CB) function \cite{1,2,3}:

\begin{equation}
p(m) \propto \begin{cases} 
e^{-\frac{1}{2} \left(\frac{m-\mu}{\sigma}\right)^2}, & \text{if } m-\mu > -a \\
A \left( B - \frac{m-\mu}{\sigma} \right)^n, & \text{otherwise}
\end{cases}
\end{equation}

where \(m\) is the free variable (the measured mass), \(\mu\) is the most probable value (the resonance mass), \(\sigma\) the resolution, \(a\) is called the transition point and \(n\) the power-law exponent. \(A\) and \(B\) are calculated by imposing the continuity of the function and its derivative at the transition point \(a\). This function consists of a Gaussian core, that models the detector resolution, with a tail on the left-hand side that parametrizes the effect of photon radiation by the final state particles in the decay. In data analysis, one may deal with events which have different uncertainties on the measured mass, therefore distorting the core of the Crystal
Ball, which will not be a Gaussian any more. This is sometimes modelled by the sum of two or three Crystal Ball functions, which is the equivalent of assuming that the per-event uncertainty is a sum of two or three delta functions. However, per-event uncertainties are usually continuous functions very different from a sum of a small number of deltas. One way of dealing with per-event uncertainties that follow a certain distribution, is to either make a p.d.f. conditional on the per-event uncertainty (if its distribution is known) or to perform the analysis in bins of the quantities that affect the per-event uncertainties (for example, particle momenta) and combine them afterwards. However, those procedures can significantly complicate the analysis, and in some cases one may prefer to simply marginalize over the mass error and have a p.d.f. that describes the final mass peak, as:

\[
p(m) \propto \int_{0}^{\infty} \frac{1}{\sqrt{v}} e^{-\frac{1}{2}(v_{e} - \frac{1}{2}v_{m} - \mu)^2} \rho(v) dv
\]  

where \(v\) is the variance and \(\rho(v)\) the prior density of the variance.

In this paper, we will define some extensions of the Crystal Ball distribution for different assumptions on \(\rho(v)\). We will fit the proposed mass models to \(J/\psi \rightarrow \mu^+ \mu^-\) toy MC samples where we can modify the relative importance of multiple scattering (MS) and detector spatial resolution (hereafter SR). Section 2 describes the generation of the toy MC samples. Section 3 defines an extension of the CB using a hyperbolic distribution core. Sections 4 and 5 generalize the function defined in Sect. 3. Section 6 gives a brief discussion of the meaning of the fit parameters. Section 7 discusses other effects on the invariant mass line-shape that are not directly related to resolution. Conclusions are drawn in Sect. 8.

2. Simulation of \(J/\psi \rightarrow \mu^+ \mu^-\) decays

We generate \(J/\psi\) events at \(\sqrt{s} = 8\) TeV using the \texttt{main17.cc} script of \texttt{Pythia8.176}\cite{4}. The \(J/\psi\)'s are then isotropically decayed into two muons. No
photons are added, as the radiative tail of the mass distribution should be well accounted by the Crystal Ball tail.

The generated muon momenta are smeared with a Gaussian resolution which has a momentum dependence:

\[ \frac{\sigma(p)}{p} = a + bp \]  

where \( a \) mimics the multiple scattering (MS) and \( b \) mimics the effect of the hit resolution. We take as typical values \( a = 3 \times 10^{-3} \) and \( b = 2 \times 10^{-5} \) GeV\(^{-1}\)c inspired by [5], although we will vary them for different tests.

3. Hyperbolic resolution model

A very flexible function that describes asymmetric unimodal p.d.f.’s defined above a certain threshold (i.e, like per-event error distributions usually look like, see for example Fig. 6 in [6]) is the so-called Amoroso distribution [7] (see Fig. [8]). If we consider the Amoroso distribution as a potential implementation for \( \rho(v) \), then the corresponding core of the invariant mass p.d.f. will be the following:

\[
\Phi(m) \propto \int_0^\infty \frac{1}{\sqrt{v}} e^{-\frac{1}{2}(m-\mu)^2} \left( \frac{v-\mu}{\theta} \right)^{\alpha \beta - 1} e^{-\left( \frac{v-\mu}{\theta} \right)^\beta} dv
\]  

