Gauss Integration over Relativistic 3–Body Phase Space for 1–Dimensional Distributions of $2 \rightarrow 3$ Reaction

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Abstract

We present the analysis of the phase space geometry of $2 \rightarrow 3$ reaction for the general case of nonzero and unequal particle masses. Its purpose is to elaborate an alternative approach to the problem of integration over phase space which does not exploit the Monte Carlo principle. The fast and effective algorithm of integration based on Gauss method is developed for treating 1–dimensional distributions in two–particle invariant variables. The algorithm is characterized by significantly improved accuracy and it can meet requirements of interactive processing.
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1 Introduction

Analysis of kinematics and integration over phase space of a reaction are basic problems which are common to both experimental and theoretical high energy physics.

In the theoretical field the integration over phase space, for example, is needed to make theoretical predictions confronting the experimental measurements and to provide fitting of experimental data. Besides, a lot of pure theoretical investigations such as statistical models of nuclear reactions, calculation of unitarity corrections, etc., rely upon the integration over phase space of final state.

At all stages of the modern experiments from designing the experimental device to determination of its characteristics and, finally, data treatment, various kinematic tools, including integration packages, are used for simulation of events, determination of acceptances and making corrections to the measured distributions.

The Monte–Carlo integration principle built into the most elaborate GEANT3 [1] system for modeling experimental devices provides subroutines for integration purposes which are universal in the sense that any number of final particles can be treated. The time–of–run and precision characteristics of the Monte-Carlo based programs are not so crucial here since, for example, determination of acceptances and other device properties is the direct problem. At the same time the majority of theoretical applications are in the field of inverse problems — to find out physical parameters some kernel built of theoretical model and device characteristics (angles, momentum cuts, etc.) must be inverted when applied to the experimental results. It is well–known that the precision requirements for determination of the kernel properties which obviously include the procedure of integration over a domain of phase space are much more stringent than in the case of the direct problem.

In contrast with experimental applications where the integration is usually being performed with empty phase space the theoretical ones operate with complicated model amplitude which itself needs considerable time for processing. The time–of–run properties of the integration routines become especially vital for creating an interactive utilities for data bases and routines for data treatment (like phase shift analysis package SAID [2]).

Therefore, development of an alternative to Monte–Carlo methods of phase space integration even at the price of loosing universality in respect to the number of particles seems to be important.

Up to now alternative to Monte–Carlo methods are used only in the simplest case of \( 2 \rightarrow 2 \) reactions (the phase space is effectively 1–dimensional and, therefore, any integration
method, in fact, applies well in this occasion). Appearing from time to time papers like [3, 4], heavily rely on simplification of phase space geometry due to equal masses or specific amplitude of the reaction.

Meanwhile the case of the $2 \rightarrow 3$ reactions which importance many times was stressed since the work [5] by Chew and Low admits almost equally complete elaboration as in the $2 \rightarrow 2$ case. The ground for such a statement might be found in the many-years-long investigations the results of which are summarized in the monographs [6, 7]. Of course, the full-scale realization of a classical integration scheme for all choices of variables of $2 \rightarrow 3$ reactions and at any kind of kinematical constraints will require an approach of artificial intelligence and computers of extraordinary power.

The main goal of the present research is the demonstration of the principal feasibility of the classical integration approach. This will be done by developing the integration algorithm for treating total cross sections and 1-dimensional distributions in two-particle invariant variables for the general case of unequal particle masses of $2 \rightarrow 3$ reaction. This problem requires extended analysis of the geometry of the phase space of the reaction.

Fortunately, almost all the necessary examinations and hints might be found in various particular chapters of the books [6, 7] — one needs to gather carefully crucial conclusions and put considerations into purposive line of algorithm. Certainly, all the key relations must be expanded in exact analytic form to provide solid programming. The presentation of principle answers is an incidental goal of the paper.

Another principle goal is to find a way beyond the standard integration algorithms. The extremely effective Gauss integration method is proved to be quite feasible in the considered case.

The paper is organized as follows. Sect. 2 introduces basic notations and the starting form of the phase space integral. The central Sect. 3 is devoted to analysis of necessary elements of geometry of the phase space. To avoid burst of formulae most of explicit expressions are concentrated in Appendix. The iterated form of the phase space integral is introduced in Sect. 4 where the most important properties of the integrated expressions are investigated to motivate the applicability of Gauss method. The specific characteristics of the FORTRAN implementation of the results of the previous sections are considered in Sect. 5. The perspectives of further development of the considered approach are discussed in Sect. Conclusion.
2 General Definitions

2.1 Variables

We consider the reaction where initial particles $a$ and $b$ create 3 particles in the final state. We use the notations for momenta of particles and for the set of basic variables which are very close to that of the book [7]. They are shown in the diagram

The choice of labels $a$ and $b$ is made for convenience of classification scheme of the forthcoming integration. Momentum transfer $t_a$ ($t_b$) inherits label of the incoming particle. For the given particle $a$ ($b$) of the diagram (1) there is the pair of associated variables $s, t_a$ ($s, t_b$) (the energy variable $s$ is assumed to be fixed in the course of integration) and there exists only one variable among the two–particle energies of the final state which is nonadjacent to the pair $s, t_a$ ($s, t_b$) — it gets the same label $a$ ($b$).

Here, we only list the definitions of invariant variables $s, s_a, s_b, t_a, t_b$ in terms of 4-momenta $p_a, p_b, q_1, q_2, q_3$ and masses $m_a, m_b, m_1, m_2, m_3$ of particles:

$$
s = (p_a + p_b)^2 = m_a^2 + m_b^2 + 2p_a \cdot p_b ,
$$
$$
s_a = (q_1 + q_2)^2 = m_1^2 + m_2^2 + 2q_1 \cdot q_2 ,
$$
$$
s_b = (q_2 + q_3)^2 = m_2^2 + m_3^2 + 2q_2 \cdot q_3 ,
$$
$$
t_a = (p_a - q_3)^2 = m_b^2 + m_3^2 - 2p_a \cdot q_3 ,
$$
$$
t_b = (p_b - q_1)^2 = m_b^2 + m_1^2 - 2p_b \cdot q_1 .
$$

The most general case of particle masses will be considered: all masses are different and nonzero — otherwise considerable simplifications are known to take place.

Every 4-momentum of a particle can enter Lorentz-invariant expression only via scalar products with another momenta (we consider the amplitude of the unpolarized experiment, so there are no other 4-vectors for constructing invariants).

Five momenta can form 10 scalar products provided the mass-shell conditions

$$
p_a^2 = m_a^2 , \quad p_b^2 = m_b^2 , \quad q_1^2 = m_1^2 , \quad q_2^2 = m_2^2 , \quad q_3^2 = m_3^2
$$

are fulfilled for all external particles of the considered reaction. It is to be noted that in a given experiment a specific variable, for example, like $(p_b - p_a) \cdot (q_1 - q_3)$, might undergo investigation. In principle, there is combinatorically large amount of invariants formed by linear combinations of scalar products of momenta of 5 particles. Here, we restrict
ourselves to the set of invariants shown in the diagram (1). We note only three features of the quoted diagram.

First, these very variables, being invariant masses of pairs of external particles, enter the pole contributions of 2-particle resonances. Therefore, these variables are common to almost every theoretical analysis.

Second, the most important property of the above variables is their independence. This means that any Lorentz-invariant function of five 4-momenta of the diagram (1) can be written in terms of these 5 invariant variables only. Avoiding lengthy proof of the independence let us simply give the explicit expressions of all 10 products in terms of variables $s, s_a, t_a, s_b, t_b$:

$$
\begin{align*}
p_a \cdot p_a &= \left( s - m_b^2 - m_b^2 \right) / 2 , \\
p_b \cdot q_1 &= -(t_b - m_b^2 - m_1^2) / 2 , \\
q_1 \cdot q_2 &= \left( s_a - m_1^2 - m_2^2 \right) / 2 , \\
q_2 \cdot q_3 &= \left( s_b - m_2^2 - m_3^2 \right) / 2 , \\
p_a \cdot q_3 &= -(t_a - m_b^2 - m_3^2) / 2 ; \\
p_b \cdot q_2 &= \left( m_1^2 + m_2^2 - m_3^2 + m_b^2 - m_b^2 \right) + 2q_1 \cdot q_2 - 2p_b \cdot q_1 + 2p_a \cdot q_3 ) / 2 , \\
p_b \cdot q_3 &= \left( -m_1^2 - m_2^2 + m_3^2 + m_b^2 + m_b^2 \right) - 2q_1 \cdot q_2 - 2p_a \cdot q_3 + 2p_b \cdot p_a ) / 2 , \\
p_a \cdot q_1 &= \left( m_1^2 - m_2^2 - m_3^2 + m_b^2 + m_b^2 \right) - 2q_2 \cdot q_3 - 2p_b \cdot q_1 + 2p_b \cdot p_a ) / 2 , \\
p_a \cdot q_2 &= \left( -m_1^2 + m_2^2 + m_3^2 - m_b^2 + m_b^2 \right) + 2q_2 \cdot q_3 + 2p_b \cdot q_1 - 2p_a \cdot q_3 ) / 2 , \\
q_3 \cdot q_1 &= \left( -m_1^2 - m_2^2 - m_3^2 + m_b^2 + m_b^2 \right) - 2q_2 \cdot q_3 - 2q_1 \cdot q_2 + 2p_b \cdot p_a ) / 2 .
\end{align*}
$$

Here, 5 relations of the first group are simple inversion of definitions (4); the relations of the second group express the rest scalar products in terms of ones of the first group.

Third, the planar character of the diagram (1) makes it convenient to introduce the notion of adjacent and nonadjacent pairs of variables. In the forthcoming analysis one will find a principal difference of the geometry of the 2-dimensional projections of the phase space for pairs of adjacent and nonadjacent variables. In the amplitude analysis the difference is displayed by the fact that variables of nonadjacent pair can simultaneously enter the two–pole contribution as invariant masses of two-particle resonances whereas variables of adjacent pair never can meet together in double-pole term.

To conclude the discussion of the choice of variables one must notice the following:

1. Along with the set of variables (1) any other set which can be defined in terms of a planar diagram will also present the set of independent variables.
2. Performing substitutions of particles

$$
(p_b, p_a, p_1, p_2, p_3) \rightarrow (p_i, p_i, p_i, p_i, p_i)
$$

with $i_a, i_b, i_1, i_2, i_3$ being any transposition of the set $\{a, b, 1, 2, 3\}$ it is possible to use all the results of the analysis of a particular case in any other planar setting. This is provided
by invariance properties of kinematical functions determining the geometry of the phase space. These properties are discussed in details in the book [7].

