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WEIGHTS BY MONTE-CARLO METHOD

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CALCULATION OF THE STATISTICAL
WEIGHTS BY MONTE-CARLO METHOD

Объединенный институт
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БИБЛИОТЕКА

ANNOTATION

A new way of calculation of repeated integrals of any multiplicity by Monte-Carlo method is proposed. Its application to the calculation of the statistical weights under multiple production process, simulating is stated. Possibilities of its application in different cases are discussed.

INTRODUCTION

Under simulating multiple production processes (see /1/), the necessity of the calculation of the statistical weights of separate reactions arises. This task was repeatedly solved for the Fermi model and now there are effective table and graphical ways (See /2/, /3/) of the calculation of the phase space volume for this model. However, simulating, you must be able to calculate phase volumes for different models of multiple production, i.e. to have a way of solution of the integral:

$$\int_n(E, 0) = \int d^3\vec{p}_1 d^3\vec{p}_2 \dots d^3\vec{p}_n F(\vec{p}_1, \vec{p}_2, \dots, \vec{p}_n) \delta(\sum \vec{p}_i) \delta(\sum \epsilon_i - E) \quad (I)$$

for any form of F^x). Monte-Carlo method may be the mean for the calculation of (I), especially, "importance of sampling," which gives the opportunity to improve sharply the convergence of approximations (as regards this, see /4/).

However, for the application of "importance of sampling," it is necessary to imagine more or less well the form of the function F ; that is impossible at the present time.

In the present paper we suggest that the other modification of Monte-Carlo method - the method of weighted disposition - should be used. It does not improve the convergence of approximations so much, as the "importance of sampling," but still, it is better than the "usual" Monte-Carlo method of the calculation and it is applicable for the arbitrary function F .

The idea concerning it was stated by M.I. Podgoretsky; the mathematical basis is given by Ju.N. Blagoveschensky [5].

x) All the designation and formulas with the numeration of the (2.12) kind are taken from the paper /1/.

I. THE CALCULATION OF REPEATED INTEGRALS

Let it be calculated

$$S = \int_{a_n} f(\rho) d\rho, \quad (2)$$

where a_n is a bounded region in n -dimensional space of the points $\rho = (\xi_1, \xi_2, \dots, \xi_n)$ and $f(\rho)$ is the continuous non-negative function of n variables.

The usual way of calculation (2) according to Monte-Carlo method begins with the fact that the point ρ is uniformly "thrown" into the rectangle A_n containing a_n , with the sides which are parallel to the coordinate axes.

Let it be

$$\hat{f} = \begin{cases} f(\rho), & \text{if } \rho \in a_n \\ 0, & \text{if } \rho \notin a_n \end{cases} \quad (3)$$

Then, an average value of \hat{f} over all the throwings under the increasing of their number tends to the ratio of S to the volume V_{A_n} . Hence, averaging the quantity $V_{A_n} \hat{f}$, we shall tend to S .

By this method of the calculation the rectangle A_n is essentially used. Whereas, it is absent in the primary integral (2). Its introducing looks not very well-grounded. Therefore the idea of refusing the sample of ρ in the rectangle A_n , and, instead of this, of throwing ρ strictly into the region a_n each time, is natural. But now it is obvious, that it is not possible to consider all the throwings equivalent during the calculation of an average \hat{f} over all of them. It is necessary to appropriate a definite "weight" to each of them; the weight would take into account the fact that while using the rectangle A_n hitting the region a_n would take place, as a rule, after repeated misses in a_n .

An average number of the similar misses must be necessarily brought in correspondence with every point $\rho \in a_n$. It determines the weight of the value $f(\rho)$.

It is clear that the weight decreases, when the number of misses increases. It is clear, too, that the weight must not depend upon the kind of the function $f(\rho)$. Instead, it must depend not only on the form of the region, but also on the succession, in which the coordinates of the point ρ are picked.

That is why such a method must be suitable by a great number of calculations of integrals of different functions over one and the same many-dimensional region. The similar situation

may be found, for example, in the task of simulating the process of multiple production, where the passage to a new model means changing of the function F in (I), and the region of integration is determined only by the kinematic relations and, therefore, remains unchanged.

Let us illustrate the proposed method of summarising with the weight according to Monte-Carlo method with the help of the following two examples. From these examples it will be easily to see the general rule, too, for the calculation of the weight.

