Notes on Phase Space
M. R. Shepherd
March 5, 2024

Motivation

Consider a typical photoproduction reaction at GlueX energies $\gamma p \to UL$ that is commonly illustrated as t-channel production of say a meson U at an "upper vertex" recoiling against a baryon L at the "lower vertex." Let's assume U and L each decay into u and ℓ stable particles, respectively. Let the phase space for the reaction is then given by $d\Phi_n(E_{cm}; p_1, \ldots, p_n)$ where $n = u + \ell$. The differential cross section for the reaction is then proportional to

$$d\sigma \propto |\mathcal{M}|^2 \times d\Phi_n(E_{cm}; p_1, \ldots, p_n). \tag{1}$$

In the above expression, the square of the matrix element $|\mathcal{M}|^2$ contains "the physics" that we are often trying to study, *e.g.* resonances that generate a peak in some invariant mass distribution m_{12}. In the absence of any interesting physics then $|\mathcal{M}|^2 = 1$, and it is generally useful to understand how phase space populates the various kinematic variables commonly used in data analysis, e.g., invariant mass. Furthermore if we intend to develop a model for $\mathcal{M}$ that we may want to use in an amplitude analysis then in order to performance an accurate Monte-Carlo integration of the model we must have a sample of events that are distributed according to this phase space.

The Problem: the Monte-Carlo generators that are commonly in use in the GlueX software stack do not properly generate n-body phase space in the above reaction. Specifically, the dependence on invariant mass of the particles at the upper and lower vertex is not phase space and often events are generated with an exponential t distribution, which is physics and not a byproduct of n-body phase space. Up until now this has not been a significant limiting factor as amplitude analyses are often performed in bins of invariant mass or by selecting narrow regions of invariant mass. Analyses can also be binned in t and the Monte-Carlo is tuned to generate a t-distribution that matches the data – in such cases the "phase space" sample is really phase space weighted by some physics that is not included in the model that is being fit to the data. However, if one intends to migrate to a fitting strategy where larger regions of invariant mass are fit, then it is important to develop generators that properly distribute the events according to phase space across these regions. This includes a practical challenge: a simple n-body phase space generator will not strongly populate regions that are heavily populated by the physics, *e.g.,* at low t. The goal is then to develop a generator suitable for doing importance sampling of the Monte-Carlo model in amplitude analysis. One should be able to seed the generator with resonance shapes at the upper and lower vertices as well as a t distribution, but it should produce events that can be weighted to be distributed according to n-body phase space.

Populating phase space

The general problem of efficiently generating n-body phase space has been solved and documented many years ago. To make use of importance sampling though, we would like to be able to draw the invariant masses at the upper and lower vertices from some defined distribution, like a sum of Breit-Wigner functions, which we can then re-weight to be uniform in phase space. In order to do this, we need to first determine how n-body phase space depends on the invariant mass at the upper and lower vertices.

It can be shown [1] that the integral over n-body Lorentz-invariant space space depends only on the center-of-mass energy and the masses of the stable particles in the final state.

$$R_n(\sqrt{s}, m_1, \ldots, m_n) = \int d\Phi_n, \tag{2}$$

and such phase space integrals can written in terms of integrals over a smaller-dimensional phase space:

$$R_n(\sqrt{s}; m_1, \ldots, m_n) = \int R_{n-\ell+1}(\sqrt{s}; M_\ell, m_{\ell+1}, \ldots, m_n) R_\ell(M_\ell; m_1, \ldots, m_\ell)\; dM_\ell^2, \tag{3}$$

where

$$M_\ell^2 = \left|\sum_{i=1}^{\ell} p_i\right|^2 \tag{4}$$

is the invariant mass squared of the ℓ particles produced at the lower vertex. Likewise, let's define M_u as the invariant mass at the upper vertex:

$$M_u^2 = \left|\sum_{i=\ell+1}^{n} p_i\right|^2 . \tag{5}$$

We can split the first term in the integral $R_{n-\ell+1}$ into an integral over $R_{n-\ell} = R_u$ and R_2 so that we have

$$R_n = \iint R_2(\sqrt{s}; M_\ell, M_u) R_u(M_u, m_{\ell+1}, \ldots, m_n) R_\ell(M_\ell; m_1, \ldots, m_\ell)\ dM_\ell^2 dM_u^2. \tag{6}$$

Using the fact that $dM^2 = 2MdM$ we see the distribution of phase space across the two invariant masses is then given by

$$\frac{d^2 R_n}{dM_\ell dM_u} = 4M_u M_\ell R_2(\sqrt{s}; M_\ell, M_u) R_u(M_u, m_{\ell+1}, \ldots, m_n) R_\ell(M_\ell; m_1, \ldots, m_\ell). \tag{7}$$

This now casts the problem in terms of the masses at the upper and lower vertex, which is useful if we desire to implement importance sampling to concentrate events in regions of M_ℓ and M_u. However, to go beyond this we need to consider how to write R_u and R_ℓ.