Unfortunately, the above integral cannot be solved analytically. It would require a numerical implementation of the core and its derivative. This would make the matching with the radiative tail difficult. Evaluating (4) numerically for different values of Amoroso parameters, we find log-densities that exhibit an hyperbolic profile. Based on that observation, we define a possible core:

\[ c(x) \propto e^{- \sqrt{1+(m-\mu)^2}/\delta} \]  

i.e, \( c(x) \) is the symmetric limit of the hyperbolic distribution. It can also be rewritten in such way that the mass resolution \( \sigma \) appears explicitly, as it will be discussed in Sect. [4]. Adding a CB-like tail to (5), we obtain the following
p.d.f.:

\[
A(m, \mu, b, \delta, a, n) \propto \begin{cases} 
  e^{-b\sqrt{1+(m-\mu)^2/\delta^2}}, & \text{if } \frac{m-\mu}{\delta} \geq -a \\
  e^{-b\sqrt{1+a^2}} \left( \frac{n\sqrt{1+a^2}}{ba(n\sqrt{1+a^2}/(ba)-a-(m-\mu)/\delta)} \right)^n, & \text{otherwise}
\end{cases}
\]

(6)

Figure 1: Example of the Amoroso distribution for a hypothetical variance \( v \). The parameters used are \( \theta = 5, \alpha = 1.5, \mu = 7, \) and \( \beta = 2.3. \)

We fit the mass peak for \( J/\psi \rightarrow \mu^+\mu^- \) decays satisfying \( p_T^{J/\psi} \in [0, 14] \text{ GeV/c}, \)
\( \theta^\mu \in [20, 300] \text{ mrad}, p^\mu > 6 \text{ GeV/c}, p^\mu_T > 0.5 \text{ GeV/c} \) (which mimics LHCb-like conditions) to the Apollonios distribution, and find a very good agreement as can be seen in Fig. 3.

Now, the good agreement between this model and the MC toys used for testing can be broken without too much effort. For example, we now repeat the exercise releasing all kinematic and acceptance cuts, and switching off the
Figure 2: Fit of the invariant mass distribution of a $J/\psi \rightarrow \mu^+ \mu^-$ generated sample with $p_T^{J/\psi} \in [0, 14]$ GeV/$c$, $\theta_\mu \in [20, 300]$ mrad, $p^\mu > 6$ GeV/$c$ and $p_T^\mu > 0.5$ GeV/$c$. The pink line corresponds to the fit to a hyperbolic distribution. The dashed black line corresponds to the fit to a Gaussian. Left: linear scale. Right: Logarithmic scale.

4. Generalized Hyperbolic resolution model

The core of (5) is a limit case of the generalized hyperbolic distribution [8]:

$$G(m, \mu, \lambda, \alpha, \beta, \delta) = ( (m - \mu)^2 + \delta^2 )^{-\frac{\lambda}{2} - \frac{1}{2}} e^{\beta(m-\mu)} K_{\lambda - \frac{1}{2}} \left( \alpha \sqrt{(m-\mu)^2 + \delta^2} \right)$$

where $K_\lambda$ are the cylindrical harmonics or special Bessel functions of third kind.

In principle, $\beta^2$ is constrained to be smaller than $\alpha^2$. In practice that condition can be ignored if the fitting range is finite, but one has to be careful that if $\beta^2 > \alpha^2$ one of the tails will start rising at some point. The generalized hyperbolic distribution also has an important limit case, the Student’s-t distribution, as indicated in Table 1.

The p.d.f. in (8) can also be obtained by marginalizing over a variance density.  

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1 The parameter $\beta$ is related to a variance-dependency of the Gaussian mean, and not to
Figure 3: Fit of the invariant mass distribution of a $J/\psi \rightarrow \mu^+\mu^-$ generated sample without any phase space restriction and without the multiple scattering term in the momentum resolution. The pink line corresponds to the fit to an hyperbolic distribution. The dashed black line corresponds to the fit to a Gaussian. Left: Fit in the full mass range. Right: Fit in a region of about two standard deviations around the mean.