3. However, one can not exploit the full $5! = 120$ transpositions when dealing with specific processes, for example,

$$\gamma p \rightarrow \pi^+ \pi^0 n.$$  \hspace{1cm} (6)

Indeed, permutations of particles belonging to initial and final states, for example, $\gamma \leftrightarrow \pi^0$ or $p \leftrightarrow n$, introduces variables for another physical processes rather than provides description of the considered process in terms of another set of variables.

Therefore, the principal number of different sets is $2! \times 3! = 12$.

4. There are many other sets of invariant variables which, being strongly nonplanar, nevertheless admit the same treatment (an example of such a set is: \{ $s, s_a, t_a, t_x = (p_b - p_a) \cdot (q_1 - q_2), t_y = (p_b + p_a) \cdot (q_1 - q_2)$ \}). Here, our discussion of the principal problem of integrating over phase space will be restricted to the case of variables described by planar diagram (1).

### 2.2 Phase space integral in invariant variables

The end point of theoretical analysis of the reaction (1) is the cross section $\sigma(a + b \rightarrow 1 + 2 + 3)$ which might be written in the form

$$\sigma = \sigma_c \frac{f}{4J} \int \prod_{j=1}^{3} \frac{d^3q_{j}}{(2\pi)^3 2q_{j0}} (2\pi)^4 \delta^4(p_b + p_a - q_1 - q_2 - q_3)|M|^2$$ \hspace{1cm} (7)

in the case of normalization convention adopted, for example, in the book [1]. Here, $\sigma_c \equiv (\hbar c)^2 = 0.38937966(23)[\text{GeV}^2 \text{mbarn}]$ is the conversion constant, $f$ — statistical factor (equal to product of $1/n_a!$ over subsets of identical particles) and

$$4J = 4 \sqrt{(p_b \cdot p_a)^2 - m_a^2 m_b^2} = 2 \sqrt{\lambda(s, m_a^2, m_b^2)}$$ \hspace{1cm} (8)

$$\lambda((p + q)^2, p^2, q^2) \equiv -4 \begin{vmatrix} p^2 & p \cdot q & q^2 \\ p \cdot q & q^2 \end{vmatrix}$$ \hspace{1cm} (9)

stands for normalization of initial state.

In the papers on particle physics different factors in the denominator of the integrand (7) like $(2\pi)^3$ or even

$$2q_{j0} \equiv 2 \sqrt{m_j^2 + |q_j|^2}$$ \hspace{1cm} (10)

sometimes are used to be hidden into the matrix element by normalization convention for particle states. Therefore, the definition of the empty phase space $R_3 \equiv R_3(|M|^2 = 1)$ is usually based on the common part of (7):

$$R_3 \equiv \int \prod_{j=1}^{3} \frac{d^3q_{j}}{2q_{j0}} \delta^4(p_b + p_a - \sum_j q_j)$$ \hspace{1cm} (11)

(energy, or, the same, $s$ variable is assumed to be fixed in (7) and (11)).

The differential cross sections are always experimentally known in terms of distributions. Thus, the integrations in equations (7) and (11) are assumed to be performed over all region of allowed momenta in the case of total cross section or over subdomain (slice),
cut out by bin bounds in the case of distribution. The dimension of a distribution of the discussed $2 \to 3$ process might be 1, 2, 3 or 4.

This directly follows from the counting of integration variables in expression (11): there are three particles in the final state; their 3-momentum components ($9 = 3 \times 3$ in total) are integrated while being restricted by 4–momentum–conservation conditions expressed by $\delta^4$– function — $5 = 9 - 4$ degrees of freedom remain.

Here, we do not consider polarization measurements. Therefore, matrix element $|M|^2$ has no dependence on the angle in the plane orthogonal to the beam axis in the laboratory frame where the target particle is at rest. Then integration over this variable is easily performed providing $2\pi$ factor.

Hence, maximal dimension of a nontrivial distribution equals 4. The reduction of the 9–dimensional integral (7) ((11)) to 4-dimensional form in terms of some sets of variables of the most interest is discussed in details in the book [7]. In particular, for the case of invariant variables (2) the result reads:

$$\sigma = \frac{\sigma_{cf}}{2\sqrt{\lambda(s, m^2_a, m^2_b)}} \frac{1}{(2\pi)^5} R_3(|M|^2); \quad R_3(|M|^2) = \frac{\pi}{4\sqrt{\lambda(s, m^2_a, m^2_b)}} r_3(|M|^2);$$

$$r_3(|M|^2) = \int ds_a dt_a ds_b dt_b \frac{\Theta(-\Delta_4)}{\sqrt{-\Delta_4}} |M|^2 . \quad (12)$$

Here, $\Delta_4$ is the Gram determinant of any four independent momenta, say $p_b, p_a, q_1, q_2$; its explicit form in terms of scalar variables (2) is given in the Appendix. In what follows we omit subscript 3 in (12), (7) pointing to the number of particles in the final state.

In practice, the overwhelming majority of experimental information on rare processes at intermediate energies is represented in the form of total cross sections and 1–dimensional distributions. The reason might be illustrated by $\pi^- p \to \pi^- \pi^+ n$ experiments [10]: 1023 full–kinematics events constitute solid ground for total cross section; 10–14 bins of 1–dimensional distribution have good filling with averaged number of 60–100 events per bin; the filling of $8 \times 8$ bins of 2–dimensional distribution is satisfactory (15 events per bin in average) while filling of $6 \times 6 \times 6$ of 3–dimensional ones and $4 \times 4 \times 4 \times 4$ 4–dimensional bins is poor.

The increase of statistics of the contemporary experiments [11] by a factor of 10 considerably improves accuracy of results of total cross sections and 1–dimensional distributions. When dealing with 4–dimensional distributions one anyway has to make difficult choice between poor binning or insufficient filling of bins.

Therefore, the minimal problem which solution provides maximal effect is the problem of integration over bins of 1–dimensional distributions (an overall integration for total cross sections is then solved by simple summation).

There is well known property (see, for example, [7]) of the nonadjacent pairs (namely, $(s_a, t_a)$ and $(s_b, t_b)$) of variables: projections of the phase space onto a plane of any such pair admits relatively simple description. This makes possible to modify considerations in such a way that integration over 1–dimensional bins might be in fact realized by adding up results of 2–dimensional distribution, known as Chew–Low plot:

$$r_A(|M|^2; j, k) = \int ds_a dt_a ds_b dt_b \frac{\Theta(-\Delta_4)}{\sqrt{-\Delta_4}} |M|^2 \chi(s_a; s_{a}^{j-1}, s_{a}^{j}) \chi(t_a; t_{a}^{k-1}, t_{a}^{k}) ; \quad (13)$$
\[ \chi(x; x_1, x_2) \equiv \Theta(x - x_1)\Theta(x_2 - x), \]

where \( s_{j-1}^a, s_j^a, t_{a-1}^k, t_a^k \) are bounds of bin \((j, k)\) in the quoted variables.

Owing to the symmetry of the phase space in the pairs of variables \((s_a, t_a) \leftrightarrow (s_b, t_b)\) which is induced by transpositions of particles: \((a \leftrightarrow b), (1 \leftrightarrow 3)\), it is sufficient to perform analysis only for the case \((13)\). To treat 1–dimensional bins in variable of \(s–\) (or \(t–\)) type one needs to rearrange particles in such a way that the variable in question becomes \(s_a\) (or \(t_a\)) variable of the diagram \((1)\) and use trivial binning in the accompanying variable of nonadjacent pair — \(t_a\) (or \(s_a\)).
3 Geometry of Phase Space

The present section deals with the equations determining the boundary of the phase space over which the integration in eqs. (7), (12), (13) has to be performed. The main goal is to display the origin of expressions for limits of the quoted above integrals when the latter are written in an appropriate successive (iterated) form. This requires treating unwieldy formulae when they are explicitly expanded. Therefore, we collect the most cumbersome final expressions in Appendix, devoting the discussion of the present section to the principal steps of analysis of the phase space geometry.

3.1 General properties of phase space of two nonadjacent variables

The conditions fixing the 3–particle phase space (physical region) of the process (1) might be written in terms of inequalities for Gram determinants $\Delta_n(p_1, \ldots, p_n)$ built of all possible sets of $n$ momenta of particles:

\[ \Delta_1(p_1) \geq 0, \quad \Delta_2(p_1, p_2) \leq 0; \]
\[ \Delta_3(p_1, p_2, p_3) \geq 0; \]
\[ \Delta_4(p_1, p_2, p_3, p_4) \leq 0; \]
\[ \Delta_5(p_1, p_2, p_3, p_4, p_5) = 0. \]

Here, $\{p_i\}$ stands for any subset of momenta $\{p_a, p_b, q_1, q_2, q_3\}$ entering diagram (1).

The thorough analysis of how these conditions arise and should be treated as well as references to original papers might be found in [7]. We only remind that

• left hand sides of conditions (14), (15), (16), (17) are invariant functions of momenta of particles; substitution of expressions (4), (5) for scalar products of momenta shows that eqs. (14), (16), (17) are conditions for $s_a, t_a, s_b, t_b$ at fixed $s$;

• conditions (14) are in fact statements that all $p_j$ describe physical particles with nonnegative mass squared ($\Delta_1(p_j) = m_j^2 \geq 0$) and positive energy ($p_0 j > 0$);

• in the given pattern of iterated integration only few of conditions (15) are necessary for due treatment (see, for example, [8]);

• the choice of momenta in the determinant $\Delta_4(p_1, p_2, p_3, p_4)$ has no influence on its value — it is the unique function of independent invariant variables;

• eq. (17) expresses the simple fact that in the 4–dimensional Minkowsky space there cannot be more than 4 linearly independent vectors.

The condition (16) is the natural starting point of analysis. The left hand side of this very condition appears in the form (11), (13) of the phase space integral when it is rewritten in terms of invariant variables. The explicit expression of $D_4 \equiv -\Delta_4(q_2, q_3, p_b, p_a)$ is given in the Appendix in terms of expansions

\[ D_4 = \sum_{\alpha, \alpha, \beta, \beta} d_{\alpha, \alpha, \beta, \beta} s_a^{\alpha} p_a^{\alpha} s_b^{\beta} t_b^{\beta}; \]

\[ = \sum_{\beta, \beta, \beta} b_{\beta, \beta, \beta} s_b^{\beta} t_b^{\beta}. \]

It is reasonable to consider $D_4$ as a function of such subset of variables in which it takes the simplest form. Being generally the form of the fourth degree the above expression is
only quadratic in any pair of nonadjacent variables. The total list of such pairs among variables of diagram (1) is: \((s_a, t_a), (s_b, t_b)\) and \((t_a, t_b)\). (Here, we do not list pairs formed with energy \(s\) which is fixed during integration.)

