Calculation of a multidimensional integral with a singularity by dividing the integration domain into subsegments.

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Calculating multidimensional integrals of type $\int ... \int f(x)/(x-c)$ is not a simple task. The methods used to calculate such an integral must effectively bypass the singularity, minimizing the error. This work presents an algorithm that, in the process of calculating the integral, analyzes the area of integration, dividing it into subsegments. Subsegments containing a singularity, as well as those located close to the singularity, are excluded during the final calculation of the integral. Integrals final calulation is carried out using the Monte Carlo integration method. The algorithm allows to calculate both one-dimensional and multidimensional integrals.

Вычисление многомерного интеграла с сингулярностью путём дробления области интегрирования на подсегменты.

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Вычисление многомерных интегралов с особенностью типа $\int ... \int f(x)/(x-c)$ — непростая задача. Методы, используемые для вычисления такого интеграла, должны эффективно обходить сингулярность минимизируя ошибку. В данной работе представлен алгоритм, который, в процессе вычисления интеграла, анализирует область интегрирования разбивая ее на подсегменты. Подсегменты содержащие особенность, а также расположенные вблизи особенности, исключаются при окончательном вычислении интеграла. Окончательный расчет интегралов осуществляется методом интегрирования Монте-Карло. Алгоритм позволяет вычислять как одномерные, так и многомерные интегралы.

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1. INTRODUCTION

The most commonly used trick for calculation of the Cauchy Principal value of $\int_a^b f(x)/(x-c)\,dx$ over a finite interval (a,b) is to eliminate the region around the singularity $x=c$. The integral is split in two smooth integrals $(a, c-\Delta)$, $(c+\Delta, b)$ which can be calculated by any numerical method suitable for the problem. For the solution to this problem can be used Wolfram Mathematica, GNU GSL Library [1], qdawc-function in the FORTRAN IMSL library [2]. There exists algorithms in QUADPACK library (a numerical integration package written by R. Piessens, E. de Doncker-Kapenga, C. Ueberhuber and D. Kahaner [3]). But the methods of those libraries are used for one-dimensionl case with the predetermined position of the singularity. And are not applicable in cases when the integral is multidimensional and the position of the singularity is not explicitly defined.

This work presents a algorithm to solve multidimensional integrals with a singularity, which is not explicitly defined.

2. ALGORITHM

The presented algorithm is based on dividing the integration domain into segments and analyzing them in such a way that sub-segments containing a singularity or that are located close to it (by a certain Δ value) are not taken into account in the final calculations.

Fig. 1 illustrates how to check whether the singularity is inside the segment or closer to it than Δ value. The algorithm strategy is to check the values of the integrand on the edges of a segment. When the minimal negative and maximal positive values appear on neighboring coordinates, the singularity is supposed to be presented in the segment. When the singularity is detected in the segment, the segment is split into equal 2^d sub-segments in accordance to its dimension d.

As can be seen from the left panel of Fig. 1, each current segment is expanded by the value Δ. This expansion guarantees that segment without singularity is sufficiently far from the singularity. In other case, the region around the singularity $x=c$ that must be removed from final calculations. The "detection-splitting" loop continues until reaches the minimum length of each edge equal (ε parameter) over every singular segment.

The smaller is ε parameter value, the more accurately it is possible to determine the position of the singularity, because the singularity with each stage enclosed in an increasingly smaller figure, which means striving towards its center (see Fig. 1, right panel). Nevertheless there should be found a balance between the segment minimal size and the permissible calculation error, as the closer the segment to the singularity, the higher the error is. At this stage, both parameters (ϵ and Δ) are chosen empirically. The choice is based on practical experiments to achieve the required smoothness of the graph and reducing the final total error calculated by Eq. (1).

