Two-, Three- and n-body Phase Space

Curtis A. Meyer Carnegie Mellon University

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Introduction

This document describes how to generate two-body, three-body and *n*-body phase space events in the rest frame of the decaying particle. Two-body phase space produces events uniform in $\cos \theta$ and π with equal and opposite momenta. In the case of three-body decays, phase space is more complicated. The note first describes how to select final state momenta that satisfy the kinematic constraints of the decay, and the how to determine the probability of that event. Using this probability, it is possible to select events that uniformly populate three-body phase space. This uniformity can also be observed in the Dalitz plot, where purely phase space distributed events uniformly populate the Dalitz plot. It finishes with a generalization of the three-body discussion to that of *n*-body decays.

Two-body Decays

We consider the decay of a particle of mass m_A to two daughter particles of masses m_a and m_b where $m_A \ge m_a + m_b$. In the rest frame of m_A , the two daughter particles come out back to back with equal and opposite three momenta; \vec{p} and $-\vec{p}$, as shown in Figure 1. The magnitude of this three momentum, p, is given in terms of the three masses as in equation 1.



Figure 1: The two-body decay of particle A with mass m_A into daughters a and b with masses m_a and m_b respectively. The two daughters have equal and opposite three-momentum \vec{p} .

$$p = \frac{1}{2m_A} \sqrt{\left[m_A^2 - (m_a + m_b)^2\right] \left[m_A^2 - (m_a - m_b)^2\right]}.$$
 (1)

In the case of $m_a = m_b$, equation 1 simplifies to

$$p = \frac{1}{2}\sqrt{m_A^2 - 4m_a^2}.$$
 (2)

Equation 1 can also be written as in equation 3 which may be computationally more compact.

$$p = \frac{1}{2m_A} \sqrt{(m_A^2)^2 - 2m_A^2 (m_a^2 + m_b^2) + (m_a^2 - m_b^2)^2}, \qquad (3)$$

which may be computationally more compact.

A convenient way to compactly represent the two-body decay momentum is with the Källen or *triangle* function as defined in equation 4.

$$\lambda(a,b,c) = a^2 + b^2 + c^2 - 2ab - 2ac - 2bc \tag{4}$$

In analogy with equation 1, the Källen function can be written as in equation 5

$$\lambda(a,b,c) = \left[a - (\sqrt{b} + \sqrt{c})^2\right] \left[a - (\sqrt{b} - \sqrt{c})^2\right], \qquad (5)$$

and in analogy to equation 3 as in equation 6.

$$\lambda(a,b,c) = a^2 - 2a(b+c) + (b-c)^2$$
(6)

Using the Källen function, the decay momentum can be compactly written as

$$p = \frac{1}{2m_A} \sqrt{\lambda \left(m_A^2, m_a^2, m_b^2 \right)}.$$
 (7)

Given the magnitude of the decay momentum, the direction of the first particle is chosen be selecting a value of $\cos \theta$ uniformly between -1 and 1, and a value of ϕ uniformly between 0 and 2π . If rndm() produces a random number between 0 and 1, then:

$$\cos\theta = 2 r ndm() - 1 \tag{8}$$

$$\sin\theta = \sqrt{1 - \cos^2\theta_i} \tag{9}$$

$$\phi = 2\pi r \mathrm{ndm}(). \tag{10}$$

With the chosen values of $\cos \theta$ and ϕ , we can express the components of the particles momentum as follows.

$$p_{1x} = p \sin \theta \cos \phi$$

$$p_{1y} = p \sin \theta \sin \phi$$

$$p_{1z} = p \cos \theta$$

We then set $\vec{p}_2 = -\vec{p}_1$, so we have

$$p_{2x} = -p\sin\theta\cos\phi$$
$$p_{2y} = -p\sin\theta\sin\phi$$
$$p_{2z} = -p\cos\theta.$$

As we move forward with three-body decays, we will utilize the two-body decay formalism in the form of equation 7.