The pair \((t_a, t_b)\) can not provide universal treatment since both momentum transfers enter the pair and only the energy variables \((s_a, s_b)\) left. On the other side the choice of any pair \((s_a, t_a)\) or \((s_b, t_b)\) can provide covering of all cases of 1–dimensional distributions.

Therefore, assuming that \(s_a\) and \(t_a\) acquire some fixed values from the allowed domain — Chew–Low plot (the explicit description will be given a little later) — it is convenient to write \(D_4\) in the matrix form

\[
D_4 = \left(\begin{array}{c} s_b \\ t_b \end{array} \right)^T \hat{b} \cdot \left(\begin{array}{c} s_b \\ t_b \end{array} \right) + b^T \cdot \left(\begin{array}{c} s_b \\ t_b \end{array} \right) + b_{00},
\]

(19)

where

\[
b \equiv \left(\begin{array}{c} b_{10} \\ b_{01} \end{array} \right); \quad \hat{b} \equiv \left(\begin{array}{cc} b_{20} & b_{11}/2 \\ b_{11}/2 & b_{02} \end{array} \right).
\]

(20)

Let us list the most important properties of the form (19):

a) determinant of the matrix \(\hat{b}\)

\[
\text{Det } \hat{b} = s_a D_{3a}/16,
\]

(21)

where explicit expression for determinant \(D_{3a} \equiv \Delta_3(q_3, p_b, p_a)\) is given by eq. \((A.11)\) of Appendix, is nonnegative in the physical region since two–particle energy \(s_a\) is positive and for the Gram determinant \(D_{3a}\) condition \((15)\) is valid;

b) trace of the matrix \(\hat{b}\) is nonpositive — analyzing the diagonal elements \(b_{02}, b_{20}\) of \(\hat{b}\) provided by eqs. \((A.4)\) one can recognize \(\lambda\)-function expressions for combinations of momenta for which the conditions \((14)\) are fulfilled;

c) when \(D_4\) is transformed to the centered form \((A.8)\) the free term \(b_c\) of the latter

\[
b_c \equiv b_{00} - \frac{1}{4} b^T \cdot \hat{b}^{-1} \cdot b = D_{2a} D_{3a}/s_a.
\]

(22)

is nonnegative in the physical domain of \(s_a, t_a\) variables — this is direct consequence of conditions \((14), (13)\) applied to the RHS of eq. \((22)\);

d) whenever determinant \(|\hat{b}|\) becomes zero \(b_c\) vanishes also; the ratio \(b_c/\text{Det } \hat{b}\) remains finite in the physical domain — by comparing \((22)\) and \((A.12)\) one has

\[
b_c/\text{Det } \hat{b} = 16 D_{2a}/s_a^2.
\]

(23)

These properties imply that condition \((16)\) determines an ellipse in the \((t_b, s_b)\) plane. Before proceeding with its analysis let us recall that \(t_a\) and \(s_a\) variables are assumed to be fixed. The location of the \((t_b, s_b)\) ellipse and orientation of its principal axes strongly depends on the latter variables: this is demonstrated by the Fig. 1 where families of ellipses are drawn in the \((t_b, s_b)\) plane for different values of \(t_a\), \(s_a\) from the allowed domain. Horizontal sequences of elliptic curves are obtained for a fixed value of \(s_a\) — from eq. \((A.7)\) given in the Appendix one can see that \(s_b^c\) coordinate of the center of the ellipse does not depend on \(t_a\) variable.
3.2 Boundaries of phase space for nonadjacent variables

The standard way to derive the bounds for the \((t_b, s_b)\) variables is to solve first the equation \(D_4 = 0\) for a single–variable form \((A.13)\) \((A.14)\) which is scanned in the Appendix:

\[
\begin{align*}
\bar{s}_b^{L,R}(t_b) &= \frac{-(b_{s1} \pm \sqrt{b_s})}{2b_{s2}}; \\
\bar{t}_b^{L,R}(s_b) &= \frac{-(b_{t1} \pm \sqrt{b_t})}{2b_{t2}}.
\end{align*}
\]

Here and in what follows we use the pattern of subscript mnemonics \((L–R), \dot{D}own–U)p, \(Ground–H)igh\) to mark the solution. Small letters will be used for boundary functions \((l, r)\) in eqs. \((24), (25)\) whereas capital ones — for absolute bounds of variables in the considered plot.

The above solutions by virtue of relations \((A.15), (A.16)\) (see subsect. 2.2 of Appendix) are expressed in terms of coefficients \(b_{\beta\beta}, b_{\beta t}\) and discriminants \(b_{s}, b_{t}\). The latter are also written out explicitly in eqs. \((A.19), (A.20)\) and \((A.21), (A.22)\) of Appendix. Note that the plus sign at square root in \((25)\) \((24)\) corresponds to the \(left\) bound of \(t_b (s_b)\) because the denominator \(b_{t2} = b_{02} (b_{s2} = b_{20})\) is already stated to be negative.

Analysis of the above discriminants and the properties a)–c) of the form \((19)\) of the previous subsection shows that all the \(necessary\) and \(sufficient\) conditions for existing a nondegenerate domain in \((t_b, s_b)\) plot are collected in the requirement that free term \((b_c)\) is positive. Because of restrictions \((14), (15)\) the only unambiguous splitting of the product \((22)\) is

\[
D_{2a} > 0; \ D_{3a} > 0.
\]

These conditions determine the Chew–Low plot in \(s_a, t_a\) variables. Its boundaries correspond to curves in \((s_a, t_a)\) plane where LHS’s of the above inequalities vanish. Because of factorization of the expression \((A.43)\) for Gram determinant \(D_{2a}\) it is easy to see that one of the boundary curve is simply the straight line

\[
s_a - (m_1 + m_2)^2 = 0
\]

and the other line provided by \(D_{2a}\)

\[
s_a - (m_1 - m_2)^2 = 0
\]
is well out of phase space for the square of two–particle energy. Here it is where an asymmetry between the momentum transfer \( t_a \) and energy variable \( s_a \) appears. The lower (left) absolute bound \( s^0_a \) for the latter does not depend on initial energy \( s \):

\[
    s^0_a = (m_1 + m_2)^2. \tag{30}
\]

Another boundary curve in \((s_a, t_a)\) plane is provided by vanishing of the \( D_{3a} \) factor of \( b_c \). This factor, being the second order form of the \( s_a, t_a \) variables, is presented in Appendix in the manner similar to that of \( D_4 \) case. Now, the quadratic form

\[
    D_{3a} = \left( \begin{array}{c} s_a \\ t_a \end{array} \right)^T \cdot \hat{A} \cdot \left( \begin{array}{c} s_a \\ t_a \end{array} \right) + A^0, \tag{31}
\]

where

\[
    A \equiv \left( \begin{array}{c} A_{10} \\ A_{01} \end{array} \right); \quad \hat{A} \equiv \left( \begin{array}{cc} A_{20} & A_{11}/2 \\ A_{11}/2 & A_{02} \end{array} \right), \tag{32}
\]

are determined by coefficients provided by eqs. (A.34) of Appendix, is of hyperbolic type. The conclusion is not so difficult to arrive to, basing on the properties of this form presented in Appendix. In particular, the roots in a variable (provided the accompanying variable is fixed) are

\[
    s_{g,h}^a(t_a) = \frac{(-A_{11}t_a + A_{10}) \pm \sqrt{A_s}}{2A_{20}}; \tag{33}
\]

\[
    t_{g,h}^a(s_a) = \frac{(-A_{11}s_a + A_{01}) \pm \sqrt{A_t}}{2A_{02}}, \tag{34}
\]

where discriminants \( A_s, A_t \) are

\[
    A_s \equiv (A_{11}t_a + A_{10})^2 - 4A_{20}(A_{02}t_a^2 + A_{01}t_a + A_{00}) = D_{2c}D_{2a} = D_{2c}(t_a - (m_a + m_3)^2)(t_a - (m_a - m_3)^2)/4; \tag{35}
\]

\[
    A_t \equiv (A_{11}s_a + A_{01})^2 - 4A_{02}(A_{20}s_a^2 + A_{10}s_a + A_{00}) = D_{2c}D_{2as} = D_{2c}(s_a - (\sqrt{s} + m_3)^2)(s_a - (\sqrt{s} - m_3)^2)/4. \tag{36}
\]

This helps to fix critical points \( t_{a}^{G,H}, s_{a}^{G,H} \) of the considered variables as roots of the above discriminants:

\[
    t_{a}^{G,H} = (m_a \mp m_3)^2 ; \tag{37}
\]

\[
    s_{a}^{G,H} = (\sqrt{s} \mp m_3)^2. \tag{38}
\]

Unlike the previous case of second–order form \( D_4 \) in \( s_b, t_b \) variables, here, the intervals between roots are nonphysical since \( D_{3a} < 0 \) there. Regions \( t_a > t_{a}^{H} \) and \( s_a > s_{a}^{H} \) are cross regions of another processes: \( a + 3 \rightarrow b + 1 + 2 \) and \( a + b + 3 \rightarrow 1 + 2 \) respectively. It is easy to see that the absolute range of variation of \( s_a \) variable is fixed in an unique way by eqs. (30) and (38):

\[
    (s_a^D \equiv s^0_a) < s_a < (s_a^U \equiv s^{G}_a). \tag{39}
\]

12
For a given \( s_a \) bounds \( t^{d,u}_a(s_a) \) of \( t_a \) interval are those given by eq. (34)

\[
t^{d,u}_a(s_a) = t^{g,h}_a(s_a) .
\]  

(40)

The absolute bounds of momentum transfer \( t_a \) are provided in a different way. It is simple to find that the lowest possible value of \( t_a \) is given by the lowest intersection point of hyperbola \( D_{3a} = 0 \) with the line \( s_a = s_a^0 \).

\[
t^D_a = t^g_a(s_a^0) .
\]  

(41)

