An algorithm for identifying of singularity in improper multidimensional integrals of a "second" type

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This paper presents an algorithm for locating singularities in improper multidimensional integrals of the "second" type when their positions are not explicitly specified. After locating these integrals can be evaluated using Monte Carlo integration (the classical methods or GSL VEGAS). The applicability of the algorithm is demonstrated by calculating the temperature dependence of the decay width of a neutral pion into two photons and by evaluating the pion transition form factor (a 6 two-dimensional integrals).

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Алгоритм выявления особенностей в несобственных многомерных интегралах «второго» типа

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1. Introduction

The calculation of scattering and decay amplitudes in particle physics often requires the evaluation of multidimensional integrals. These integrals are typically of the second type with singularities such as $1/(x-c)$. Mathematicallyy such integrals are defined via the Cauchy Principal Value, where symmetric region of size Δ is excises around the singularity before taking the limit $\Delta \to 0$. Numerical solution for such integrals is possible using well-known libraries such as the GNU GSL Library [1], and the qdawc-function in the FORTRAN IMSL library [2]. These algorithms are generally applicable to the one-dimensional case with a predetermined position of the singularity in the integration domain. Practically, however, the problem is more complex: the integrals are multidimensional (making Monte Carlo algorithms the natural choice) and the singularity's location is typically not known.

Our previous work proposed an algorithm for locating singular region by partitioning the integration domain into sub-segments, applying this algorithm to calculate the two-photon decay of the neutral pion $\pi^0 \to \gamma\gamma$ within the extended Nambu-Jona-Lasinio model [3]. In this paper, we present a major revision: the search for singularities in the integration domain is now reduced to a binary search, which significantly cuts the algorithm's running time and the volume of data processed during the integral calculation. The developed two-stage algorithm first isolates singular points and subsequently computes the integral using the Vegas GNU Library, integrating over the full domain, excluding small region near the identified singular points. The proposed algorithm is applied to the calculation of the pion decay width and to

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the calculation of the pion transition form factor $\pi^0 \to \gamma\gamma^*$, which requires the evaluation of six two- dimensional integrals.

2. The algorithm for identification of singular points

The algorithm is designed for the evaluation of multidimensional integrals with constant integration limits. The procedure for locating singular points in the domain consists of the following steps:

- For every edge of the N-dimensional integration domain (numbering $2^{N-1}N$ in total), M uniformly distributed points are sampled (Fig. 1 step 2). The integrand is computed at each of these points (Fig. 1 step 3). The behavior of the function across this set of points is analyzed. If an anomaly of the function's behavior is detected between two adjacent points, the sub-segment connecting them is flagged for further inspection (Fig. 1 step 4).

- The each flagged segment is then analyzed using a binary search: the integrand is evaluated at the segment's boundaries and its midpoint. By comparing these function values, the algorithm determines which half of the segment is likely to contain the singular point. This segment is bisected again. The process iterates until the minimum size is reached. The midpoint of the remaining segment is taken as the singularity location (unless it was not found by chance). If the function exhibits regular behavior on the segment, the entire segment, search is terminated (Fig. 1 step 5).

- The second stage involves searching for singular points inside the integration domain. The initial edge point is designated as a center, and a local N-dimensional figure of size θ is constructed around that (Fig. 1 step 7). The edge-search algorithm is then repeated on this region boundary. The singular point found then becomes the next center and the process repeats until the full integration volume is covered.

Binary search significantly reduces the number of operations required to find a singularity. The output is a set of singular points.

3. The calculation of the integral

The multidimensional integral is computed numerically using the well-known Monte Carlo VEGAS method [1], implemented in the GNU Scientific Library (GSL). A key modification is introduced in the function calling the integrand: for each random point generated by the VEGAS algorithm, the algorithm verifies whether it lies within a prescribed exclusion region surrounding any previously detected singular point. These exclusion zones are defined as hypercubes of size Δ centered on each singularity (similar to