Three-body Decays

Decay Momentum

We have a particle at rest of mass m_A that decays to three final state particles of masses m_a , m_b and m_c , where the available decay energy Q is given as

$$Q = m_A - m_a - m_b - m_c \,. \tag{11}$$

For this decay as seen in the rest frame of A, the total three momentum must be zero,

$$0 = \vec{p}_a + \vec{p}_b + \vec{p}_c \,, \tag{12}$$

and the total energy of the final three particles must satisfy

$$(m_A c^2)^2 = \sum_{i=a,b,c} (\vec{p}_i \cdot \vec{p}_i c^2 + m_i^2 c^4) .$$
(13)

Schematically, this decay is shown in Figure 2. Because of the constraints imposed by equations 12 and 13, it is not possible to simply randomly select values for the three decay momentum, \vec{p}_a , \vec{p}_b and \vec{p}_c . A more sophisticated procedure using quasi two-body decays is needed.



Figure 2: The three-body decay of particle A with mass m_A into daughters a, b and c with masses m_a , m_b and m_c respectively. The sum of the three daughter's three-momentum adds to zero.

This more sophisticated procedure treats the three-body decay as a pair of two-body decays. First A decays to particles with invariant masses m_{ab} and m_c . Then the particle of mass m_{ab} decays to particles of masses m_a and m_b . This is shown in Figure 3. To perform this, a the mass m_{ab} is chosen uniformly between $m_a + m_b$ and $m_A - m_c$.

$$m_a + m_b \leq m_{ab} \leq m_A - m_c \tag{14}$$

Clearly, at the lower limit, the decay momentum, \vec{p}_a , of the particle of mass m_{ab} will be zero and at the upper limit, the decay momentum \vec{p}_{ab} of the initial decay to particles of mass m_{ab} and m_c will also be zero. For all other values of m_{ab} , both of these momenta will be non zero.

From equation 7 we have the magnitude of \vec{p}_{ab} given in equation 15.

$$p_{ab} = \frac{1}{2m_A} \sqrt{\lambda \left(m_A^2, m_{ab}^2, m_c^2\right)}$$
(15)

In the rest frame of the particle of mass m_{ab} , the magnitude of the decay momentum \vec{p}_a is given by equation 16.

$$p_a = \frac{1}{2m_{ab}} \sqrt{\lambda \left(m_{ab}^2, m_a^2, m_b^2\right)}$$
(16)



Figure 3: The three-body decay of particle A with mass m_A as a pair of two-body decays. The particle of mass m_A first decays into daughters of mass m_{ab} and m_c . The particle of mass m_{ab} subsequently decays to daughters of masses m_a and m_b .

Choosing $\cos \theta_{ab}$ uniformly between -1 and 1 and ϕ_{ab} uniformly between 0 and 2π , we have in the rest frame of A

$$\vec{p}_{ab} = (p_{ab} \sin \theta_{ab} \cos \phi_{ab}, p_{ab} \sin \theta_{ab} \sin \phi_{ab}, p_{ab} \cos \theta_{ab})$$

$$\vec{p}_{c} = -(p_{ab} \sin \theta_{ab} \cos \phi_{ab}, p_{ab} \sin \theta_{ab} \sin \phi_{ab}, p_{ab} \cos \theta_{ab}).$$
(17)

In the rest frame of the particle of mass m_{ab} , we throw $\cos \theta_a$ and ϕ_a as above, which then yields

$$\vec{p}_{a} = (p_{a} \sin \theta_{a} \cos \phi_{a}, p_{a} \sin \theta_{a} \sin \phi_{a}, p_{a} \cos \theta_{a})$$

$$\vec{p}_{b} = -(p_{a} \sin \theta_{a} \cos \phi_{a}, p_{a} \sin \theta_{a} \sin \phi_{a}, p_{a} \cos \theta_{a}).$$
(18)

To express these latter two momentum in the rest frame of A, we need to perform a Lorentz boost along the direction of \vec{p}_{ab} using

$$\vec{\beta} = \frac{\vec{p}_{ab}c}{\vec{p}_{ab} \cdot \vec{p}_{ab} c^2 + m_{ab}^2 c^4} \,. \tag{19}$$

This procedure yields a set of moment for the three daughter particles as seen in the rest frame of A that satisfy the constraints given in equations 12 and 13. Unfortunately, the are not generated uniformly in three-body phase space, We assumed that all possible values of m_{ab} have the same probability, while for a phase space distribution, this is not true.