For determination of the upper bound it is crucial whether the common point

\[
s^T_a \equiv \left\{ s(m_a - m_3) + m_3(m_3m_a + m^2_b - m^2_a) \right\}/m_a
\]

of the tangent line \( t_a = t^D_a \) and the hyperbola belongs to the physical region \( [33] \) of \( s_a \) variable or is located below. In the former case the value \( t^G_a \) is never attained. The discussed condition depends on the particular relations of the particle masses (and energy region); the relevant classification might be found in the paper \([8]\). For the purpose of calculations it is sufficient simply to compare \( s^T_a \) with \( s_a^0 \). Then the upper bound \( t^U_a \) is given by eqs.

\[
\begin{align*}
\text{if } s^T_a < s^0_a & \text{ then } t^U_a = t^h_a(s_a^0) \quad \text{(43)} \\
\text{else} & \quad t^U_a = t^G_a. \quad \text{(44)}
\end{align*}
\]

The behavior of the \( s_a \) bounds \( s^{d,u}_a \) at given \( t_a \) follows the similar scheme:

\[
\begin{align*}
s^u_a(t_a) = s^h_a(t_a) ; \\
\text{if } t_a < t^h_a(s_a^0) \text{ then } s^d_a(t_a) = s_a^0 \quad \text{(46)} \\
\text{else} & \quad s^d_a(t_a) = s^g_a(t_a). \quad \text{(47)}
\end{align*}
\]

The variety of labels is dictated by the need of avoiding overlappings when reproducing for the case of \((s_b, t_b)\)–plot. The symmetry

\[
a \leftrightarrow b , \quad 1 \leftrightarrow 3
\]

(48)

of diagram (1) allows to use all the formulae of the current subsect. with the substitution \([8]\) made for all indices and labels containing \(\{a, b, 1, 2, 3\}\).

To resume this Sect. one should note that the symmetry in two–particle energy and momentum transfer variables which is perfect for \( s_b, t_b \) at fixed \( s_a, t_a \) (eqs. \([24], [25], [27]\), \([26]\) following from the symmetric representation \([19]\) of boundary function \( D_4 \)) is broken in the resulting description of Chew–Low plot: \([36], [40] \) versus \([13], [17]\). This must be carefully implemented into algorithms performing integration over phase space.
4 Gauss Integration

4.1 Iterated form of phase space integral

The analysis of the phase space geometry provided by the previous section makes it possible to write the phase space integral \((12)\) (\((13)\)) in a number of iterated forms. There is the natural splitting of 4-dimensional integral into internal integral over \(s_b, t_b\) variables

\[
 r_b(|M|^2) = \int ds_b dt_b \frac{\Theta(-\Delta_4)}{-\Delta_4} |M|^2 \tag{49}
\]

and the integral over the rest ones, the final form of \((13)\) being

\[
 r_A(|M|^2; j, k) = \int ds_a dt_a \frac{\Theta(-\Delta_4)}{-\Delta_4} \chi(s_a; j^{j-1}, s_a^j) \chi(t_a; t_a^{k-1}, t_a^k) r_b(|M|^2) \tag{50}
\]

Basing on the calculated boundary functions \((24), (25), (27), (26)\) the internal integral might be written in two iterated forms, namely:

\[
 r_b(|M|^2) = \int_{s_b^R}^{s_b^L} ds_b \int_{t_b^R}^{t_b^L} \frac{\Theta(-\Delta_4)}{-\Delta_4} |M|^2 \tag{51}
\]

and

\[
 r_b(|M|^2) = \int_{t_b^R}^{t_b^L} dt_b \int_{s_b^L(t_b)}^{s_b^R(t_b)} ds_b \frac{\Theta(-\Delta_4)}{-\Delta_4} |M|^2 \tag{52}
\]

There are no reasons to prefer one form or another basing on pure geometric arguments — the \(s_b, t_b\) domain was stated to be quite symmetric. However, the integrated amplitude \(M\) might have different behavior in the discussed variables. For example, the amplitude might have poles in two-particle energy \(s_b\) (shifted to complex plane from the real axe) and cuts whereas there should be no such reason of rapid variation with momentum transfer \(t_b\) in the integration domain. Since there is maximal step limit among the parameters terminating the calculations of integrating procedures it is reasonable to perform the integration over "smooth" variable \(t_b\) first — otherwise all the rest integrations are expected to be performed at maximal step number as well.

As to external integral \((50)\) the difference in the description of \((s_a, t_a)\)-plot in the variables which was discussed at the end of previous section makes it more convenient to choose the order

\[
 r_A(|M|^2; j, k) = \int_{s_b^L}^{s_b^R} ds_a \int_{t_a^L(s_a)}^{t_a^R(s_a)} dt_a \frac{\Theta(-\Delta_4)}{-\Delta_4} \chi(s_a; j^{j-1}, s_a^j) \chi(t_a; t_a^{k-1}, t_a^k) r_b(|M|^2) \tag{53}
\]

to simplify the program logic. The order

\[
 r_A(|M|^2; j, k) = \int_{t_b^L}^{t_b^R} dt_a \int_{s_b^L(t_a)}^{s_b^R(t_a)} ds_a \frac{\Theta(-\Delta_4)}{-\Delta_4} \chi(s_a; j^{j-1}, s_a^j) \chi(t_a; t_a^{k-1}, t_a^k) r_b(|M|^2) \tag{54}
\]

which directly provide 1-dimensional distribution in momentum transfer \(t_a\) is less attractive from the point of view of amplitude behavior and, what is more important, it causes
considerable complications of the program logic which must trace all details of conditions 
(43–47). Because of these complications the program for calculation of 1–dimensional \( t_a \) 
distribution based on representation (54) is found to be equivalent to the program for 
processing 2–dimensional distribution according to eq. (53).

When we have written the explicit form (53), (51) of the phase space integral (13), the 
problem of calculation of all 1–dimensional distributions in two–particle invariant variables 
is, in principle, solved by an universal procedure which is designed in a straightforward 
way according to the discussed formulae (and boundary eqs. of the previous section 
written in terms of quantities explicitly given in the Appendix). Even with the use of 
integration routines based on Simpson or other standard algorithm the procedure is much 
more effective when compared to the Monte Carlo based analog.

In the rest part of the current section we shall consider the implementation of the Gauss 
integration method for the integral in question. The possibility of further improvement 
of characteristics of the program comes from the following observations:

1) the presence of denominator in eq. (49) which vanish at the boundary of the phase 
space makes it evident that the standard integrating routines waste almost all the time 
processing this (integrable) singularity (one can avoid the difficulty by a change of vari-
bles. This results in minor complications of transfer of arguments from the integrating 
procedure to the user amplitude. It is the loss of universality for further development 
of algorithms processing 3– and 4– dimensional distributions which makes this way of 
correction less attractive);

2) the integrated matrix element \( |M|^2 \) is usually smooth enough (at least, piecewise) 
function of the variables and it might be well approximated by a polynomial.

Therefore, calculating the phase space integral in question, one deals with a classical 
case for which the Gauss integration method proved its unprecedented effectiveness.

Let us note that there might be different approaches of implementation of Gauss 
method to the considered integral. One can try to find the set of orthogonal functions or 
polynomials of all four variables appropriate for the 4–dimensional integral in question. 
This is very interesting and yet unsolved problem. Its solution should help much especially 
in the case when the integration must be performed over all the phase space (for example, 
when analyzing unitarity relation for the considered amplitude). However, when the 
integration is to be performed only over a part (bin) of the phase space or over a sequence 
of bins one easily finds that the set of functions providing calculations by the Gauss 
method must be distinct for every bin. This makes impossible to use once precalculated 
roots and corresponding weights of the polynomial system of the method.

Here, we shall follow the way which can allow, in principle, to deal with all kinds of 
distributions in invariant variables: 1–, 2–, 3– and 4–dimensional. The separate treatment 
of all four integrals will be found to require only two types of orthogonal polynomials in 
every variable to be considered in the most general case.
4.2 Standard singularities of iterated integrals

To find the polynomial basis which is most suitable for the integral in question one must analyse the properties of all four iterated integrals in expressions (51), (53).

Since it is the phase space induced specifics of the considered integral which is of interest we can take the amplitude in the expressions (51), (53) as smooth as we like, say, polynomial.

The singularity structure of the most interior integral over $t_b$ in eq. (51) is evident. The theta–function cuts the entire interval between the roots $(t^l_b, t^r_b)$ of $D_4$ in this variable.

In the case of a polynomial matrix element $|M|^2$ this integral is an elementary one and it might be calculated analytically for every monomial term

$$I_n \equiv \int_{t^l_b}^{t^r_b} \frac{t^n_b \, dt_b}{\sqrt{-D_4}} = \frac{1}{\sqrt{-b_{22}}} \int_{t^l_b}^{t^r_b} \frac{t^n_b \, dt_b}{\sqrt{(t_b - t^l_b)(t^r_b - t_b)}} \quad (55)$$

by recurrent relation

$$I_n = -\frac{2n - 1}{n} \frac{b_{11}}{2b_{22}} I_{n-1} - \frac{n - 1}{n} \frac{b_{00}}{b_{22}} I_{n-2}. \quad (56)$$

This relation uniquely defines $I_n$ in terms of coefficients $b_{00}$, $b_{11}$, $b_{22}$ of the single–variable form (A.14) of $D_4$. The values of the two starting members of the recurrent sequence

$$I_0 = \frac{\pi}{\sqrt{-b_{22}}}, \quad I_1 = -\frac{b_{11}}{2b_{22}} I_0 \quad (57)$$

show that integrand of eq. (51), being polynomial in $s_b$, remains polynomial after first integration since the quantity $b_{22}$, entering both the square root and denominator of expressions (56), (57), does not depend on $s_b$.

This leads to the important conclusions, namely:

1. The natural weight function for the integral over $t_b$ is given by

$$\mu_b(t_b) = \left[ \sqrt{(t_b - t^l_b)(t^r_b - t_b)} \right]^{-1}. \quad (58)$$

2. There is no nontrivial weight function for the next integration over $s_b$.

It is to be noted that the above conclusions are determined by the integration order chosen. The inverted conclusions will be made if one chooses the order of eq. (52): it is the integral over $s_b$ which acquires the weight function, originating from square root of $D_4$, the second integral in $t_b$ being free from nontrivial weight function.

In the course of integration via relations (55), (57) the irrationality

$$\sqrt{-b_{22}} \quad (59)$$

appears. It depends on $s_a, t_a$ variables and might be imagined to be important for analysis of the subsequent integrations. In fact, it must be modified by the following integration over $s_b$ and the final answer appears to be more symmetric in terms of components of the elliptic form (19).