Let (Fig. I, the plane $\xi_1, 0 \leq \xi_2$) the integral over the quadrant Q_2 with the radius I in the plane $\xi_1, 0 \leq \xi_2$ be calculated.

Let us circumscribe the square A_2 with a side I round Q_2 .

We shall choose the coordinates of the point $P(\xi_1, \xi_2)$ not simultaneously, but in consecutive order. The coordinate ξ_1 of the points $P \in Q_2$ must be picked uniformly in the interval $(0,1)$. The coordinate ξ_2 in the former method also must be picked in $(0,1)$ uniformly. Then, by the fixed ξ_1 , a portion of a number of points hits Q_2 , from their general number, would be equal to the ratio of segments KK_1/KK_2 , in other words, $\sqrt{1-\xi_1^2}$. It is obvious, that if one chooses ξ_2 strictly uniformly on the segment KK_1 , so that all the points $P \in Q_2$, then the points P must be taken with the weight $W(P) = \frac{KK_1}{KK_2}$ in other words, $W(P) = \sqrt{1-\xi_1^2}$ then, as before, we calculate in every point $f(P)W(P)$ and average over all P .

Now, let the integral over a part of the sphere $Q_3: \xi_1, \xi_2, \xi_3 \geq 0$ of the radius I (Fig. I) be calculated. We circumscribe the cube A_3 with a side I , round it.

Let ξ_1 be picked uniformly in $(0,1)$. Then, while choosing uniformly ξ_2 on KK_1 , every point $P(\xi_1, \xi_2, 0)$ must be taken with the weight KK_1/KK_2 . Further, obtaining ξ_1 and ξ_2 , it is necessary to pick, besides this, ξ_3 on the segment LL_1 , instead of LL_2 ; from the whole number of the points, which were picked according to "canonical" method, first, on KK_2 and then on LL_2 , a portion

$$W(P) \equiv (KK_1/KK_2) \cdot (LL_1/LL_2) = \sqrt{1-\xi_1^2} \sqrt{1-\xi_1^2-\xi_2^2} \quad (4)$$

would hit the segment LL_1 .

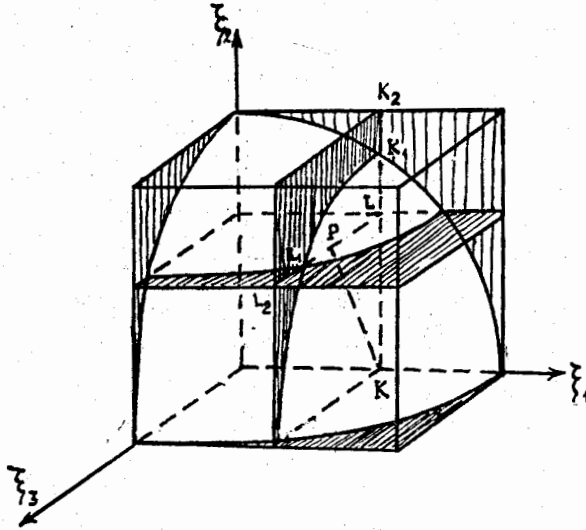


Fig. 1

It is necessary to appropriate such a weight to any point of $P \in \mathcal{L}_2$ and to any function of this point.

May be, here, it is suitable to underline the dependence of the weight upon the procedure of simulating; so, if we obtain ξ_1 and sample the distance PK and the angle $\angle K_2KP$ in the intervals $(0, \sqrt{1-\xi_1^2})$ and $(0, \pi/2)$, accordingly, then the weight of each point P would be determined by the ratio of the circle area of the radius $\sqrt{1-\xi_1^2}$ and the square area with the side 1 in other words, it would be equal to $\frac{\pi}{4} (1-\xi_1^2)$.

Now we may proceed to the general case.

Let the coordinates of the point $P = (\xi_1, \dots, \xi_n)$ be uniformly sampled in the order of numeration: in other words ξ_k is uniformly sampled within the bounds ξ_k', ξ_k'' , which essentially depend on the results of the previous samplings. It is inductively clear from the above-mentioned examples that $f(P)$ in the point P must be taken with the weight:

$$w(P) = \prod_{k=1}^n (\xi_k'' - \xi_k') \tag{5}$$

and the value of the integral may be obtained as a limit of the consequence S_N' , in other words:

$$S = \lim_{N \rightarrow \infty} S_N' = \lim_{N \rightarrow \infty} \frac{1}{N} \sum f(P) w(P) \tag{6}$$

where the summarizing is carried out by all the N points of the sampling.