Table 1: Limit cases of the generalized hyperbolic distribution

| Distributions                  | $G(m, \mu, \lambda, \alpha, \beta, \delta)$ |
|-------------------------------|---------------------------------------------|
| Hyperbolic                    | $\lambda = 1, \alpha \delta = b$           |
| Symmetric hyperbolic          | $\lambda = 1, \beta = 0, \alpha \delta = b$|
| Student’s t                   | $\lambda = -\frac{\nu}{2}, \alpha = 0, \beta = 0, \delta = \sqrt{\nu}$ |
| Non-standardized Student’s t  | $\lambda = -\frac{\nu}{2}, \alpha = 0, \beta = 0$ |
\[ \rho(v, \lambda, \alpha, \delta) \propto v^{\lambda-1}e^{-[\alpha^2 v + \delta^2 / v]} \]  \hspace{1cm} (9)

The distribution (9) is the generalized inverse Gaussian distribution and describes very well the density we find for \( \sigma_{\mu \mu}^2 \), for the example in Fig. 3. This is shown in Fig. 4, together with the good agreement between the simulated data and the generalized hyperbolic distribution. We find that (9) fits well the mass variance distribution for all the generated \( J/\psi \rightarrow \mu^+ \mu^- \) samples that we have tested, although one needs to add an overall offset to the per-event error, i.e., to change \( v \) by \( v - v_0 \) in (9). The effect of an overall displacement of the per-event error distribution is further discussed in Sect. 5.

The following re-parametrization \( \{\alpha; \delta\} \rightarrow \{\sigma; \zeta\} \):

\[ \zeta = \alpha \delta \]  \hspace{1cm} (10)

\[ \sigma^2 = \delta^2 \frac{K_{\lambda+1}(\zeta)}{K_{\lambda}(\zeta)} = \delta^2 A_{\lambda}^{-2}(\zeta) \]  \hspace{1cm} (11)

is more suitable for fitting purposes as it allows us to specify the rms (\( \sigma \)) of the distribution in the symmetric case (\( \beta = 0 \)) as an explicit parameter. \( A_{\lambda}^2 = \frac{\zeta K_{\lambda}(\zeta)}{K_{\lambda+1}(\zeta)} \) is introduced for further convenience. In that parametrization:

\[ G(m, \mu, \sigma, \lambda, \zeta, \beta) \propto \left( (m - \mu)^2 + A_{\lambda}^2(\zeta) \sigma^2 \right)^{\frac{\lambda}{2} - \frac{1}{4}} e^{\beta(m - \mu)} K_{\lambda-\frac{1}{2}} \left( \zeta \sqrt{1 + \left( \frac{m - \mu}{A_{\lambda}(\zeta)\sigma} \right)^2} \right) \]  \hspace{1cm} (12)

Figure 4 shows \( G(m, \mu, \sigma, \lambda, \zeta, \beta) \) for different values of \( \zeta \) and \( \lambda \).

Using (12) as the core of a CB-like function, we define:

\[ I(m, \mu, \sigma, \lambda, \zeta, \beta, a, n) \propto \left\{ \begin{array}{ll} \left( (m - \mu)^2 + A_{\lambda}^2(\zeta) \sigma^2 \right)^{\frac{\lambda}{2} - \frac{1}{4}} e^{\beta(m - \mu)} K_{\lambda-\frac{1}{2}} \left( \zeta \sqrt{1 + \left( \frac{m - \mu}{A_{\lambda}(\zeta)\sigma} \right)^2} \right) , & \text{if } \frac{m - \mu}{\sigma} > -a \\ \frac{G(m - a\sigma, \mu, \sigma, \lambda, \zeta, \beta)}{1 - m/(n \sigma G(m - a\sigma, \mu, \sigma, \lambda, \zeta, \beta))} , & \text{otherwise} \end{array} \right. \]  \hspace{1cm} (13)

the per event variance distribution. For the purpose of this paper \( \beta \) can be considered zero.
Figure 4: $G(m, \mu, \sigma, \lambda, \zeta, \beta)$ is plotted for standard values of $\mu, \sigma, \beta$ and different values of $\zeta$ and $\lambda$. 