Let us shift the $s_b, t_b$ variables to make the answer less immense. The coordinates $s^c_b, t^c_b$ of the ellipse center do depend on the $s_a, t_a$ variables. Fortunately, they were found
to be smooth in the physical domain (see eqs. (A.7)). The standard monomial in both variables is then

$$|M|^2 = M_{nm} \equiv (s_b - s^c_b)^n(t_b - t^c_b)^m.$$ \hspace{1cm} (60)

By means of elementary calculations the details of which it is reasonable to omit, the integral

$$r_{nm} \equiv r_b(M_{nm})$$ \hspace{1cm} (61)

can be brought to the form (provided $n + m$ is even; otherwise integral $r_{nm}$ is zero):

$$r_{nm} = \frac{2\pi}{(n + m + 1)!!} \sqrt{\frac{b_{c}}{\text{Det } \hat{b}}} \left( \frac{b_{c}}{\text{Det } \hat{b}} \right)^{\frac{n+m}{2}} (-b_{02})^{\frac{n-m}{2}} \times$$

$$\times \sum_{l=1}^{[\frac{m}{2}]} C^2_l (n + m - 2l - 1)!!(2l - 1)!!(\text{Det } \hat{b})^l [b_{11}/2]^{m-2l},$$ \hspace{1cm} (62)

or, changing the order of integration, to the equivalent form:

$$r_{nm} = \frac{2\pi}{(n + m + 1)!!} \sqrt{\frac{b_{c}}{\text{Det } \hat{b}}} \left( \frac{b_{c}}{\text{Det } \hat{b}} \right)^{\frac{n+m}{2}} (-b_{20})^{\frac{m-n}{2}} \times$$

$$\times \sum_{l=1}^{[\frac{n}{2}]} C^2_l (n + m - 2l - 1)!!(2l - 1)!!(\text{Det } \hat{b})^l [b_{11}/2]^{n-2l}.$$ \hspace{1cm} (63)

At first glance the quantity $b_{02}$ ($b_{20}$) appears in the denominator of eq. (62)((63)) when $m > n$ ($n > m$). Then eq. (63)((62)) helps to avoid the algebraic proof that the quantity in the denominator is exactly cancelled by the factor from the sum.

Taking into account that coefficients $b_{\alpha\beta}$, entering the answer, are (second order) polynomials of the $s_a$, $t_a$ variables, one easily continues analysis of properties of the iterated integrals:

3. The true irrationality generated by integration over $s_b$, $t_b$ variables is

$$\sqrt{\frac{b_{c}}{\text{Det } \hat{b}}} = 2\sqrt{\frac{[s_a - (m_1 + m_2)^2][s_a - (m_1 - m_2)^2]}{s_a}}.$$ \hspace{1cm} (64)

4. Polynomial matrix element in $t_a$ variable remains polynomial after the considered internal integration; there is no nontrivial weight function for the next integration in $t_a$ variable.

5. The discussed in the previous section asymmetry of the description of the phase space in the variables $s_a$, $t_a$ appears to be deeper after the internal integration; the generic polynomial of $s_a$ variable acquires irrationality with the critical point just at the boundary of $(s_a, t_a)$–plot

$$s_a = (m_1 + m_2)^2 = s_a^0$$ \hspace{1cm} (65)

multiplied by a rational function of $s_a$.

6. The position of the only pole of this rational function

$$s_a = 0$$ \hspace{1cm} (66)
is distant from the physical region, an expansion or polynomial approximation being allowed (in the potentially dangerous case of vanishing masses \( m_1, m_2 \) both the pole and the irrationality disappear — see eq. (64)).

Turning to the integration over \( t_a \) variable one should remind that integration in eq. (53) is assumed to be performed over domain cut out from the \((s_a, t_a)\)-plot by rectangle defined by bounds \( s_j^{j-1}, s_j^{j}, t_k^{k-1}, t_k^{k} \) of bin \((j, k)\). Whenever the rectangle is exactly inside the Chew–Low plot integration of any \( t_a \) polynomial will provide only constant (in \( s_a \)) contribution. If there is an interval in \( t_a \) for which an arc of hyperbola \( D_{3a} = 0 \) enters the integration domain as a part of boundary the \( t_a \) integration results in an expression containing the term \( \sqrt{A_t} \) from the boundary function (34). The expression (36) for discriminant \( A_t \) shows that it is the absolute bound \( s_a^U = (\sqrt{s} - m_3)^2 \) where the analyticity might be lost due to the above square root — another critical point \( s_a^H = (\sqrt{s} + m_3)^2 \) is well outside the physical region. (And again, the condition \( m_3 = 0 \) bringing \( s_a^H \) to the boundary simultaneously kills the square root itself.)

Depending on the given binning in the \( s_a, t_a \) variables, the absolute bounds \( s_a^0, s_a^U \) might be unattainable at all, only one might be attained and, at last, for a specific bin of a \( t_a \) distribution in the case of some energy and particle masses both bounds might happen to undergo due counting. The bounds must always be taken into account when the total cross section is being calculated.

Combining with the point 5. of the previous conclusion one can find that the last integration in (53) must be performed either

a) with the two–point singular expression

\[
\sqrt{[s_a - (m_1 + m_2)^2] \left[ (\sqrt{s} - m_3)^2 - s_a \right]},
\]

or

b) with

\[
\sqrt{[s_a - (m_1 + m_2)^2]},
\]

or

c) with

\[
\sqrt{[ (\sqrt{s} - m_3)^2 - s_a]},
\]

or

d) without square root singularity.

Now, it is easy to realize that cases b) and c) admit a simple change of variables

\[
s_a = s_a^0 + x^2,
\]

\[
s_a = s_a^U - x^2,
\]

respectively, which helps to get rid of singularity. Of course, the price is the doubling of the effective power of integrand (i.e. the power of approximating polynomial for the smooth factor of integrand). This looks quite acceptable. In contrast, the case a) needs a nonpolynomial (trigonometric) substitution providing no guarantee for estimated rate of convergence.

Finally, we can state that
7. Depending on the given binning the last integration has the weight function given by eq. (67), namely,

\[ \mu_A(s_a) = \sqrt{(s_a - s_0^b)(s_a' - s_a)} \]

(72)
or might be processed with the trivial weight function; in the latter case a change of variable might be required.

To resume the current subsection one should reread the discussed above points 1., ..., 7. and note that there is no principal difference between the weight function \( \mu_b(t_b) \) of eq. (58) and \( \mu_A(s_a) \). Indeed, by multiplication of numerator and denominator of integrand by \( \mu_A(s_a) \) one increases the effective power of the latter by one and converts the irrationality to the form of \( \mu_b \). Therefore, only two distinct sets of orthogonal polynomials are required for implementation of the Gauss method to the integration over the phase space in question, namely, the set, corresponding to the (normalized to the unit interval) weight function \( \mu_b \) of eq. (58), and the set, corresponding to the unit weight function.
5 Principal Features of FORTRAN Code

5.1 Outlines of the Gauss method; specifics of realization

To proceed with implementation of results of the previous analysis let us briefly recall
the basic formulae of the Gauss method [12]. More details might be found in almost any
book on numeric integrating. For example, see [13].

Suppose we have to calculate integral of the type

$$\int_{-1}^{1} f(x)\mu(x)dx ,$$

(73)

where \( f(x) \) is a smooth enough function and \( \mu \) — positive weight function which might
have integrable singularities at the points \( \pm 1 \). Such weight function uniquely defines
the set of polynomials \( \{\phi_n\} \), \( (n \geq 0) \) orthogonal to each other with this weight function
provided a normalization convention is adopted. Then the Gauss formula reads

$$\int_{-1}^{1} f(x)\mu(x)dx \simeq \sum_{k=1}^{n} w_k^{(n)} f(x_k^{(n)}) \equiv G_n .$$

(74)

Here, the weights \( \{w_k^{(n)}\} \) and points \( \{x_k^{(n)} \in (-1, 1)\} \) are assumed to be chosen in such
a way that relation (74) turns into equality for any \( f \) being a linear combination of the
first \( n + 1 \) functions \( \phi_m \) from the system \( \{\phi_m\} \). In this case \( x_k^{(n)} \) should be the roots of
the polynomial \( \phi_n \).

The function \( f \) being a smooth function possesses rapidly decreasing Fourier coefficients \( c_n \):

$$f(x) = \sum_{n \geq 0} c_n \phi_n(x) ;$$

(75)

$$c_m = \int_{-1}^{1} f(x)\phi_m\mu(x)dx .$$

(76)

The convergence rate of the integral sums \( \{G_n\} \) depends on that of \( \{c_n\} \) and, consequently,
on the choice of the system \( \{\phi_n\} \) — this opens the possibility to hide singularities of
an overall integrand into the weight function \( \mu(x) \).

According to the conclusion of the previous section the two cases of weight functions
are peculiar to the iterated integrals over phase space, namely,

$$\mu(x) = (1 - x^2)^{-1/2}$$

(77)

and

$$\mu_0(x) = 1 .$$

(78)

In the first case the orthogonal functions are the Chebyshev polynomials

$$T_n(x) = \cos (n \arccos x) ,$$

(79)

for which there are exact expressions for roots and weights:

$$x_k^{(n)} = \cos \frac{\pi (2k - 1)}{2n} ;$$

(80)
\[ w_k^{(n)} = \frac{\pi}{n}, \quad (81) \]

the quadrature formula (74) being
\[ \int_{-1}^{1} f(x)(1-x^2)^{-1/2} \, dx \simeq \sum_{k=1}^{n} \frac{\pi}{n} f \left( \cos \left( \frac{2k-1}{2n} \right) \right). \quad (82) \]

The unit weight function defines the set of the well–known Legendre polynomials
\[ P_n(x) = \frac{1}{2^n n!} \frac{d^n}{dx^n} (1-x^2)^n. \quad (83) \]

In this case the roots \( X_k^{(n)} \) of the Legendre polynomial \( P_n \) for \( n \geq 10 \) are to be found only by numerical solution of algebraic equation \( P_n(x) = 0 \). The corresponding weights \( W_k^{(n)} \) are then given by the expression
\[ W_k^{(n)} = 2[1 - (X_k^{(n)})^2]^{-1} \left[ \frac{d}{dx} P_n(x) \bigg|_{x=X_k^{(n)}} \right]^{-2}. \quad (84) \]

Explicit expression for the considered integral is
\[ \int_{-1}^{1} f(x) \, dx \simeq 2 \sum_{k=1}^{n} [1 - (X_k^{(n)})^2]^{-1} \left[ \frac{d}{dx} P_n(x) \bigg|_{x=X_k^{(n)}} \right]^{-2} f(X_k^{(n)}). \quad (85) \]

The formulae (82), (85) are the basis of the central subroutines of the integrating program, namely, \texttt{CHIN} and \texttt{ZNIN}. To avoid problems with recurrent calls in the course of processing iterated integrals the subroutines were simply cloned: identical copies \texttt{CHIN1}, \texttt{CHIN4} and \texttt{ZHIN1}, \texttt{ZHIN2}, \texttt{ZHIN3} were used to be called at the corresponding level of integration.