Dalitz Plots

As noted at the end of previous section, we can generate a set of three momentum that satisfies our kinematic constraints, but more work is needed to uniformly populate three-body phase space. In order to do this, we will consider that the Dalitz plots of our decay of particle A to particles a, b and c. The Dalitz plot show invariant masses of pairs of particles plotted against each other. Given four vectors for the three daughter particles, \mathcal{P}_a , \mathcal{P}_b , \mathcal{P}_c , there are three possible pairs of invariant masses

$$m_{ab}^2 = \left(\mathcal{P}_a + \mathcal{P}_b\right)^2 \tag{20}$$

$$m_{ac}^2 = \left(\mathcal{P}_a + \mathcal{P}_c\right)^2 \tag{21}$$

$$m_{bc}^2 = \left(\mathcal{P}_b + \mathcal{P}_c\right)^2. \tag{22}$$

Based on the kinematics, there is an overall constraint between all the of masses given in equation 23.

$$m_A^2 + m_a^2 + m_b^2 + m_c^2 = m_{ab}^2 + m_{ac}^2 + m_{bc}^2$$
(23)

Given this constraint, there are only two independent pairs of invariant masses, the third can always be determined from equation 23. Hence the plots of one pair's invariant mass versus another. A Dalitz plot shows the squares of invariant masses are plotted agains each other, where one of the three possible Dalitz plots is sketched in Figure 4.

For that shown, m_{ac}^2 is plotted against m_{ab}^2 . The minimum possible value for these is just the sum of the masses, while the maximum possible value is related to the total mass minus the remaining mass.

$$(m_a + m_b)^2 \leq m_{ab}^2 \leq (m_A - m_c)^2$$
 (24)

$$(m_a + m_c)^2 \leq m_{ac}^2 \leq (m_A - m_b)^2$$
 (25)

$$(m_b + m_c)^2 \leq m_{bc}^2 \leq (m_A - m_a)^2$$
 (26)

The kinematic limits given by these are shown as the dashed lines on the Dalitz plot. If the entire retangular region defined by the kinematic limits were allowed, then the momenta we generated in the previous section would be uniform in phase space. Unfortunately, the actual allowed kinematics are defined by an oval region inside the boundaries defined by the limits. This region is shown schematically as the solid oval shaped region in Figure 4. Rather, for a given m_{ab}^2 , the pase space is limited by the bottom and top of the shaded region, which is smaller than the height of the box. At the left and right edges, that height is zero, while it is maximum somewhere near the center of the box. To uniformly populate phase space, we need to choose m_{ab}^2 with a probability proportional to the height of the shaded region for that value of m_{ab} .



Figure 4: One of three possible Dalitz plots for the decay of A to a, b and c. This plots the invariant mass of a and c against the invariant mass of a and b. Kinematic limits are show as dotted lines, while the allowed phase space is shown as the solid oval shape.

The height of that line can be shown to be proportional to the product of the two decay momentum as given in equations 15 and 16. To make sure that when we take the product, we have a value that is between 0 and 1, we normalize that product by the maximum values of those two momentum. These occur at the left and right edges of the allowed region in the Dalitz plot.

$$p_{ab}^{max} = \frac{1}{2m_A} \sqrt{\lambda (m_A^2, (m_a + m_b)^2, m_c^2)}$$
$$p_a^{max} = \frac{1}{2(m_A - m_c)} \sqrt{\lambda ((m_A - m_c)^2, m_a^2, m_b^2)}$$

Putting everything together, we get the scaled weight for our choice of m_{ab} is given by equation 27.

$$w_{ab} = \frac{m_A - m_c}{m_{ab}} \sqrt{\frac{\lambda(m_A^2, m_{ab}^2, m_c^2) \lambda(m_{ab}^2, m_a^2, m_b^2)}{\lambda(m_A^2, (m_a + m_b)^2, m_c^2) \lambda((m_A - m_c)^2, m_a^2, m_b^2)}}.$$
(27)