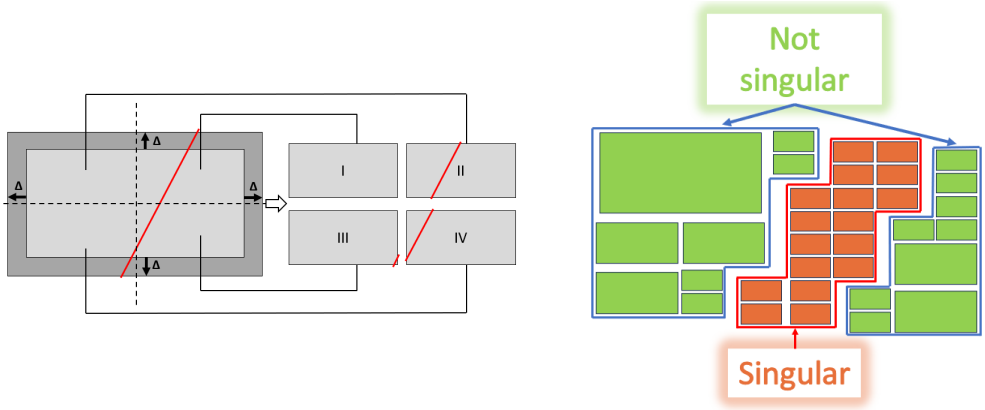

Fig. 1: Left panel: splitting current segment into equal segments (dashed area shows the expansion of current segment). Right panel: Getting singular and non-singular segments from initial integration domain

At each step of algorithm non-singular and singular segments are distinguished. Non-singular segments saved in storage to calculate they in the end of algorithm work. After completion of splitting of the integral region into segments, algorithm calculates results and errors for each non-singular segment and combines them to get total result and total error of initial integration domain:

$$Res_{\text{tot}} = \sum_{n=1}^{k} res_i, \quad Err_{\text{tot}} = \sum_{n=1}^{k} err_i \cdot c_i, \tag{1}$$

where $c_i = V_i/V_{total}$ and V_i is volume of segment, and err_i is error upper bound by [4].

3. NUMERICAL RESULTS AND OUTLOOKS

In theoretical physics integrals of a kind $f(x) = f(x)/(x-c)$ appear at a study of hadronization processes, scattering, and decay processes at decomposing Feynman diagrams at the one-loop level. Low-temperature calculation of such integrals has some approaches (the Feynman parametrization or low-momentum expansion [5]), but the finite-temperature calculation meets some problems due to appearing of the imaginary part and the singularity in the denominator after the temperature reaches some critical value.

In our previous work we examined the photoproduction of neutral pions $\pi_0 \to \gamma\gamma$ in the framework of Nambu-Jona-Lasinio model [6].

$$|A(q_1^2, q_2^2, P)|^2 = 512\alpha^2\pi^2 g_{\pi qq}^2 (\frac{M_\pi^4}{m^2}) m^4 |I_3(q_1^2, q_2^2, P)|^2, \tag{2}$$

where $\alpha = e^2/4\pi$, $g_{\pi qq}$ is the pion coupling constant, M_π is pion mass and m is the quark mass, q_1, q_2 are four-momentum for γ-s. For the calculation of the photoproduction we used $q_1^2 = 0$, $q_2^2 = 0$ in the pion rest frame $\vec{P} = 0$.

For this case an integral I_3 in Eq.2 turns into the one-dimensional integral (see for details [6, 7]).

In this work more general case $\pi_0 \to \gamma\gamma^*$ with $q_1^2 = 0, q_2^2 \neq 0$ in the pion rest frame $\vec{P} = 0$ is examined. Omitting theoretical calculations, we give the resulting expression ReI_3 for the finite-temperature case:

$$\begin{aligned}
\mathrm{Re}I_3 &= \frac{1}{8\pi^2}\int_m^{\sqrt{m^2+\Lambda^2}} |\vec{p}|dE\Big\{ \\
&- \frac{f(E-\mu)}{4q_{10}q_{20}}\int_{-1}^{1} dx \frac{1}{E-|\vec{p}|x}\frac{1}{E+\frac{q_2^2}{2q_{20}}+\frac{|\vec{p}|q_{10}}{q_{20}}x} - \\
&+ \frac{f(E-\mu)}{2P_0q_{10}}\frac{1}{2E+P_0}\int_{-1}^{1} dx \frac{1}{E-|\vec{p}|x} - \\
&+ \frac{f(E-\mu)}{2P_0q_{20}}\frac{1}{2E-P_0}\int_{-1}^{1} dx \frac{1}{E-\frac{q_2^2}{2q_{20}}+\frac{|\vec{p}|q_{10}}{q_{20}}x} - \\
&- \frac{f(-E-\mu)}{4q_{10}q_{20}}\int_{-1}^{1} dx \frac{1}{E+|\vec{p}|x}\frac{1}{E-\frac{q_2^2}{2q_{20}}-\frac{|\vec{p}|q_{10}}{q_{20}}x} + \\
&- \frac{f(-E-\mu)}{2P_0q_{10}}\frac{1}{2E-P_0}\int_{-1}^{1} dx \frac{1}{E+|\vec{p}|x} + \\
&- \frac{f(-E-\mu)}{2P_0q_{20}}\frac{1}{2E+P_0}\int_{-1}^{1} dx \frac{1}{E+\frac{q_2^2}{2q_{20}}-\frac{|\vec{p}|q_{10}}{q_{20}}x}\Big\},
\end{aligned} \tag{3}$$