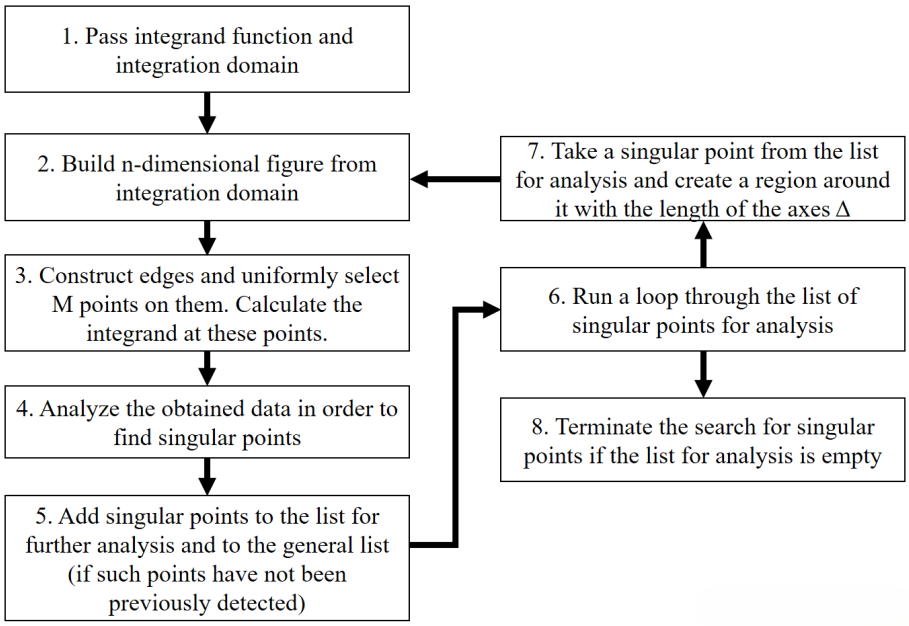

Fig. 1: The figure shows a diagram of the algorithm for finding singular points in the integration domain.

Cauchy's principle). If the generated point falls inside such a region, the integrand is assigned a value of zero (Fig. 2 step 5). This procedure effectively excises the singular region from the integration domain and allows for numerical calculation of the integral using any integral calculation method, including those not designed for improper integrals.

Checking a large set of singular points for every sampling point generated by the VEGAS algorithm incurs significant computational overhead. To accelerate the calculation, the integration domain can be partitioned into independently calculated subsegments (Fig. 2 step 2). For each subsegment, a precomputed list of singular regions that intersect it is created (Fig. 2 step 3). This optimization significantly reduces the number of checks required per subsegment, especially for those with no intersections. Furthermore, this approach allows for parallel computation.

The application of the proposed algorithm to complex physical problems is presented in the following section.

4. The $\pi^0 \to \gamma\gamma$ decay and transition form factor

Photoproduction of the neutral pion $\pi_0 \to \gamma\gamma$ is widely described, including the framework of NJL-like models [4]. The amplitude of the pion photodecay is as

$$T(P^2; q_1^2, q_2^2) \;=\; 2\epsilon_{\mu\nu\alpha\beta}\epsilon_1^\mu \epsilon_2^\nu q_1^\alpha q_2^\beta N_c \frac{4e^2}{3} g_{\pi qq} m I_3(P, q_1, q_2), \qquad (1)$$

q_1, q_2 are photon momenta, e is electron charge and $g_{\pi qq}$ is the pion coupling constant.

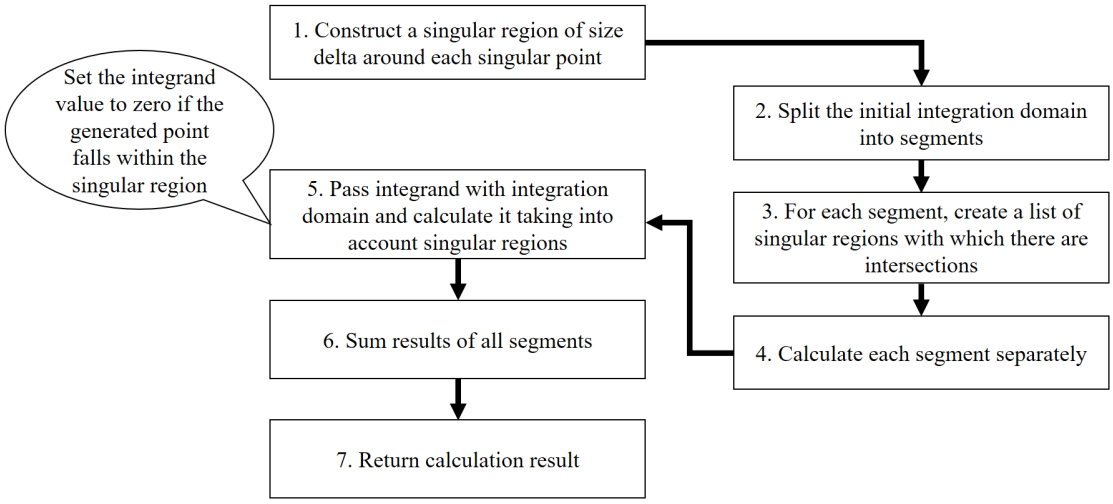

Fig. 2: The figure shows a diagram of a parallel integral calculation (see text).