Generating N-body phase space

Following the notes James [1], let's make a brief digression to discuss how to express multi-body phase space in terms of two-body phase space. Assume that you have N particles, each with mass m_i and four-momentum p_i. We can define the invariant mass of a subset of these particles as

$$M_j^2 = \left|\sum_{i=1}^{j} p_i\right|^2 . \tag{8}$$

Working in the center of mass, the total energy available for the decay is then M_N, and we can picture the decay as a chain of sequential two-body decays. At the first level the masses of the two particles are m_N and M_{N-1}, *i.e.,* the rest mass of the N^{th} particle and the invariant mass of all the other particles. Then at the second level M_{N-1} decays into m_{N-1} and M_{N-2}, and so on. The result one can write R_N with repeated use of Eq. 3 (choosing $\ell = 2$) as

$$R_N = \int dM_{N-1}^2 \ldots \int dM_2^2 \prod_{i=1}^{N-1} R_2(M_{i+1}; m_i, m_{i+1}). \tag{9}$$

As above, we can change variables from $M^2 \to M$ and write, equivalently,

$$R_N = \int \ldots \int \frac{1}{2m_1} \prod_{i=1}^{N-1} \{2M_i R_2(M_{i+1}; M_i, m_{i+1})\}\ dM_{N-1} \ldots dM_2. \tag{10}$$

There are a variety of ways to write the integral of two-body phase space:

$$R_2(M; m_1, m_2) = \frac{p_{\text{cm}}}{4\pi M} = \frac{\sqrt{\lambda(M^2, m_1^2, m_2^2)}}{8\pi M^2}, \tag{11}$$

where $p_{\rm cm}$ is the magnitude of the momentum of one of the particles in the center-of-mass frame. This is often expressed in terms of the Källén function which has a variety of representations. One relatively compact form is

$$\lambda(a,b,c) = (a-b-c)^2 - 4bc. \tag{12}$$

Using Eqs. 11 and 10 we can write an equivalent expression for R_N:

$$R_N = \int \dots \int \frac{1}{M_N} \prod_{i=2}^{N} \left\{ \frac{1}{2\pi} p_{{\rm cm};i} \right\} \, dM_{N-1} \dots dM_2, \tag{13}$$

where $p_{{\rm cm};i}$ is the center-of-mass momentum for the decay $M_i \to m_i + M_{i-1}$. The above equation provides the recipe for generating N body phase space decays of a particle of mass M_N. One throws invariant masses $M_2, \dots, M_{N-1}$ and then weights each event by the product of the center-of-mass momenta of the individual decays. The factors of 2π and M_N are constant and can be ignored in generation. This technique, and the procedure discussed below for choosing the M_i, is known as the "Raubold-Lynch method" and is documented extensively in Ref. [1]. This is also the procedure implemented in the ROOT class `TGenPhaseSpace` which is the basis for the `NBodyPhaseSpaceGenerator` that appears in the GlueX software stack.

Special care must be taken in throwing the invariant masses. The kinematic limits are

$$M_{i-1} + m_i < M_i < M_{i+1} - m_{i+1}. \tag{14}$$

However, generating M_i sequentially based on some value of M_{i+1} will lead to bias. The set $M_2, \dots, M_{N-1}$ must all be generated independently. If the specific values of M_i do not land within the kinematic boundary, then *the entire set must be discarded* and regenerated. One can write a less restrictive bound on M_i:

$$\sum_{j=1}^{i} m_j < M_i < M_N - \sum_{j=i+1}^{N} m_j \tag{15}$$

This boundary now only depends on the fixed initial mass of the system and the masses of the N particles in the final state and none of the other generated M_i. One can choose M_i by selecting a random number r_i from $0 \to 1$ and then setting

$$M_i = r_i \left(M_N - \sum_{j=i+1}^{N} m_j \right) + \sum_{j=1}^{i} m_j, \tag{16}$$

where the term in parentheses is the difference between the maximum and minimum values of M_i. One then chooses a set of $N-2$ values of r_i independently. It can be shown that the more restrictive kinematic limits of Eq. 14 can be met if and only if the r_i are in ascending order. This can be accomplished by discarding every random set that is not ordered (which would be very inefficient for large N) or by reordering the r_i which can be done without bias. The latter approach is used and results in efficient generation of N-body phase space.