where $\vec{p} = \sqrt{E^2 - m^2}$.

The integral ReI_3 was calculated as function of temperature using of the described algorithm. To check the correctness of calculations, we compare results for Eq.3 at $q_1^2 = 0$, $q_2^2 = 0.0001$ with the results of previous research [7], where the special kinamatics $q_1^2 = q_2^2 = 0$ was used. Calculations in the work [7] were made using simple Monte-Carlo method and the correctness of calculations was checked by GNU GSL QUADPACK package [1]. As can be seen Fig. 2, the algorithm and Monte-Carlo integration method are applicable to calculate of the integral.

As shown in Fig. 2, both results are almost same at low T, but after reaching $T = 0.25$ the results of the algorithm become unstable, that is expressed in significant jumps in the graph. The algorithm did not cope with the task very well with parametres $\Delta = 0.01, \varepsilon = 0.001$. The total errors of integrals are shown in the Fig. 2 with dashed lines. Right panel Fig.2 shows 2-dimensional integral Eq.3 for different values of q_2^2: $q_2^2 = 0.0001$,$q_2^2 = 0.001$, $q_2^2 = 0.01$.

The algorithm is planned to be revised on the step of the selecting segments for the final calculation by identifying small segments containing a singularity and expanding their integration limits by the Δ parameter for further exclusion from the initial integration domain. The smaller is ε parameter (segments minimum length of each edge), the more accurately is possible to determine the location of the singular region. But reducing the ε parameter causes exponential growth of segments count, which affects the calculation time. One way to solve this problem, is to implement into code parallelization methods to significantly reduce total calculation time. Also there should be found a balance between the segment minimal size and the permissible calculation error, as the closer the segment to the singularity, the higher the error is.

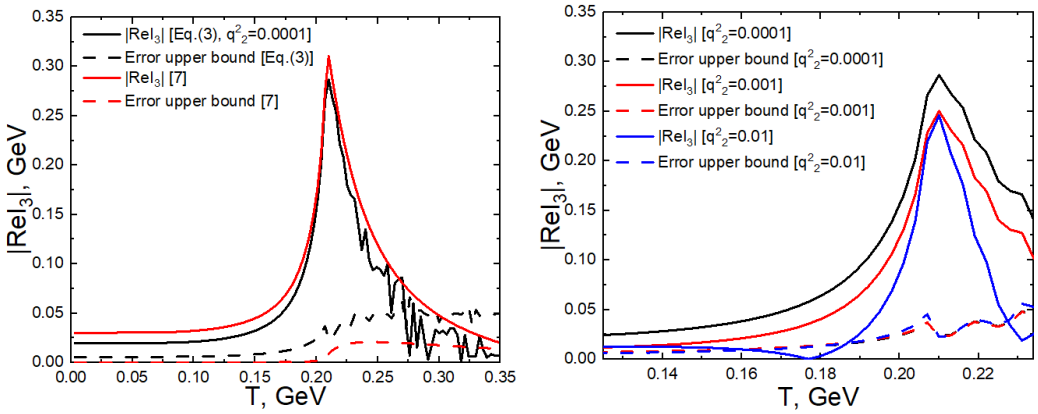

Fig. 2: Left panel: comparison of results for 1-dimensional integral from the work [7] and Eq.3 with their error upper bounds (dashed lines). Right panel: 2-dimensional integral Eq.3 $q_2^2 = 0.0001$,$q_2^2 = 0.001$, $q_2^2 = 0.01$.The errors for all three results are approximately the same with minor differences.

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