*Top:* $\zeta$ is fixed to 0.1 and $\lambda$ is varied. 

*Bottom:* $\lambda$ is fixed to -0.5 for the left plot and 0.5 for the right plot and $\zeta$ is varied.
Figure 5: Left: Per-event mass error squared fitted to $\sigma^2$ in a $J/\psi \rightarrow \mu^+\mu^-$ sample generated without MS. Right: Fit to the mass distribution on the same sample. The pink solid line shows the generalized hyperbolic. The dot-dashed blue line the Student’s-t case, and the dashed red line the hyperbolic distribution.

hereafter referred to as Hypatia distribution, where $G'$ is the derivative of the $G$ defined in (8).

The generalized hyperbolic core can describe most of the examples that were generated (see Fig. 4, right), but can also be broken with high statistic samples if $J/\psi \rightarrow \mu^+\mu^-$ events are taken all over the phase space without any kinematic or acceptance requirement, as it can be seen in Fig. 5.

5. Effect of the offset

We have seen that $f$ is a flexible function that can parametrize mass variance distributions if an offset is added to it. Yet, by adding the offset, the marginalization does not yield a generalized hyperbolic distribution for the most general case. We can see that adding an offset to the per-event error distribution
is equivalent to performing a convolution:

$$\int_0^\infty \frac{1}{\sqrt{v}} e^{-\frac{1}{2} (m-\mu)^2} \rho(v-v_0) \, dv = \int_0^\infty \frac{1}{\sqrt{v_0+\Delta}} e^{-\frac{1}{2} (v_0+\Delta)(m-\mu)^2} \rho(\Delta) \, d\Delta =$$

$$\int_0^\infty \left( \int_{-\infty}^{+\infty} \frac{1}{\sqrt{v_0}} e^{-\frac{1}{2} (m-t)^2} \frac{1}{\sqrt{\Delta}} e^{-\frac{1}{2} \Delta (t-\mu)^2} \, dt \right) \rho(\Delta) \, d\Delta =$$

$$\int_{-\infty}^{+\infty} \frac{1}{\sqrt{v_0}} e^{-\frac{1}{2} (m-t)^2} \left( \int_0^\infty \frac{1}{\sqrt{\Delta}} e^{-\frac{1}{2} \Delta (t-\mu)^2} \rho(\Delta) \, d\Delta \right) \, dt =$$

$$\frac{1}{\sqrt{v_0}} e^{-\frac{1}{2} (m)^2} \ast \left( \int_0^\infty \frac{1}{\sqrt{\Delta}} e^{-\frac{1}{2} \Delta (t-\mu)^2} \rho(\Delta) \, d\Delta \right) \quad (14)$$

The convolution of a generalized hyperbolic distribution with a Gaussian is not in general another generalized hyperbolic. However, we can argue that if \( v_0 \gg \Delta \), we will have a single Gaussian (that is a limit case of the generalized hyperbolic) and, on the contrary, that if \( v_0 \ll \Delta \) in most of the \( \Delta \) range, we will recover the generalized hyperbolic distribution. One can also argue that as we are looking for corrections to the Gaussian distribution, the convolution properties of the Gaussian function still hold approximately. Yet, it will not be exact, and therefore a smeared Hypatia distribution:

$$\Upsilon(m, \mu, \sigma^{SR}, \lambda, \zeta, \beta, a, n, v_0) = \frac{1}{\sqrt{v_0}} e^{-\frac{1}{2} (m)^2} \ast I(m, \mu, \sigma^{SR}, \lambda, \zeta, \beta, a, n) \quad (15)$$