The method under suggestion, which called by us, "the weighted disposition" method, has with the usual Monte-Carlo method one and the same property, that the sampling of ξ_k takes place uniformly; it is similar to the "importance of sampling" in the presence of the

weight $w(\rho)$, which is determined, however, not by the function $f(\rho)$, but by the position of the point ρ in A_n .

Let us estimate the probable deviation of S'_n about S in the method under suggestion. According to the Chebyshev's inequality:

$$P\{|S'_n - S| \leq \varepsilon\} \geq 1 - \frac{D S'_n}{\varepsilon^2}, \quad (7)$$

where

$$D S'_n = \frac{D\{f(\rho)w(\rho)\}}{N} = \frac{1}{N} \left\{ \int_{A_n} f^2(\rho)w(\rho)d\rho - S^2 \right\}. \quad (8)$$

In other words, the probability of the fact that the deviation of the average S'_n over N samplings about the value of the integral S does not exceed ε differs from the unity by the magnitude:

$$\delta = \frac{\int_{A_n} f^2(\rho)w(\rho)d\rho - S^2}{N\varepsilon^2}$$

The corresponding magnitude δ_1 for the usual Monte-Carlo method by N' throwing into the rectangle A_n is equal to:

$$\delta_1 = \frac{V_{A_n} \int_{A_n} f^2(\rho)d\rho - S^2}{N'\varepsilon^2},$$

where V_{A_n} is the volume of the rectangle A_n . It is possible to neglect the second term in comparison with the first one for many of multi-dimensional integrals. Then, taking into account the above-mentioned for δ and δ_1 , we shall obtain the following approximate expressions for $V_{A_n} = 1$:

$$\delta \approx \frac{\int_{A_n} f^2(\rho)w(\rho)d\rho}{N\varepsilon^2}; \quad \delta_1 \approx \frac{\int_{A_n} f^2(\rho)d\rho}{N'\varepsilon^2}. \quad (9)$$

By the same accuracy ε and the same number of throwings $N' = N$ the diminution of δ arises only for account of the substitution $w < 1$ for 1.

So, essential economy on the scale of the calculations will appear only by $w \ll 1$

It is obvious, that this diminution of dispersion sets in for the reason that the points, which had been previously thrown about the whole of A_n , are now concentrated only in the region of a_n , and the contraction of the region of throwings of the point ρ leads to the decrease of the dispersion about the values of $f(\rho)$.

To estimate numerically the diminution of δ with respect to δ_i , the magnitude $\omega_n = \delta_i / \delta$ was calculated for $n=3$ and $n=10$, when a_n - n -dimensional sphere with the radius R , A_n - circumscribed round it n -dimensional cube and $f(\rho) \equiv 1$

The values are as follows: $\omega_3 \approx 1,5$; $\omega_{10} \approx 7,5$

The diminution of dispersion leads to the diminution of the time, which is necessary for the calculation of the integral with a given error. Besides, it is necessary to notice, that if the calculation of the limits of the integration is more difficult than the checking of the fact of the hitting of the point ρ the region a_n , this diminution may not be observed. However, in many cases the weighted disposition method has the real advantage in comparison with the usual Monte-Carlo method.

The case, when for the checking of the setting of the point ρ in the region a_n it is necessary to calculate the limits of integration, since the bounds of the region are given by them, is especially suitable with respect to it. In this case the diminution of the dispersion leads to the diminution of the time, which is necessary for the calculation of the integral by the use of the method under suggestion.

2. THE CALCULATION OF PHASE VOLUMES

To apply the "weighted disposition" method to the calculation of (I), it is necessary to place the limits of the integration in (I). This may be done in different ways, depending on the choice of variables and the order of integration. As it was previously mentioned the limits are determined only by kinematic relations between the secondary particles, and not by the form of F .