The weight is clearly 0 for the two limits, $m_a = M - m_3$ and $m_a = m_1 + m_2$ and has a value between0 and 1 those two limits. If we know that maximum value of w_{ab} , w_{ab}^{max} , then the probability of a particular value of m_{ab} is given by

$$P(m_{ab}) = \frac{w_{ab}}{w_{ab}^{max}}.$$
(28)

Phase Space Weighting

We could analytically try to find the value of m_{ab} that yields the maximum of value of equation 27. Essentially, we would set

$$\frac{dw_{ab}}{dm_{ab}} = 0$$

and solve for m_{ab} . Unfortunately, one needs to solve a fifth order equation in m_{ab} and there are no obvious tricks to solve it. It is likely that only a numerical solution can be found. To explore this, we built a toy model where a particle A decays to $\eta \pi^+ \pi^-$. The mass of A, $m_{\eta\pi\pi}$ is then chosen uniformly between $m_{\eta} + m_{\pi} + m_{\pi}$ and $2.5 \, GeV/c^2$. For each value of $m_{\eta\pi\pi}$, we then sampled 10000 values of $m_{\pi\pi}$ between the limits of $2m_{\pi}$ and $m_{\eta\pi\pi} - m_{\eta}$ and identified the the value of $m_{\pi\pi}$ that yielded the maximum value of equation 27. In Figure 5(left) we plot $(m_{\pi\pi})_{max}$ versus $m_{\eta\pi\pi}$. The data are very close to being linear, and can be well described by the equation

$$(m_{\pi\pi})_{\rm max} = 0.624523 \, m_{\eta\pi\pi} - 0.250057 \, .$$

We can see that the linear curve, shown as the red line, does not exactly follow the data, but is very close. In Figure 5(right) is shown the difference between the true maximum value and that predicted by the linear fit. At the left hand edge, the prediction is small by about 1%, then for larger values of $m_{\eta\pi\pi}$ oscillates between over and under predicting, always by amounts that are smaller than 1%. Thus, except for values of $m_{\eta\pi\pi}$ with 2 to 3% of threshold, the linear model can safely predict the value of $m_{\pi\pi}$ that would yield the maximum weight.

Generalizing to n-body Decays

The procedure described in the earlier section on three-body decays can be fairly easily generalized to more than three particles. In the general case, we would have a system of mass M that decays into n daughter particles of masses m_1, m_2, \dots, m_n where by definitions,

$$M > m_1 + m_2 + m_3 + \dots + m_n \,. \tag{29}$$

Following the example of the three-body decay, we have a particle at rest of mass M that decays to N final state particles of masses m_1, m_1, \cdots and m_n , where the available decay energy Q is similar to equation 11 where

$$Q = M - \sum_{i=1}^{n} m_i \,. \tag{30}$$

For this decay as seen in the rest frame of M, as in equation 12, the total three momentum must be zero,

$$0 = \sum_{i=1}^{n} \vec{p}_{i}, \qquad (31)$$



Figure 5: Left: a linear fit to the data for the value of $m_{\pi\pi}$ that gives the maximum weight versus the mass of the three-meson system, $m_{\eta\pi\pi}$. The data are reasonable well described by the line $(m_{\pi\pi})_{\text{max}} = 0.624523 m_{\eta\pi\pi} - 0.250057$. Right: the difference between the value of m_{12} that gives the maximum weight and the value predicted by the linear model shown in Fig. 5. As with the previous figure, the left-hand plot is for 100 samples and the right-hand plot is for 10,000 samples. The model undershoots the true value near threshold in $m_{\eta\pi\pi}$, and in fact predicts m_{12} values that are smaller than the mass of two pions.

and as in equation 13, the total energy of the final three particles must satisfy

$$(Mc^2)^2 = \sum_{i=1}^n \left(\vec{p}_i \cdot \vec{p}_i c^2 + m_i^2 c^4 \right).$$
(32)

Choosing Invariant Masses

The general procedure starts by choosing a consistent set of multi-particle invariant masses that would correspond to progressively lighter sets of particles. The heaviest would be a mass that could decay to m_1 through m_{n-1} that would recoil against m_n .