Whereas the programming of a subroutine of the \texttt{CHIN} type (based on Chebyshev polynomials) is straightforward \texttt{ZHIN} subroutines require calculation of roots of Legendre polynomials and the corresponding weights in much more complicated manner. Therefore, to avoid significant losses of time during integration runs the way of using precalculated values was chosen.

The roots of Legendre polynomials have the following property: any root of every subsequent polynomial is located between corresponding roots of the previous Legendre polynomial. Hence, the Newton method of determination of roots is the most suitable in this case. It operates with function and its derivative. Legendre polynomials \( P_l \) and the derivatives \( D_l \) might be easily calculated by the well–known recurrent formulae:
\[ lP_l(x) = xP_{l-1}(x)(2l - 1) - P_{l-2}(x)(l - 1); \quad (86) \]
\[ D_l(x) = (2l - 1)P_{l-1}(x) + D_{l-2}(x), \quad (87) \]
starting the recurrence from \( P_0 = 1, P_1 = x \) and \( D_0 = 0, D_1 = 1 \).

As soon as the roots are found the values of corresponding weights are determined by eq. (84) in terms of roots and derivatives (87).

Since the above calculations are needed to be performed only once the time of run is not of much importance but the precision is, because it directly determines the accuracy of the integration method. To avoid complicated analysis of the influence of the uncertainties of roots and weights on the final answer the latter were calculated at the maximal precision allowed by VAX/VMS PASCAL. The present realization contains common block \texttt{RTWT} with roots and weights for Legendre polynomials up to 50 order (up to 100 — available); in practice, the maximal order 16 appears to be called.
5.2 Implementation

The principle structure of the program is simple: User defined MAIN manipulates with User database to provide necessary parameters, calls integration subroutine WTFF and performs appropriate output of results. There must be another User routine which is called by WTFF, namely, matrix element USRF.

The numeric integration over 4-dimensional phase space is performed by subroutine WTFF. It returns the value of integral and its absolute difference with the value of previous iteration which are the variables of the argument list. The list of physical variables to be passed to this procedure includes energy \( s \), particle masses \( m_a, m_b, m_1, m_2, m_3 \) and bounds of 2-dimensional bin \( s_{a_{j-1}}, s_{a_{j}}, t_{a_{k-1}}, t_{a_{k}} \). Only the bounds were chosen to be included into the list of arguments — other variables are accessible through the COMMON blocks. This is because of the following reasons: a) along with the value of \( s \) some other totally equivalent precalculated quantities \( T_{BEAM}, E_{BEAM}, P_{BEAM} \), etc. are necessary also for calculation of matrix element provided by User; b) according to the described in the end of section 2 universal way of treating bins in one or another variable the above list of masses realizes some transposition of particle masses of the User reaction; a manipulation is needed to pass true arguments to the amplitude which should not know anything about this.

Apart the above physical variables the subroutine WTFF operates with a number of control parameters including terminating value EPS of attained accuracy and 4 limits of iterations for all 4 integrals.

The WTFF algorithm exploits the crucial property of phase space which is expressed by the fact that at any given values of variables \( s_a \) and \( t_a \) the allowed domain of variables \( s_b, t_b \) is the ellipse. Parameters of the latter are determined by masses of external particles and the values of \( s_a \) and \( t_a \) — the corresponding functions and subroutines are built according to the formulae given in section 3 and in Appendix.

The integration domain in the plain \((s_a, t_a)\) is the intersection of the given rectangle

\[
\begin{align*}
& s_{a_{j-1}} \leq s_a \leq s_{a_{j}}, \\
& t_{a_{k-1}} \leq t_a \leq t_{a_{k}},
\end{align*}
\]

\[ (88) \]

with the region

\[
\begin{align*}
& s_{a_D} \leq s_a \leq s_{a_U}, \\
& t_{a_{g}(s_a)} \leq t_a \leq t_{a_{h}(s_a)}
\end{align*}
\]

\[ (89) \]

(see eqs. \( (39), (34) \)).

The properties of the resulting domain determine the integration method (based on Legendre or Chebyshev polynomials) to be applied to the \( s_a \) variable. In the most general case we have to split exterior integration into up to 4 processes (intervals) \((SINTA, ..., SINTD)\) so that boundaries of the internal integration over \( t_a \) have smooth dependence on \( s_a \) on each interval. Thus every process performs integration of the smooth function FWA, FWB, FWC or FWD (which are specified below) and admits an exact method.

As it is discussed in subsection 4.2 almost each of the four intervals might contain singularities at their ends classified by the cases a), b), c) and d). So, depending on the relative values of integration interval bounds and absolute bounds \( (39) \), the calculation of each of integrals SINTA, ..., SINTD is processed by different algorithms, using procedures
The algorithms call the corresponding functions FWA, FWB, FWC or FWD depending on the case of singularities classified by a), b), c), d). These functions realize appropriate changes of variable $s_a$ and make this problem hidden for the next integration over variable $t_a$.

The analysis of the previous section (see points 1., ..., 7.) shows that the next two integrations over any bin in variable $t_a$ and over the complete range $(s_b^L, s_b^R)$ of $s_b$ variable are performed by Gauss method with Legendre polynomials. The algorithms in question are realized by identical subroutines ZHIN2 and ZHIN3.

According to the quoted above analysis the last integration is processed by subroutine CHIN4 which realizes a simple algorithm of Gauss integration with Chebyshev polynomials over unnormalized interval $(t_b^L, t_b^R)$ given by eq. (23). The call of the User matrix element USRF of $(s_a, t_a, s_b, t_b)$ arguments arises at this stage. Prior to the call the initialization of all ten scalar products (4), (5) is performed. The scalar products (like the particle masses) are available via COMMON block. This must simplify the calculation of the considered amplitude which is usually derived according to Feynman rules. However, User must provide appropriate rearrangement of the scalar products if variables of the diagram (1) are a permutation of the User ones.

In total, the discussed program contains about four dozens of functions and subroutines handling various kinematic calculations. The detailed description will follow the specifics of the phase space geometry discussed in Sect. 3 and collection of formulae given in Appendix.
6 Conclusion

In the result of analysis of the geometry of relativistic 3–particle phase space and implementation of integration algorithm the principal solvability of the integration problem appears to be demonstrated. Besides, it becomes evident that the considered case of 2 → 3 reaction is likely to be the last one permitting a treatment outside the framework of Monte Carlo approach. This is due to combinatorical growth of the number of kinematical variables (as free as well as dependent ones) characterizing the reaction (as compared with 2 → 2 case) and the complication of geometry which is displayed by growing algebraic power of definition equations. Given more than 3 particles in the final state other methods of analysis, like the artificial intelligence ones, become necessary.

The integration problem has been solved here for 1–dimensional distributions in any of $10^9$ two–particle invariant variables (i.e. without counting initial energy $s$) of the considered reaction on the base of the fast integration algorithm implementing the Gauss method. The algorithm needs to process the calculation of matrix element in few thousands of points in phase space (compared with tens of millions ones and even more in the Monte Carlo routines) and provides the accuracy which will be never attainable by Monte Carlo calculations.

It goes without saying that the solution was possible due to the extensive coverage of the 2 → 3 case by preceding investigations (the reader had been already advised to look the books [7, 6] for an overview). The same reason might be used for motivation of further researches in this field. At least two directions of the researches might be proposed: 1) a generalization of the approach for the case of noninvariant variables (like angles and 3–momenta); 2) its extension to treat 2–, 3– and 4–dimensional distributions.

While the first direction seems to be closer to the needs of specific experiments the second one appears to be more attractive. Indeed, now it is not so difficult to form almost any distribution (hence, in invariant variables as well) from full–kinematics data with the help of modern tools like GEANT–3. The capability of comparison of different measurements will be opened then and the phenomenological parameters describing specifics of distributions will get an universal status.

The field of application of the considered integration algorithm might include a large variety of processes at intermediate energies like $\pi D \to \pi pn$, $\pi N \to \pi \pi N$, $\gamma p \to \pi \pi N$, etc. One can also try the approach at high energies as well (at least for control of accuracy of the ultra–relativistic approximation for phase space).

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8 Appendix: Gram Determinants

8.1 Two–variable matrix form of $D_4$

The fourth order Gram determinant $D_4$ does not depend on the choice of particle momenta. Let us define it as follows:

$$D_4 \equiv -\Delta_4(q_2, q_3, p_b, p_a)$$

$$= - \left| \begin{array}{cccc}
 q_2 & q_2 & q_2 & q_2 \\
 q_2 & q_3 & q_2 & q_3 \\
 q_3 & q_3 & q_3 & q_3 \\
 p_b & p_b & p_a & p_a \\
 p_a & p_a & p_b & p_b \\
 p_a & p_a & p_a & p_a
\end{array} \right| .$$

(A.1)

Here, all scalar products depending on $s_b$ and $t_b$ variables are underlined (see eqs. (4), (5)). This makes evident that $D_4$ is only quadratic in $s_b$ and $t_b$. By virtue of the symmetry $(a \leftrightarrow b, 1 \leftrightarrow 3)$ the same conclusion is valid for $(s_a, t_a)$ pair as well.

