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Regularized computation of oscillatory integrals with stationary points

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ABSTRACT

Ability to calculate integrals of rapidly oscillating functions is crucial for solving many problems in optics, electrodynamics, quantum mechanics, nuclear physics, and many other areas. The article considers the method of computing oscillatory integrals using the transition to the numerical solution of the system of ordinary differential equations. Using the Levin's collocation method, we reduce the problem to solving a system of linear algebraic equations.

In the case where the phase function has stationary points (its derivative vanishes on the interval of integration), the solution of the corresponding system becomes an ill-posed task. The regularized algorithm presented in the article describes the stable method of integration of rapidly oscillating functions at the presence of stationary points. Performance and high accuracy of the algorithms are illustrated by various examples.

1. Introduction

Let us consider the method for the evaluation of the oscillatory integral

$$I = \int_a^b f(x)e^{i\omega g(x)}\,\mathrm{d}x \equiv \int_a^b F(x)\,\mathrm{d}x, \qquad (1)$$

assuming that the constant of oscillations $\omega \gg 1$ is a "large" value; and in the domain if integration the amplitude $f(x)$ and phase $g(x)$ are sufficiently smooth functions.

This type of integrals is of great interest and is of fundamental importance for the solution of many applied problems. Rapidly oscillating phenomena occur in electromagnetics, quantum theory, fluid dynamics, acoustics, electrodynamics, molecular modeling, computerized tomography and imaging, plasma transport, celestial mechanics and many other areas [1]. A great number of studies are devoted to the numerical integration of highly oscillating functions that appears very frequently in a wide range of practical applications, such as engineering applications, Fourier transform, signal processing, image recognition, fluid dynamics and electrodynamics.

This type of oscillatory integrals may be useful in investigation of the interaction of atoms and molecules with external electric (laser) fields [2–4]. The processes in which a fast ion captures one or several electrons colliding with an atomic target is studied in [5].

The multiple ionization of atoms and molecules by photon or charged-particle impact is of considerable interest in many branches of physics, such as plasma physics, astrophysics and radio-physics. Such processes are also important to understand the electronic structure, the ionization mechanisms and to probe electron-electron correlation in the case of double ionization which is the main cause of this process [6,7]. All of these studies deal with the problem of numerical integration of highly oscillating functions.

Such a wide use of integrals from rapidly oscillating functions makes development of adequate methods and algorithms of their numerical calculation quite urgent. Examples of such researches

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include the solution of highly oscillatory differential equations via the modified Magnus expansion [8,9], boundary integral formulations of the Helmholtz equation [10], the evaluation of special functions and orthogonal expansions (Fourier series, modified Fourier series) [11], ODEs/PDEs with oscillating and quasi-periodic coefficients [12–14], and some other types of oscillatory functions [15,16].

The traditional methods of quadrature mentioned above are well studied and work well in cases where the phase function has no stationary points. However, in the case where the phase function has stationary points (its derivative vanishes at the interval of integration) and calculating the corresponding integral becomes an ill-posed problem.

For solving this problem, various methods are proposed [17–20], but their practical use is not an easy work. We would like to present more general and much simpler approach.

The integrals of this type can be effectively calculated using the following methods: the Levin-type method [21,22,17], the method of steepest descent [18]. For integrands with linear phase Filon method [23,24] is often used, which works reliably. It is based on building composite quadrature formulas in which at each partial interval an interpolation polynomial of low degree is used to approximate the amplitude $f(x)$.

The Levin collocation method is suitable for finding the oscillatory integrals with complex amplitude and phase functions. It consists in moving on to finding the antiderivative $p(x)$ of the integrand satisfying the condition

$$\frac{\mathrm{d}}{\mathrm{d}x}[p(x)e^{i\omega g(x)}] = f(x)e^{i\omega g(x)}. \tag{2}$$

Knowing the a particular solution $p(x)$ on the interval of integration (or more precisely, at the end points of this interval), one can calculate the value of the integral of the oscillating function with the formula

$$I[f] = \int_a^b fe^{i\omega g}\ \mathrm{d}x = \int_a^b \frac{\mathrm{d}}{\mathrm{d}x}[pe^{i\omega g}]\ \mathrm{d}x = p(b)e^{i\omega g(b)} - p(a)e^{i\omega g(a)}. \tag{3}$$

In the collocation method the problem of calculating the integral is replaced by the "equivalent" problem of finding the values of the function antiderivative at two points at the ends of the integration interval $[a, b]$, allowing to calculate the value of the integral $I[f]$ with the formula (3). Note that the method does not use the boundary conditions for the solution of the problem (2), because any particular solution allows to calculate the value of the definite integral [22].