Before returning to the problem of GlueX Monte-Carlo generation it is worth emphasizing a few key features of N-body phase space generators.

- Generation is done a series of sequential two-body decays, where one of the two bodies is a stable particle and the other is a "particle" formed from all remaining particles.
- The weight of each event is given by the product of the center-of-mass momentum of all of the two-body decays. Weighted events properly populate N-body phase space. Alternatively, one can use an accept/reject algorithm on the weight to generate N-body phase space events with a weight of unity.
- The allowable region for generating the invariant masses in the intermediate steps is defined in terms of the total available energy M_N and the masses of all of the final state particles. (See Eq. 16.)

We will see that this last point is problematic when trying embed the results of a phase space generator into a higher-dimensional problem.

Populating phase space for a typical GlueX reaction

Let's now take the result expressed in Eq. 13 and use it to rewrite R_u and R_ℓ in Eq. 7. Neglecting constant factors of 2π, we have (for $n > 2$)

$$\frac{d^{n-2}R_n}{dM_\ell dM_u(dM_{\ell;2}\ldots dM_{\ell;\ell-1})(dM_{u;2}\ldots dM_{u;u-1})} \propto R_2(\sqrt{s}; M_\ell, M_u)\left[\prod_{i=2}^{\ell} p_{\mathrm{cm};\ell;i}\right]\left[\prod_{i=2}^{u} p_{\mathrm{cm};u;i}\right], \tag{17}$$

where we have used $M_\ell; i$ and $p_{\mathrm{cm};\ell;i}$ to index the center-of-mass momenta and intermediate invariant mass at the i^{th} decay step of the lower vertex and similarly for the upper vertex.

This now provides a recipe for populating phase space. We need to independently draw the $n-2$ intermediate invariant masses M_ℓ, M_u, $M_{\ell;2},\ldots,M_{\ell;\ell-1}$, $M_{u;2},\ldots,M_{u;u-1}$ and then weight the event by the RHS of Eq. 17. As with before, we should draw the masses from a range that is defined independently of any of the other masses and keep only events that land within the kinematic boundary. In a similar fashion as Eq. 15 we can write loose limits that are suitable for drawing the set of invariant masses.

$$\sum_{j=1}^{\ell} m_j^\ell < M_\ell < \sqrt{s} - \sum_{j=1}^{u} m_j^u \tag{18}$$

$$\sum_{j=1}^{i} m_j^\ell < M_{\ell;i} < \sqrt{s} - \sum_{j=1}^{u} m_j^u - \sum_{j=i+1}^{\ell} m_j^\ell \tag{19}$$

Here we have used $m_j^{\ell(u)}$ to refer to the mass of the j^{th} particle at the lower (upper) vertex. The limits on M_u and $M_{u;i}$ can be likewise be obtained by changing $\ell \to u$ in the above equations. One a full set of invariant masses are generated then they must be checked to ensure they land within the kinematic limits. If they do not, an entire new set of masses must be chosen. *In the relations above we see that proper generation of the upper vertex invariant masses depends on knowing the masses of the final state particles at the lower vertex and vice versa.*

How to do it the wrong way...

Equation 17 suggests a tempting solution. One could draw M_ℓ and M_u uniformly between the bounds provided by Eq. 18. Then one could use two standard phase space generators to generate ℓ-body and u-body phase space at the lower and upper vertex. Each of these generators would return one of the weights in brackets on the RHS of Eq. 17. One could then apply an additional weight of $R_2(\sqrt{s}; M_\ell, M_u)$, and the result would be distributed according to overall n-body phase space. However, *this is not correct* because the generation of invariant masses in the subsequent ℓ-body or u-body phase space is biased by the choice of M_ℓ and M_u. Each of those generators will choose masses according to limits specified by Eq. 15, which is more restrictive than the limits in Eq. 19. The result is that if ℓ or u are greater than 2 then the distribution of M_ℓ and M_u will be biased. (In cases where ℓ and u are equal to two there are no subsequent invariant masses to randomly choose beyond M_ℓ and M_u.)

References

[1] F. James, "Monte Carlo Phase Space," Lectures given in the Academic Training Program of CERN, CERN 68-15 (1968).