Taking into account the fact that each of the variables of the integration \vec{p}_k has three components, we write (I) in the following way:

$$S = \dots \int d\xi_k \int d\eta_k \int d\zeta_k \dots \Psi(\dots, \xi_k, \eta_k, \zeta_k, \dots) \quad (10)$$

Then the formula for the calculation S' according to the "weighted disposition" method has the following form:

$$S' = \lim_{N \rightarrow \infty} \frac{1}{N} \sum w \Psi \quad (11)$$

where

$$\Psi = \Psi(\dots, \xi_k, \eta_k, \zeta_k, \dots) \quad (12)$$

$$W = \prod_{\kappa=1}^n (\xi_{\kappa}'' - \xi_{\kappa}') (\eta_{\kappa}'' - \eta_{\kappa}') (\zeta_{\kappa}'' - \zeta_{\kappa}') \quad (13)$$

In [1] it is shown, that (I) is transformed as follows:

$$S = \int d^3 \vec{p}_1 \dots d^3 \vec{p}_{n-2} d\rho_{n-1} d\varphi_{n-1} \rho_{n-1} \frac{E_n}{p_{n-1}} \mathcal{F}(\vec{p}_1, \dots, \vec{p}_{n-1}, -\sum_1^{n-1} \vec{p}_{\kappa}) \quad (14)$$

while using the spherical system of the coordinates, introduced there. According to the choice of the order and of the variables of integration it is possible to give the three algorithms of the calculation (I): α), β), γ)

α) Let us determine in (14)

$$p_{\kappa} = \xi_{\kappa}, \quad \cos \theta_{\kappa} = \eta_{\kappa}, \quad \varphi_{\kappa} = \zeta_{\kappa} \quad (15)$$

and sample $\xi_{\kappa}, \eta_{\kappa}, \zeta_{\kappa}$ in the order of numeration from ξ_1 up to $\xi_{\kappa-1}$. Then, the limits of the integration are given by the following formulae:

$$\xi_{\kappa}'' = \frac{E_{\kappa}^* p_{\kappa} + p_{\kappa}^* E_{\kappa}}{M_{\kappa}}, \quad \xi_{\kappa}' = \begin{cases} 0, & \text{if } \frac{E_{\kappa}}{M_{\kappa}} \leq \frac{E_{\kappa}^*}{m_{\kappa}} \quad \text{and } \kappa < n-1 \\ \frac{|E_{\kappa}^* p_{\kappa} - p_{\kappa}^* E_{\kappa}|}{M_{\kappa}} & \text{in other cases} \end{cases} \quad (16)$$

$$\eta_{\kappa}'' = \begin{cases} 1, & \text{if } \frac{E_{\kappa}}{M_{\kappa}} < \frac{E_{\kappa}^*}{m_{\kappa}} \quad \text{and } p_{\kappa} < \frac{p_{\kappa}^* E_{\kappa} - p_{\kappa} E_{\kappa}^*}{M_{\kappa}} \\ \frac{M_{\kappa} E_{\kappa}^* - E_{\kappa} p_{\kappa}}{p_{\kappa} p_{\kappa}^*} & \text{in other cases} \end{cases} \quad (17)$$

$$\eta_{\kappa}' = -1$$

$$\zeta_{\kappa}'' = 2\pi; \quad \zeta_{\kappa}' = 0 \quad (\kappa = 1, 2, \dots) \quad (18)$$

and

$$\Psi = p_{n-1} \frac{E_n}{p_{n-1}} \mathcal{F}(\vec{p}_1, \vec{p}_2, \dots, \vec{p}_{n-1}, -\sum_1^{n-1} \vec{p}_{\kappa}) \prod_1^{n-2} p_{\kappa}^2 \quad (19)$$

x/ All the designations and formulas with the numeration of the (2.I2) kind are taken from the paper /I/.

β) If one changes the order of integration, using, as before the spherical system of the coordinates, in other words, takes

$$\cos \theta_k = \xi_k, \quad p_k = \eta_k, \quad \varphi_k = \zeta_k \quad (20)$$

then, Ψ , as before, is calculated according to (19). It follows from §2 [I], that the limits of the integration over ξ_k and η_k are:

$$\xi_k' = -1; \quad \xi_k'' = +1; \quad \eta_k' = 0; \quad \eta_k'' = p_{k \max} \quad \text{if } \frac{E_k}{M_k} \leq \frac{E_k^*}{m_k} \quad (21)$$

$$\xi_k' = -1; \quad \xi_k'' = \xi_{k \max}; \quad \eta_k' = p_{k \min}; \quad \eta_k'' = p_{k \max}, \quad \text{if } \frac{E_k}{M_k} \geq \frac{E_k^*}{m_k} \quad (22)$$