can provide a better fit than \( I(m, \mu, \sigma, \lambda, \zeta, \beta, a, n) \) for some complicated cases with high statistics, without a real increase in the number of fit parameters (\( \sqrt{v_0} \) can be fixed in a somewhat arbitrary point at the start-up of the mass error distribution), although at the cost of a numerical convolution. The later can be done in RooFit by calling the RooFFTConvPdf class on top of the implementation of \( I(m, \mu, \sigma, \lambda, \zeta, \beta, a, n) \). If written this way, \( \sqrt{v_0} \) can be interpreted as an estimate of the mass resolution due to multiple scattering, \( \sigma^{SR} \) the dispersion caused by the spatial resolution of the detector given the kinematics of the final state, and the total resolution would be \( \sigma = \sqrt{v_0 + (\sigma^{SR})^2} \). Fig. 5 shows a fit of \( I(m, \mu, \sigma, \lambda, \zeta, 0, \infty, 1) \) and \( \Upsilon(m, \mu, \sigma^{SR}, \lambda, \zeta, 0, \infty, 1, 6.5 \text{ MeV/c}^2) \) to the simulated \( J/\psi \to \mu^+ \mu^- \) data, for the full sample without any kinematic constraint, i.e., where very low momentum (MS dominated) and very high momentum (hit resolution dominated) coexist. The fitting range corre-
Figure 6: Fit of $I(m, \mu, \sigma, \lambda, \zeta, 0, \infty, 1)$ (red dashed) and $\Upsilon(m, \mu, \sigma^{SR}, \lambda, \zeta, 0, \infty, 1, 6.5 \text{MeV}/c^2)$ (solid blue) to the simulated $J/\psi \rightarrow \mu^+\mu^-$ data, for the full sample without any kinematic constraint.

...responds to about eleven standard deviations. An excellent agreement between $\Upsilon(m, \mu, \sigma^{SR}, \lambda, \zeta, 0, \infty, 1, 6.5 \text{MeV}/c^2)$ and the simulated data is found. We failed to find any subsample of the $J/\psi \rightarrow \mu^+\mu^-$ data that could not be fitted by $\Upsilon(m, \mu, \sigma^{SR}, \lambda, \zeta, 0, \infty, 1, \nu_0)$.

6. Properties of $\lambda$

We have seen that using the Hypatia $\Upsilon$ distribution we can factorize the mass resolution modelling into MS and SR. The first part is governed by a resolution parameter $\sigma_0$ that can be estimated from the start-up of the per-event variance distribution. The second part is governed by the parameters $\zeta, \lambda, \sigma$ of the generalized hyperbolic distribution, where $\sigma$ corresponds to the resolution introduced by SR and where, empirically, we have found that $\zeta$ is in most cases small. In this chapter we will derive a physical meaning for $\lambda$, at least in the small $\zeta$ limit.

In the $\alpha = 0$ ($\rightarrow \zeta = 0$) limit case, the generalized hyperbolic distribution becomes a Student’s-t distribution, which can be understood as a marginalization
over a per-event variance density:

\[ \rho(v) \propto v^{\lambda-1} e^{-b/v} \]  

(16)

The mean \((M)\) and mode \((\mu)\) of \((16)\) are:

\[ M = \frac{b}{-\lambda - 1}; \quad \mu = \frac{b}{-\lambda + 1} \]  

(17)

thus

\[ \lambda = \frac{1 + M(v)/\mu(v)}{1 - M(v)/\mu(v)} < 0 \]  

(18)

and we can get an estimate of \(\lambda\) by looking at the per-event error (squared) distribution, and making the ratio of its mean and mode after shifting it to start at zero. But, we can further exploit this relation. From \((3)\) we can suppose that the per-event uncertainty will be strongly correlated with the particle momenta. Indeed, Fig. 6 supports this.

\[ \sigma_{i}^{SR} \approx c_{i} e \times p_{J/\psi,i} \]  

(19)

If this is the case, then \(M(v_{SR})/\mu(v_{SR}) \approx M(p_{J/\psi,i}^{2})/\mu(p_{J/\psi,i}^{2})\) and \(\lambda\) does not depend on detector effects, only on particle kinematics. This is an interesting result, because if we have a MC simulation with a good description of the momentum distribution of the particles in the lab frame, then the values of \(\lambda\) obtained in simulation should be reasonably valid for data, regardless of having an accurate description of detector simulation.