$$\sum_{i=1}^{n-1} m_i \leq m_a \leq M$$

In the rest system of M, the magnitude of the decay momenta of m_a and m_n would be given as

$$p_a = \frac{1}{2M} \sqrt{\lambda(M^2, m_a^2, m_n^2)}.$$
(33)

Next, we consider the decay of m_a to a system with mass m_b between $\sum_{i=1}^{n-1} m_i$ and m_a ,

$$\sum_{i=1}^{n-2} m_i \leq m_b \leq m_a \,,$$

where is the rest frame of m_a , the momentum of both m_b and m_{n-1} is given as

$$p_b = \frac{1}{2m_a} \sqrt{\lambda(m_a^2, m_b^2, m_{n-1}^2)} \,. \tag{34}$$

This procedure continues until we reach the last two-body system. If we refer to this as m_q , we know this decays into m_1 and m_2 with decay momentum

$$p_q = \frac{1}{2m_q} \sqrt{\lambda(m_q^2, m_1^2, m_2^2)} \,. \tag{35}$$

This procedure yields a set of n-1 invariant masses: m_a, m_b, \cdots and m_q as well as their decay momenta in the relevant rest frame: p_a, p_b, \cdots and p_q . As a computational note, it is advisable to make sure that none of the decay momentum are less than or equal to zero. If that happens, it is suggested you choose a different mass for the decaying particle.

Choosing Helicity-frame Angles

For each of the n-1 decays that we calculated in the previous section, we now want to choose a direction of the unstable daughter particle in the helicity frame of decaying particle. This procedure follows what was done in equations 17 and 18. We choose $\cos \theta_i$ to be uniform between -1 and 1 and ϕ_i to be uniform between 0 and 2π as per equations 8 and 10. Doing this, we can create a list vector particle momenta as expressed in a series of rest frames.

For the case of M decaying to m_a and m_n , the momentum vectors are in the rest frame of M and given as

$$\vec{p}_{a} = (p_{a} \sin \theta_{a} \cos \phi_{a}, p_{a} \sin \theta_{a} \sin \phi_{a}, p_{a} \cos \theta_{a})$$

$$\vec{p}_{n} = -(p_{a} \sin \theta_{a} \cos \phi_{a}, p_{a} \sin \theta_{a} \sin \phi_{a}, p_{a} \cos \theta_{a}).$$
(36)

In the rest frame of m_a , we have the momentum vectors for m_b and m_{n-1} . These are given as

$$\vec{p}_b = (p_b \sin \theta_b \cos \phi_b, p_b \sin \theta_b \sin \phi_b, p_b \cos \theta_b)$$

$$\vec{p}_{n-1} = -(p_b \sin \theta_b \cos \phi_b, p_b \sin \theta_b \sin \phi_b, p_b \cos \theta_b).$$
(37)

This continues until we get to the last two-body decay in the rest frame of the q^{th} mass. Here we have

$$\vec{p}_{2} = (p_{q}\sin\theta_{q}\cos\phi_{q}, p_{q}\sin\theta_{q}\sin\phi_{q}, p_{q}\cos\theta_{q})$$

$$\vec{p}_{1} = -(p_{q}\sin\theta_{q}\cos\phi_{q}, p_{q}\sin\theta_{q}\sin\phi_{q}, p_{q}\cos\theta_{q}).$$
(38)

Boosting to a Single Frame

At this point, we have a set of decay momenta magnitudes in various reference frames. In each of those frames, after we have choosen a direction for the back-to-back pair of particles, and then boost them back into the rest frame of their mother particle. In this procedure, we start with the very last decay where m_q decays into m_1 and m_2 and define a boost as in equation 19 that will transform the momenta of the two particles into the moving frame of q.

$$\vec{\beta}_1 = \frac{\vec{p}_q c}{\vec{p}_q \cdot \vec{p}_q c^2 + m_q^2 c^4} \,. \tag{39}$$

We now perform a Lorentz boost along $\vec{\beta}_1$ to yield $(\vec{p}_1)^{b_1}$ and $(\vec{p}_2)^{b_1}$ in the moving frame of q. At this point we have the particle momenta for the first three particles in the rest frame of q: $(\vec{p}_1)^{b_1}$, $(\vec{p}_2)^{b_1}$ and \vec{p}_3 . We now compute the factor $\vec{\beta}_2$ that will boost these three momenta into the rest frame of particle q-1.