Let us consider the problem of finding the antiderivative of the integrand, or, more precisely, of the function $p(x)$ satisfying the condition (2) at certain points on the interval $[a, b]$. Let us dwell on spectral methods of finding the unknown function in the problem of integrating the rapidly oscillating functions. These spectral methods use a representation of the function as an expansion in series

$$p(x) = \sum_{k=0}^{\infty} c_k\varphi_k(x) \tag{4}$$

over the basis $\{\varphi_k(x)\}_1^\infty$ in the Hilbert space. To achieve an acceptable accuracy of the approximation it is often necessary to use a sufficiently large number $(n+1)$ of terms in the series. Consider the "operator" $L[p] = p' + i\omega g'p$ and the equation $L[p](x) = f(x)$. Its solution has to be such that with certain coefficients c_k, $k = 1, \ldots, n$ the following equalities should be fulfilled

$$L\left[\sum_{k=0}^{n} c_k\varphi_k(x_j)\right] = f(x_j), \quad j = 0, \ldots, n \tag{5}$$

at collocation points $\{x_0, \ldots, x_n\}$, i.e. coefficients c_k can be defined as the solution of the system of equations of the collocation method:

$$\begin{cases} L[p](x_0) = f(x_0), \\ \ldots \\ L[p](x_n) = f(x_n). \end{cases} \tag{6}$$

While determining the approximate value of the integral $I[f]$ in the form

$$Q^L[f] = \int_a^b L(p)e^{i\omega g}\ \mathrm{d}x = \int_a^b \frac{\mathrm{d}}{\mathrm{d}x}[pe^{i\omega g}]\ \mathrm{d}x = p(b)e^{i\omega g(b)} - p(a)e^{i\omega g(a)} \tag{7}$$

the following estimate of the approximation error is valid [24]:

$I[f] - Q^L[f] = O(\omega^{-1})$ — in the case where the boundary points are not included in the number of grid nodes;
$I[f] - Q^L[f] = O(\omega^{-2})$ — in the case where the boundary points are included in the number of grid nodes.

These estimates imply very simple practical conclusion that inclusion of the boundary points in the number of grid nodes allows to increase by an order the accuracy of the solution.

Thus, the problem of the approximate calculation of the integral (1) from rapidly oscillating function can be reduced to solving the system of equations (6). By an appropriate choice of the approximation points, i.e. their location within the range of integration and their number, it is possible to improve the accuracy of the solution.

2. Approximation of a (sought antiderivative) function by the Chebyshev polynomials. Differentiation matrix in the frequency and physical spaces

Among many basis systems of polynomials used to approximate functions on finite intervals the Chebyshev polynomials of the first kind have proven well for practical calculations. We assume that the interval of integration is $[a, b] = [-1, 1]$. And we consider the Chebyshev polynomials of the first kind $T_k(x)$, $k = 0, \ldots, n$ as basis functions. Suppose that we know the values of some polynomial $p(x)$ of the nth degree at $(n+1)$ points $\mathbf{x} = (x_0, \ldots, x_n)$. Then these values define the polynomial uniquely and hence uniquely determine the values $p'(x) = \mathrm{d}p(x)/\mathrm{d}x$ of its derivatives at these points. Furthermore, the value of the derivative at every point can be represented as a linear combination of values of the polynomial at these points. This dependence can be written in matrix form [25] as

$$\mathbf{p}'(\mathbf{x}) = \mathbf{D}\mathbf{p}(\mathbf{x}). \tag{8}$$

The matrix $\mathbf{D} = \{d_{kj}\}$ is called the differentiation matrix in the physical space.

If the basis functions are the Chebyshev polynomials of the first kind, and grid points are the Gauss–Lobatto nodes

$$x_j = \cos\frac{j\pi}{N}, \quad j = 0, \ldots, N, \tag{9}$$

then the elements of antisymmetric Chebyshev differentiation matrix are calculated as follows [25]:

$$d_{kj} = \begin{cases} \dfrac{c_k}{c_j}\dfrac{(-1)^{k+j}}{(x_k - x_j)}, & k, j = 0, \ldots, N, \quad k \neq j, \\ -\displaystyle\sum_{\substack{n=0 \\ n \neq k}}^{N} d_{kn}, & k = j. \end{cases} \tag{10}$$

Note. It is easy to check that the sum of the columns of the Chebyshev matrix is the zero vector, therefore, the differentiation matrix $\mathbf{D} = \{d_{kj}\}$ is *degenerate* [25].