Here $\xi_{k \max}$ is the cosine of the limit angle (See, for ex., (1.12) from /I/)

$$\xi_{k \max} = - \frac{\sqrt{E_k^2 p_k^{*2} - e_k^2 p_k^2}}{m_k p_k} \quad (23)$$

and $p_{k \max}$ - are the limit values of the momenta at the angle θ_k (See, for ex., (I, 9₁), (1,10) from /I/)

$$p_{k \min} = \frac{-E_k^* M_k p_k \cos \theta_k \pm \sqrt{E_k^2 (M_k^2 p_k^{*2} - m_k^2 p_k^2 \sin^2 \theta_k)}}{E_k^2 - p_k^2 \cos^2 \theta_k} \quad (24)$$

γ) Let us make use of the rectangle coordinates, determining

$$\vec{p}_k = \{ \xi_k, \eta_k, \zeta_k \} \quad (25)$$

Then,

$$\Psi = p_{n-1} \frac{E_n}{p_{n-1}} \mathcal{F}(\vec{p}_1, \dots, \vec{p}_{n-1}, -\sum_1^{n-1} \vec{p}_k) \quad (26)$$

To find the limits of integration, let us take into account, that (See /I/) the region of the permitted values of ρ_κ is the three-dimensional ellipsoid of revolution. The extreme values of the coordinate ξ for the three-dimensional ellipsoid with the matrix of the coefficients (a_{ij}) $i, j = 1, \dots, 4$ are equal to:

$$\xi', \xi'' = \frac{(\Delta_{14} \pm \sqrt{-\Delta_2^{(1)} \Delta_4})}{\Delta_{44}} \quad (27)$$

Here Δ_4 is a determinant of the matrix (a_{ij}) by $i, j = 1, \dots, 4$

$\Delta_2^{(1)}$ is a determinant of the matrix (a_{ij}) by $i, j = 2, 3$.

Δ_{ij} is a cofactor to the element a_{ij} of the matrix (a_{ij}) ; $i, j = 1, \dots, 4$.

In ellipsoid under consideration the matrix (a_{ij}) has the following form:

$$(a_{ij}) = \begin{pmatrix} E_\kappa^2 - X_\kappa^2 & -X_\kappa Y_\kappa & -X_\kappa Z_\kappa & X_\kappa M_\kappa E_\kappa^* \\ -X_\kappa Y_\kappa & E_\kappa^2 - Y_\kappa^2 & -Y_\kappa Z_\kappa & Y_\kappa M_\kappa E_\kappa^* \\ -X_\kappa Z_\kappa & -Y_\kappa Z_\kappa & E_\kappa^2 - Z_\kappa^2 & Z_\kappa M_\kappa E_\kappa^* \\ X_\kappa M_\kappa E_\kappa^* & Y_\kappa M_\kappa E_\kappa^* & Z_\kappa M_\kappa E_\kappa^* & E_\kappa^2 m_\kappa^2 - M_\kappa^2 E_\kappa^{*2} \end{pmatrix} \quad (28)$$

Therefore,

$$\left. \begin{matrix} \xi'_\kappa \\ \xi''_\kappa \end{matrix} \right\} = \frac{-X_\kappa E_\kappa^* \mp \rho_\kappa \sqrt{M_\kappa^2 + X_\kappa^2}}{M_\kappa} \quad (29)$$

Within these limits the magnitude of the component ξ_κ of the vector ρ_κ may change. If ξ_κ is already obtained, then the section of the ellipsoid by the plane $\xi = \xi_\kappa$ will be the ellipse with the matrix of the coefficient (a_{ij}) : $i, j = 1, 2, 3$

$$(a_{ij}) = \begin{pmatrix} E_\kappa^2 - Y_\kappa^2 & -Y_\kappa Z_\kappa & Y_\kappa (M_\kappa E_\kappa^* - X_\kappa \xi_\kappa) \\ -Y_\kappa Z_\kappa & E_\kappa^2 - Z_\kappa^2 & Z_\kappa (M_\kappa E_\kappa^* - X_\kappa \xi_\kappa) \\ Y_\kappa (M_\kappa E_\kappa^* - X_\kappa \xi_\kappa) & Z_\kappa (M_\kappa E_\kappa^* - X_\kappa \xi_\kappa) & E_\kappa^2 (\xi_\kappa^2 + m_\kappa^2) - (M_\kappa E_\kappa^* - X_\kappa \xi_\kappa)^2 \end{pmatrix} \quad (30)$$

For the ellipse, the extreme values of the coordinate η_κ are expressed by the following formula:

$$\eta'_\kappa, \eta''_\kappa = \frac{\Delta_{13} \mp \sqrt{-\Delta_{11} \Delta_3}}{\Delta_{33}} \quad (31)$$

where Δ_3 - is a determinant of the matrix (a_{ij}) under $i, j = 1, 2, 3$.