Expression for $D_4$ in terms of expansion in $s_a, t_a, s_b, t_b$:

$$D_4 = \sum_{\alpha_a, \alpha_t, \beta_b, \beta_t} d_{\alpha_a, \alpha_t, \beta_b, \beta_t} s_a^{\alpha_a} t_a^{\alpha_t} s_b^{\beta_b} t_b^{\beta_t}$$

(A.2)

$$= \sum_{\beta_b, \beta_t} b_{\beta_b, \beta_t} s_b^{\beta_b} t_b^{\beta_t}$$

(A.3)

is determined by nonzero coefficients

$$d_{0000} = (-2((m_b^2 + m_a^2 - s)m_3^2 + m_b^2m_a^2 - m_a^4 + m_a^2s)m_2^2 - m_3^4m_2^2$$

$$+ m_3^2m_3^2m_2^2) + 2((m_3^2 + s) + m_3^2s)m_3m_3^2m_2^2$$

$$+ (m_3 + m_3m_3)m_1^4 + m_3^2m_2^2 - 2m_3^2m_2^2 - m_3^2 - s)m_2^4$$

$$+ m_3^4m_2^2)/16 ;$$

$$d_{0001} = (((2m_b^2 - m_a^2 - s)m_3^2 + m_3^2m_3^2) + m_3^2m_2^2 - m_3^2m_2^2m_2^2)$$

$$- ((m_b^2 - m_a^2 + s)m_3^2 + m_3^2m_2^2 + m_3^2m_2^2m_2^2)$$

$$+ m_3^2m_2^2 - 2m_3^2m_2^2m_2^2)/8 ;$$

$$d_{0010} = -((m_a^2 + s) - 2m_3^2 + m_3^2m_2^2)$$

$$+ m_3m_3m_3m_3^2 + m_3^2m_2^2m_2^2)/8 ;$$

$$d_{0011} = -(m_3^2 - s)m_2^2)/8 ;$$

$$d_{0100} = -m_3^2)/16 ;$$

$$d_{0100} = (((2m_b^2 - m_a^2 - s)m_3^2 + m_3^2m_3^2) + m_3^2m_2^2 - m_3^2m_2^2m_2^2)$$

$$+ (m_b^2 + m_3^2m_3^2)m_4^4 - (m_3^2 + m_a^2 - s)m_3^2m_2^2 + m_3^2m_2^2m_2^2)/8 ;$$

$$d_{0101} = -((m_3^2 + s)m_1^2 - 2m_3^2m_2^2m_2^2 - s^2)/8 ;$$

$$d_{0110} = -((m_3^2 + m_3^2m_3^2) - 2m_3^2m_2^2)$$

$$+ (m_3^2 - m_3^2 + s)m_1^2 + m_3^2m_2^2m_2^2)/8 ;$$

$$d_{0111} = (m_3^2 - s)/8 ;$$

$$d_{0120} = m_3^2)/8 ;$$

26
\[
\begin{align*}
    d_{0200} &= \frac{(-(m_1^2 - s)^2)}{16}; \\
    d_{0210} &= \frac{(m_1^2 + s)}{8}; \\
    d_{0220} &= \frac{(-1)}{16}; \\
    d_{1000} &= \frac{(((2m_2^2 - m_3^2 + m_2^2)m_1^2 - (m_2^2 - m_a^2 + s)m_2^2 + m_3^2m_a^2)}{8}; \\
    d_{1001} &= \frac{(-((m_2^2 + m_a^2)m_1^2 + (m_2^2 + m_a^2 - 2s)m_3^2)}{8}; \\
    d_{1002} &= \frac{(m_2^2 + s)}{8}; \\
    d_{1010} &= \frac{((m_3 + m_a)(m_3 - m_a)m_1^2}{8}; \\
    d_{1011} &= \frac{(-((m_2^2 + m_a^2 - 2m_a^2 + s)}/8; \\
    d_{1020} &= \frac{m_2^2}{8}; \\
    d_{1100} &= \frac{(-((m_1^2 - s)m_a^2)}{8}; \\
    d_{1101} &= \frac{((m_1^2 - s)}{8}; \\
    d_{1110} &= \frac{(-((m_2^2 - 2m_a^2 + m_a^2 + s))}{8}; \\
    d_{1111} &= \frac{(-1)}{8}; \\
    d_{1120} &= \frac{1}{8}; \\
    d_{2000} &= \frac{(-m_4^2)}{16}; \\
    d_{2001} &= \frac{m_a^2}{8}; \\
    d_{2002} &= \frac{(-1)}{16}; \\
    d_{2010} &= \frac{m_a^2}{8}; \\
    d_{2011} &= \frac{1}{8}; \\
    d_{2020} &= \frac{(-1)}{16}.
\end{align*}
\]

Coefficients \(b_{i\alpha, j\beta}\) are built of combinations of the latter ones with corresponding powers of \((s_a, t_a)\):

\[
\begin{align*}
    b_{00} &= \frac{(-2((m_2^2 + m_a^2 - s)m_a^2 + (m_a^2 - t_a)m_a^2)}{8}; \\
    &\quad + (s - 2s_a + t_a)m_a^2 - m_a^2 + st_a)m_a^2 \\
    &\quad + ((m_a^2 + t_a)m_a^2 + (s_a - 2t_a)m_a^2 + st_a)m_a^2 \\
    &\quad + (s + s_a)m_a^2 t_a - m_a^2 t_a - m_a^2 s_a - st_a)m_a^2 \\
    &\quad + 2((m_a^2 + s - m_b^2)m_a^2(m_3^2m_b^2 - ((2s - s_a)m_a^2 - st_a)m_a^2} \\
    &\quad + (s_a + t_a)m_a^2 s - m_a^2 s_a - s^2 t_a)m_a^2 \\
    &\quad + (m_3^2 + 2m_3m_a + m_a^2 - t_a)(m_3^2 - 2m_3m_a + m_a^2 - t_a)m_a^2 \\
    &\quad + (m_2^2 + 2m_2m_a + m_a^2 - s)(m_2^2 - 2m_2m_a + m_a^2 - s)m_a^2 \\
    &\quad + 2m_a^2 s_a + st_a)m_a^2(m_3^2m_b^2 + m_4^2m_b^2 + m_a^2s_a^2 - 2m_a^2 s_a t_a + s^2 t_a^2))~/16; \\
    b_{01} &= \frac{(((2m_2^2 - m_3^2 - s - s_a - t_a)m_a^2} + (s - s_a)m_a^2 + m_4^2 - st_a + s_a t_a)m_a^2 \\
    &\quad + (s_a - 2t_a)s - s^2)t_a^2} \\
    &\quad + ((m_2^2 - m_2^2 + s)m_3^2 + (s + s_a)m_a^2 + (s - s_a)m_a^2} \\
    &\quad + (s_a - 2t_a)s - s^2)t_a^2} \\
    &\quad + ((m_2^2 - s_a + t_a)m_a^2 - (m_a^2 - t_a)m_a^2} \\
    &\quad + (s_a - 2t_a)s - s^2)t_a^2} \frac{8}{8}; \\
    b_{10} &= \frac{(-((m_2^2 - s_a + t_a)m_a^2 - (m_a^2 - t_a)m_a^2}
\[(s_a + t_a)m_a^2 - 2st_a + sa_t a - t_a^2)m_a^2\]
\[+((m_a^2 + s + s_a + t_a)^2 + (m_a^2 - s)(s_a - t_a) - 2m_3^2m_b^2 - m_b^4)m_2^2\]
\[+((s_a + t_a) - m_b^2)m_2^2 + (m_a^2s_a + st_a - 2s_a t_a)m_2^2\]
\[-(m_a^2s_a - st_a)(s_a - t_a))/(8;\]
\[b_{11} = -((s_a - t_a) + m_b^2)m_2^2 - (s - s_a)m_b^2 + (s_a + t_a)s\]
\[-(s_a - t_a)s_a - 2m_2^2s_a)/8;\]
\[b_{02} = (2(s + s_a)m_3^2 - m_3^2 - s^2 + 2ss_a - s_a^2)/16;\]
\[b_{20} = (2(s_a + t_a)m_2^2 - m_b^4 - s_a^2 + 2s_at_a - t_a^2)/16.\] (A.4)

When considered as form of \((s_b, t_b)\) variables \(D_4\) might be written as

\[D_4 = \begin{pmatrix} s_b \\ t_b \end{pmatrix}^T \cdot \hat{b} \cdot \begin{pmatrix} s_b \\ t_b \end{pmatrix} + b_00 ,\] (A.5)

where

\[b \equiv \begin{pmatrix} b_{10} \\ b_{01} \end{pmatrix} \text{ ; } \hat{b} \equiv \begin{pmatrix} b_{20} \\ b_{11}/2 \\ b_{02} \end{pmatrix} .\] (A.6)

Eliminating the linear terms in the form \((A.5)\) by shift of variables

\[\begin{pmatrix} s_b \\ t_b \end{pmatrix} = \begin{pmatrix} s'_b \\ t'_b \end{pmatrix} + \begin{pmatrix} s^c_b \\ t^c_b \end{pmatrix} ,\]

where

\[\begin{pmatrix} s^c_b \\ t^c_b \end{pmatrix} = -\frac{1}{2} \hat{b}^{-1} \cdot b\] (A.7)

\[= \begin{pmatrix} (-s - s_a - m_b^2)m_1^2 + (s + s_a - m_b^2)m_2^2 + (s - s_a + m_b^2)s_a)/(2s_a) \\
((s_a + t_a - m_b^2)m_1^2 + (s_a - t_a + m_b^2)m_2^2 - (s_a - t_a - m_b^2)s_a)/(2s_a) \end{pmatrix},\]

it is possible to rewrite \(D_4\) as the centered form

\[D_4 = \begin{pmatrix} s'_b \\ t'_b \end{pmatrix}^T \cdot \hat{b} \cdot \begin{pmatrix} s'_b \\ t'_b \end{pmatrix} + b_c .\] (A.8)

The free term \(b_c\) of this form is

\[b_c = b_00 - \frac{1}{4} \hat{b}^T \cdot \hat{b}^{-1} \cdot b = D_{2a}D_{3a}/s_a .\] (A.9)

Here, \(D_{2a}\) and \(D_{3a}\) are the Gram determinants

\[D_{2a} \equiv -\Delta_2(q_1, q_2) = (s_a - (m_1 + m_2)^2)(s_a - (m_1 - m_2)^2)/4 ,\] (A.10)

\[D_{3a} \equiv \Delta_3(q_3, p_b, p_a) = (-s_a m_a^4 - t_a s_a^2 + t_a s_a + t_a)(s_a - t_a)\]
\[+((m_a^2 + s + s_a + t_a)m_b^2 + (m_a^2 - s)(s_a - t_a) - m_b^4)m_3^2\]
\[+((s_a + t_a)s - s_a^2 + s_a t_a)m_a^2 - (m_a^2 - t_a)(s - s_a)m_b^2 - m_b^4m_3^2)/4.\] (A.11)

In its turn the determinant of the matrix \(\hat{b}\) of the quadratic form \((A.5)\) which remains the same for the centered case \((A.8)\) also contains the \(D_{3a}\) factor:

\[\text{Det} \hat{b} = s_aD_{3a}/16 .\] (A.12)
8.2 Single–variable form of $D_4$

When considered as function of a single variable (because of symmetry $a \leftrightarrow b$ the variable is reasonable to choose $s_b$ or $t_b$) $D_4$ is determined by expansions

$$D_4 = b_{s2}s_b^2 + b_{s1}s_b + b_{s0} \ , \quad (A.13)$$

$$D_4 = b_{t2}t_b^2 + b_{t1}t_b + b_{t0} \ , \quad (A.14)$$

where

$$b_{s2} = b_{20} ;$$

$$b_{s1} = b_{11}t_b + b_{10} ;$$

$$b_{s0} = b_{02}t_b^2 + b_{01}t_b + b_{00} \quad (A.15)$$

and

$$b_{t2} = b_{02} ;$$

$$b_{t1} = b_{11}s_b + b_{01} ;$$

$$b_{t0} = b_{20}s_b^2 + b_{10}s_b + b_{00} \quad (A.16)$$

are defined by expressions \([A.4]\) for coefficients $b_{3, \beta_i}$.