$$\vec{\beta}_2 = \frac{\vec{p}_{q-1} c}{\vec{p}_{q-1} \cdot \vec{p}_{q-1} c^2 + m_{q-1}^2 c^4} \,. \tag{40}$$

Applying this boost to the previous three momenta, we will have the momenta of the first four particles in this frame: $(\vec{p}_1)^{b2}$, $(\vec{p}_2)^{b2}$, $(\vec{p}_3)^{b2}$ and \vec{p}_4 . We continue this procedure until all n particles are in the rest frame of M. We now have a set of n vector momenta for the n final state particles all in the same frame.

Computing Event Weights

While we have a valid set of final state momenta, the event has not been selected uniformly in phase space. We now need to determine a relative weight for this, if we generate a set of events and weights, the weighted events would be uniform in n-body phase space. This procedure follows what was done in equation 27, but is generalized from 3 to n particles. Generalizing equation 27, which are just products of decay momentum.

The factors in the numerator are just the products of the actual decay momenta as evaluated in equations 33 through equation 35.

$$n_{a} = \frac{1}{2M} \sqrt{\lambda(M^{2}, m_{a}^{2}, m_{n}^{2})}$$
$$n_{b} = \frac{1}{2m_{a}} \sqrt{\lambda(m_{a}^{2}, m_{b}^{2}, m_{n-1}^{2})}$$

which continues until we get to the final decay, where we have

$$n_q = \frac{1}{2m_q} \sqrt{\lambda(m_q^2, m_2^2, m_1^2)}$$

The denominator is the product of decay momenta that are based on the minimum and maximum possible masses for each two-body decays we considered. For the first decay of M to m_a and m_m , the minimum values of m_a is $\sum_{i=1}^{n-1} m_i$, so the term will be

$$d_a = \frac{1}{2M} \sqrt{\lambda \left(M^2, \left[\sum_{i=1}^{n-1} m_i \right]^2, m_n^2 \right)}.$$

For the next decay, the maximum value for the m_a is $M - m_n$ and the minimum value for m_b is $\sum_{i=1}^{n-2} m_i$, so the factor will be

$$d_b = \frac{1}{2(M-m_n)} \sqrt{\lambda \left([M-m_n]^2, \left[\sum_{i=1}^{n-2} m_i \right]^2, m_{n-1}^2 \right)}.$$

This procedure continues with

$$d_c = \frac{1}{2(M - m_n - m_{n-1})} \sqrt{\lambda \left(\left[M - m_n - m_{n-1} \right]^2, \left[\sum_{i=1}^{n-3} m_i \right]^2, m_{n-2}^2 \right)},$$

until we get to the decay of the last pair of particles,

$$d_q = \frac{1}{2(M - \sum_{i=3}^n m_i)} \sqrt{\lambda \left(\left[M - \sum_{i=3}^n m_i \right]^2, m_1^2, m_2^2 \right)}.$$

Putting all of this together, the relative weight for this event will be

$$w_e = \frac{n_a \cdot n_b \cdots n_q}{d_a \cdot d_b \cdots d_q} \tag{41}$$

Weighting the events by this relative weight will generate distributions of events that are uniformly weighted in phase space. If one would like to choose a set of events that is itself uniformly distributed in phase space, then one needs to determine the maximum value of w_{max} for a given M, m_1 , m_2 , \cdot , m_n . We can then produce a normalized event weight,

$$w_e^{norm} = \frac{w_e}{w_{max}},$$

which will have a value between 0 and 1. One can just compare the normalized weight to a uniformly distributed random number and keep the event if the normalized weight is larger than the random number.

As we saw earlier in the three-body decay, there is no easy analytic way to determine w_{max} . We found a cute trick for a specific case that let us interpolate this over a range of M values for a particular decay, but things may not be so simple in the *n*-body case. Generally, one needs to step through the range of possible M values being considered, and brute force evaluate equation 41 for a reasonably large number of events. We then assume that the maximum value found is w_{max} . These values of w_{max} over a range of values of M and then creating an interpolation function give the correct w_{max} for a given M.