The width of the photoproduction is calculated by the simple relation

$$\Gamma(\pi^0 \longrightarrow \gamma\gamma) = \frac{M_\pi^3}{64}|32\alpha\pi g_{\pi qq} m I_3(0,0,P^2)|^2, \tag{2}$$

$\alpha = e^2/4\pi$ is the fine structure constant, m is the mass of light quarks. The integral I_3 is

$$I_3(q_1^2, q_2^2, P^2) = \int \frac{dp}{(2\pi)^4} \frac{1}{(p_0^2 - E^2)((p_0 - q_{10})^2 - E_1^2)((p_0 + q_{20})^2 - E_2^2)}. \tag{3}$$

For the calculation of the photodecay width $\Gamma_{\pi^0\gamma\gamma}$ both photons are considered as real with $q_1^2 = 0$, $q_2^2 = 0$ and the pion rest frame $\vec{P} = 0$ is used. In the framework of the NJL model, the integral I_3 becomes an one-dimensional integral with the imaginary part occurring when $M_\pi > 2m$. Numerically, it means that integral has singularities after the temperature reaches the critical value $T > T_c$.

The transition form factor for $\pi^0 \to \gamma^*\gamma$ can be defined from Eq. (2) for the case when one of photons is off-shell:

$$F_{\pi\gamma}(Q^2) = 8 g_{\pi qq} m I_3(0, Q^2, P^2) \tag{4}$$

with the integral I_3 considered in kinematics $q_1^2 = 0, q_2^2 \neq 0, \mathbf{P} = 0, P_0 = \sqrt{s} = M_\pi$. This kinematics gives more complicated expression for the integral I_3 and is transformed in three-dimensional integral with singularities.

The temperature dependence of the decay width is shown in the left panel of Fig.3 for different values of the NJL cut-off parameter Λ. Here we used $\Lambda = 0.639$ GeV, which follows from the model parametrization, and $\Lambda = 3.07$ GeV, which reproduces the experimental data (for details see [4, 5]). The space-like behavior of the transition form-factor $Q^2 F_{\pi\gamma}(Q^2)$ is presented in

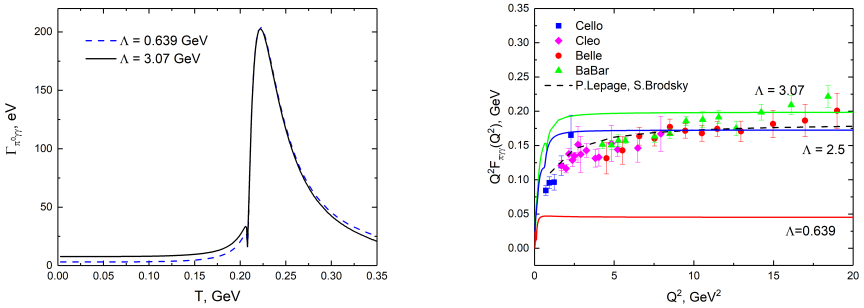

Fig. 3: Left side: the temperature behavior of the pion photo-decay width for various values of the cut-off parameter Λ. Right side: transition form factor as function of transferred momentum for for different choices of Λ.

the right panel of Fig. 3 as a function of Q^2. The transition form factor (TFF) is calculated within the NJL model using $\Lambda = 0.652, 2.5$ and $\Lambda = 3.07$ GeV, where the last value reproduces the experimental result for $\Gamma_{\pi^0\gamma\gamma}$.

5. Results

An algorithm for detecting singularities in improper integrals of the second type has been developed. The resulting algorithm demonstrates a significant increase in convergence compared to the earlier algorithm based on sub-division of the entire integration domain into sub-segments [3]. The resulting list of identified singular points is used for the numerical integration producing results with acceptable error. The implementation of a parallelization strategy significantly reduces computation time.

The proposed algorithm was applied to calculate the temperature dependence of the two-photon decay width of the neutral pion $\Gamma(\pi^0 \to \gamma\gamma)$ and the pion transition form factor as a function of the transferred momentum in the framework of the Nambu-Jona-Lasinio model. The obtained results reproduce the results of previous theoretical research and experimental data, when appropriate cut-off parameter is chosen.

The calculations were carried out on the Govorun supercomputer. The calculations were carried out on the heterogeneous cluster [6] of the Joint Institute for Nuclear Research and supercomputer Govorun [7].

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