To calculate the roots of the second order polynomials \([A.13], [A.14]\) one needs in fact only coefficients $b_{s2}$ and $b_{s1}$ ($b_{t2}$ and $b_{t1}$) provided the discriminants of \([A.13], [A.14]\)

$$b_s = b_{s1}^2 - 4b_{s2}b_{s0} \ , \quad (A.17)$$

$$b_t = b_{t1}^2 - 4b_{t2}b_{t0} \quad (A.18)$$

are known. The relevant discussion of Jacobi reduction theorem for symmetric determinants of arbitrary dimension might be found, for example in \([14, 15]\). In our particular case of the fourth order Gram determinant $D_4$ the results might be verified by direct calculation to be the products of Gram determinants

$$b_s = D_{3a}D_{3as} \ , \quad (A.19)$$

$$b_t = D_{3a}D_{3at} \ , \quad (A.20)$$

where explicit expression for $D_{3a}$ is given in \([A.11]\) and the ones for $D_{3as}, D_{3at}$ are

$$D_{3as} = \{(m_b^2 - s_a + t_a)m_2^2 - (t_b - t_a)m_b^2 + (s_a + t_a)t_b + s_at_a - t_a^2)m_1^2$$

$$+ ((m_b^2 + s_a + t_a)m_b^2 + (s_a - t_a)t_b - m_b^4)m_2^2$$

$$+ (t_b - t_a)m_b^2s_a - (s_a - t_a)t_b s_a - m_1^4t_a - m_2^4m_b^2 - t_b^2s_a) / 4 ; \quad (A.21)$$

$$D_{3at} = \{(m_a^2 + s - s_a)m_a^2 + (s + s_a + s_b)m_a^2 - m_a^4 - s s_b + s_a s_b)m_1^2$$

$$+ ((s - s_b)m_a^2 + (s_a + s_b)s - s^2 + s_a s_b)m_2^2$$

$$- (s - s_b)m_a^2s_a - m_1^4m_2^2 - m_2^4s + s s_2s_b - s_a s_b - s_a s_b^2) / 4 \quad (A.22)$$

For processing the boundaries of $(s_b, t_b)$–plot at given fixed values of $s_a$ and $t_a$ variables the similar treatment of $D_{3as}$ and $D_{3at}$ determinants is necessary. Expanding the latter in the form

$$D_{3as} = b_{st2}t_b^2 + b_{st1}t_b + b_{st0} \quad (A.23)$$
\[ D_{3at} = b_{ts2}s_b^2 + b_{ts1}s_b + b_{ts0}, \]  

where

\[ b_{st0} = \{(m_b^2 - s_a + t_a)m_b^2 + m_b^2 t_a + s_a t_a - t_a^2\}m_1^2 + (s_a + t_a) - m_b^2 m_b^2 - m_1^4 t_a - m_1^2 m_a^2 - m_b^2 s_a t_a\} / 4; \]  

\[ b_{st1} = \{(m_b^2 + s_a - t_a)m_b^2 - (m_b^2 - s_a - t_a)m_1^2 + m_b^2 s_a - s_a t_a\} / 4; \]

\[ b_{st2} = -s_a / 4; \]

along with coefficients \( b_{st2}, b_{st1}, b_{ts2}, b_{ts1} \) one needs to know the discriminants of (A.23), (A.24):

\[ b_{st} \equiv b_{st1}^2 - 4b_{st2}b_{st0} \]

\[ = -(2(s_a + t_a)m_b^2 - m_b^4 - s_a^2 + 2s_a t_a - t_a^2)(m_1^2 + 2m_1 m_2 + m_2^2 - s_a)(m_1^2 - 2m_1 m_2 + m_2^2 - s_a) / 16; \]

\[ b_{ts} \equiv b_{ts1}^2 - 4b_{ts2}b_{ts0} \]

\[ = -(2(s + s_a)m_3^2 - m_3^4 - s^2 + 2s s_a - s_a^2)(m_1^2 + 2m_1 m_2 + m_2^2 - s_a)(m_1^2 - 2m_1 m_2 + m_2^2 - s_a) / 16. \]

### 8.3 Two–variable matrix form of \( D_{3a} \)

It is again convenient to determine the Gram determinant \( D_{3a} \) defined by eq. (A.11) as expansion in its variables \( s_a, t_a \):

\[ D_{3a} = \sum_{\alpha, \alpha'} A_{\alpha, \alpha'} s_a^{\alpha} t_a^{\alpha}. \]

Explicit expressions for coefficients are

\[ A_{00} = \{(m_b^2 + s - m_b^2)m_3^2 - m_3^4 - m_b^2 s - s^2\}/4; \]

\[ A_{01} = \{(m_b^2 - m_a^2 + s)m_3^2 + m_b^2 s + m_a^2 s - s^2\}/4; \]

\[ A_{10} = \{(m_b^2 + m_a^2 - s)m_3^2 + m_b^2 m_a^2 - m_b^2 s - s^2\}/4; \]

\[ A_{02} = (-s)/4; \]

\[ A_{11} = -(m_b^2 - m_a^2 - s)/4; \]

\[ A_{20} = -m_a^2)/4. \]
The matrix $\hat{A}$ of the quadratic form (A.33)

$$D_{3a} = \left( \begin{array}{c} s_a \\ t_a \end{array} \right)^T \cdot \hat{A} \cdot \left( \begin{array}{c} s_a \\ t_a \end{array} \right) + A^T \cdot \left( \begin{array}{c} s_a \\ t_a \end{array} \right) + A_{00}, \quad \text{(A.35)}$$

where

$$A \equiv \left( \begin{array}{cc} A_{10} \\ A_{01} \end{array} \right); \quad \hat{A} \equiv \left( \begin{array}{cc} A_{20} & A_{11}/2 \\ A_{11}/2 & A_{02} \end{array} \right), \quad \text{(A.36)}$$

has the determinant which up to a constant coincides with the Gram determinant

$$D_{2c} \equiv -\Delta_2(p_a, p_b) = (s - (m_a + m_b)^2)(s - (m_a - m_b)^2)/4, \quad \text{(A.37)}$$

namely,

$$A_2 \equiv \text{Det} \hat{A} = -D_{2c}/16. \quad \text{(A.38)}$$

The free term $A_c$ of the corresponding to (A.35) centered form

$$A_c = A_{00} - \frac{1}{4} A^T \cdot \hat{A}^{-1} \cdot A \quad \text{(A.39)}$$

also is expressed via $D_{2c}$:

$$A_c = -m_3^2 D_{2c} = -m_3^2 (s - (m_a + m_b)^2)(s - (m_a - m_b)^2)/4. \quad \text{(A.40)}$$

Let us give for completeness the coordinates of geometrical center of the conic section determined by the form $D_{3a}$:

$$\left( \begin{array}{c} s_a^c \\ t_a^c \end{array} \right) = -\frac{1}{2} \hat{A}^{-1} \cdot A = \left( \begin{array}{c} s + m_3^2 \\ m_3^2 + m_a^2 \end{array} \right). \quad \text{(A.41)}$$

### 8.4 Second–order Gram determinants

To control absolute bounds of $s_b$, $t_b$ variables one should add to the list of determinants $D_{2c}$, $D_{2a}$, $D_{2as}$, $D_{2at}$

$$D_{2c} \equiv -\Delta_2(p_a, p_b) \quad \text{(A.42)}$$

$$D_{2a} \equiv -\Delta_2(q_1, q_2) \quad \text{(A.43)}$$

$$D_{2as} \equiv -\Delta_2(q_1 + q_2, q_3) \quad \text{(A.44)}$$

$$D_{2at} \equiv -\Delta_2(p_a, q_3) \quad \text{(A.45)}$$

already used in previous considerations the analogues of $D_{2a}$, $D_{2as}$, $D_{2at}$ obtained by transposition of particles $1 \leftrightarrow 3$, $a \leftrightarrow b$.

All these determinants treated as functions of quantities entering their bodies are in fact represented by the same standard kinematical function $\lambda$ ( cf. eq. (4))

$$\Delta_2(p, q) \equiv \text{Det} \left( \begin{array}{cc} p^2 & p \cdot q \\ p \cdot q & q^2 \end{array} \right) = -\frac{1}{4} \lambda((p + q)^2, p^2, q^2) \quad \text{(A.46)}$$

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with

\[ \lambda(x, y, z) = x^2 + y^2 + z^2 - 2xy - 2yz - 2zx \tag{A.47} \]

\[ = \left( x - (\sqrt{y} + \sqrt{z})^2 \right) \left( x - (\sqrt{y} - \sqrt{z})^2 \right) \]

\[ = \left( y - (\sqrt{z} + \sqrt{x})^2 \right) \left( y - (\sqrt{z} - \sqrt{x})^2 \right) \]

\[ = \left( z - (\sqrt{x} + \sqrt{y})^2 \right) \left( z - (\sqrt{x} - \sqrt{y})^2 \right). \]

The same applies to \( D_{3a}, D_{3as}, D_{3at} \) (and, generally speaking, to \( D_4 \) as well) — there are many forms in which the so called kinematical \( G \)-function might be represented and many elegant properties of it which then follow. Having in mind quite utilitarian goal we display only few of them in the simplest possible terms. For more details reader can look into [7].