7. Mass constraints on intermediate resonances

Up to now we have described resolution effects. In more complicated cases, it is sometimes very useful to apply constraints on the decay products. For example, one can significantly improve the invariant mass resolution of \(B_{s}^{0} \rightarrow J/\psi\phi\) by constraining the two muons to have the PDG \(J/\psi\) mass \([9]\). This kind of approach, although great at improving the overall resolution, can also generate tails on the mass distribution, due to the photon energy radiated in
Figure 7: Per-event mass uncertainty versus $J/\psi$ momentum. Left: with multiple scattering. Right: only detector resolution.

Table 2: Results of a fit to $T(m, \mu, \sigma^{SR}, \lambda, 0, 0, 1, \sigma^{MS})$ for toy MC $J/\psi$ events smeared with different values of $a$ and $b$ in [3]. The parameter $\sigma^{MS}$ is fixed at the start-up of the per-event variance. The parameter $\lambda$ is found to be very stable with respect to smearing parameters, which are varied by 100%. However the uncertainty on $\lambda$ varies significantly, and increases with $a/b$.

| $a \times 10^{-3}$ | $b$ GeV/c$^{-1}$ | $\lambda$   | $\sigma^{MS}$ (MeV/c$^2$) | $\sigma^{SR}$ (MeV/c$^2$) |
|-------------------|------------------|-------------|--------------------------|--------------------------|
| 3                 | $2 \times 10^{-5}$ | $-2.40 \pm 0.06$ | 6.81                     | $4.75 \pm 0.02$          |
| 1.5               | $2 \times 10^{-5}$ | $-2.10 \pm 0.03$ | 3.53                     | $3.71 \pm 0.01$          |
| 6                 | $2 \times 10^{-5}$ | $-2.67 \pm 0.16$ | 13.3                     | $6.3 \pm 0.05$           |
| 3                 | $4 \times 10^{-5}$ | $-2.11 \pm 0.03$ | 7.07                     | $7.53 \pm 0.03$          |
| 3                 | $1 \times 10^{-5}$ | $-2.65 \pm 0.15$ | 6.67                     | $3.06 \pm 0.03$          |
the $J/\psi \rightarrow \mu^+\mu^-$ decay. Let’s consider a simple case in which the constraint is just applied by substituting the mass of the dimuon by the mass of the $J/\psi$.

$$m_c^2 = m_{J/\psi}^2 + m_{KK}^2 + 2 \left( \sqrt{m_{J/\psi}^2 + p_{J/\psi}^2} \sqrt{m_{KK}^2 + p_{KK}^2} - p_{J/\psi}p_{KK} \cos(\theta) \right)$$  

(20)

while ideally one would have wanted to implement:

$$m_{true}^2 = m_{J/\psi}^2 + m_{KK}^2 + 2 \left( \sqrt{m_{J/\psi}^2 + p_{J/\psi}^2} \sqrt{m_{KK}^2 + p_{KK}^2} - p_{J/\psi}p_{KK} \cos(\theta) \right)$$  

(21)

The difference $m_c^2 - m_{true}^2$ is not zero but rather function of the energy of the photons generated in the $J/\psi \rightarrow \mu^+\mu^-$ decay. This difference can be greater than zero, generating a tail on the right-hand side. Hence, even with a perfect detector resolution, the combination of the mass constraint and the photon radiation will generate non-Gaussian tails. In practice, this effect is expected to be small because the $J/\psi \rightarrow \mu^+\mu^-$ decays are selected with a mass window cut that allows only low energy photons. Otherwise, it can be partially accommodated either by the resolution model (e.g. [8]) or by using a CB-like tail on the right-hand side (i.e., using a double-sided Hypatia). A further discussion that goes beyond the scope of this paper is to provide models marginalized over per-event errors.

8. Conclusions

We have presented a generalization of the Crystal Ball function that gives an excellent description of mass resolution non-Gaussian tails. This function, that we name the Hypatia distribution, $I$, corresponds to a CB-like tail with a generalized hyperbolic core. The smeared Hypatia distribution, $\Upsilon$ provides an improved description of mass peaks and its fit parameters have clearer fundamental meaning, although the price to pay is a numeric convolution. A second, right-hand side CB-like tail can be added in cases where one has other non-resolution effects, such as those coming from constraining the mass of intermediate resonances of a decay.
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