At last, when within the limits (31) the value η_κ is uniformly picked, the possibility for the component ξ_κ within the segment with the ends $\xi_\kappa', \xi_\kappa''$ remains.

For all the three pairs of limits $(\xi_\kappa', \xi_\kappa'')$, $(\eta_\kappa', \eta_\kappa'')$, $(\xi_\kappa', \xi_\kappa'')$ it is possible to write the only formula:

$$\left. \begin{matrix} \xi, \eta', \xi' \\ \xi'', \eta'', \xi'' \end{matrix} \right\} = \frac{AB \mp \sqrt{(C+A^2)(B^2-CD)}}{C} \quad (32)$$

where the values of all the quantities are taken from the following table:

Table I.

	ξ	η	ξ
A	X_κ	Y_κ	Z_κ
B	$-M_\kappa E_\kappa^*$	$X_\kappa \xi_\kappa - M_\kappa E_\kappa^*$	$X_\kappa \xi_\kappa + Y_\kappa \eta_\kappa - M_\kappa E_\kappa^*$
C	M_κ^2	$M_\kappa^2 + X_\kappa^2$	$M_\kappa^2 + X_\kappa^2 + Y_\kappa^2$
D	m_κ^2	$m_\kappa^2 + \xi_\kappa^2$	$m_\kappa^2 + \xi_\kappa^2 + \eta_\kappa^2$

(33)

The limits of integration over p_{n-1} and y_{n-1} are calculated according to (16) and (18). Expressions for Ψ (19), (26) lose the sense by $p_{n-1} = 0$. But it is easily to show that, for example, (19) under $p_{n-1} = 0$ may be replaced by

$$\Psi = 2 \prod_1^{n-2} p_\kappa^2 \mathcal{F}(\vec{p}_1, \dots, \vec{p}_{n-2}, \vec{p}_{n-1}^*, -\sum_1^{n-2} \vec{p}_\kappa - \vec{p}_{n-1}^*) \cdot \frac{(E_{n-1} - E_{n-1}^*) E_{n-1}^* p_{n-1}^*}{M_{n-1}} \quad (34)$$

if only to exclude the factor $(p_{n-1}'' - p_{n-1}')^2$ in w. (13):

$$w = \left[\prod_{\kappa=1}^{n-2} (\xi_\kappa'' - \xi_\kappa') (\eta_\kappa'' - \eta_\kappa') (\xi_\kappa'' - \xi_\kappa') \right] \cdot (\xi_{n-1}'' - \xi_{n-1}') \quad (35)$$

and, in this way, to evaluate the indeterminate form. It is difficult to estimate beforehand, which of the algorithms, either α), β) or γ) gives the more effective way of computing S' .

Let it, for example, be $F \equiv 1$. Then, in α) and β) it is possible to integrate over all the ξ_k , and the dimension of the region of the integration should diminish in one and a half time, that must improve the convergence; in γ) of the similar diminution of dimensions will not take place.

However, Ψ (26) in the algorithm γ) depends upon only the three variables.

$$P_{n-1}, E_{n-1}, P_{n-1} \quad \text{and} \quad \Psi \quad (\text{see } (19))$$

in α) and β) also upon P_1, \dots, P_{n-2} .

Therefore, the spread of the values Ψ in α) and β) must essentially (the calculation shows, that by several orders) exceed the spread of the values Ψ in γ). This leads to the increase of the dispersion.

A priori, it is not clear, which of the factors - the increase of the dispersion of values of the integrand or the diminution of the dimension of the integration region - influences strongly.

The described way does not pretend for the satisfactory solution of the problem of the calculation of the statistical weights under the simulating of the multiple production process.

It, as well as the usual way of the calculation according to Monte-Carlo method, requires a large scale of work, though, in some cases, it is essentially profitable. Under multiple production with a great number of particles the statistical weights of separate reactions approximately become equal to each other and for the calculation of them by the methods of the theory of probability it is necessary to carry out a large scale of computation. However, under the calculation of comparatively great statistical weights the "weighted disposition" method may be more useful.

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