

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.

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1. Introduction

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

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

assuming that the constant of oscillations $\omega \gg 1$ is a "large" value; and in the domain of 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

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

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

$$I[f] = \int_a^b f e^{i\omega g} dx = \int_a^b \frac{d}{dx}[p e^{i\omega g}] dx = p(b)e^{i\omega g(b)} - p(a)e^{i\omega g(a)}. \quad (3)$$

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

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

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 $c_k, k = 1, \dots, n$ the following equalities should be fulfilled

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

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

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

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

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

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 $T_k(x), k = 0, \dots, n$ as basis functions. Suppose that we know the values of some polynomial $p(x)$ of the n th degree at $(n+1)$ points $\mathbf{x} = (x_0, \dots, x_n)$. Then these values define the polynomial uniquely and hence uniquely determine the values $p'(x) = dp(x)/dx$ 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

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

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

$$x_j = \cos \frac{j\pi}{N}, \quad j = 0, \dots, N, \quad (9)$$

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

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

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].

Approximation of the function by the Chebyshev polynomials of the first kind is remarkable by the fact that it allows to easily calculate the coefficients of the function derivative in the expansion in terms of the same polynomials. Thus, if $p(x) = \sum_{k=0}^n a_k T_k(x)$, then the coefficients b_k , $k=0, \dots, n$ of the derivative of the function $p(x)$

$$\frac{d}{dx} p(x) = \frac{d}{dx} \left(\sum_{k=0}^n a_k T_k(x) \right) = \sum_{k=0}^n b_k T_k(x) \quad (11)$$

can be calculated using recurrent relations $T_k(x) = 2xT_{k-1}(x) - T_{k-2}(x)$, $k=2, 3, \dots$, together with the initial conditions $T_0(x)=1$, $T_1(x)=x$, as the solution of the simple tridiagonal system of linear algebraic equations [26, p. 6, 162].

From the relation (11) one can [26] derive a formula linking these coefficients in the “reverse” order by using the upper triangular differentiation matrix \mathbf{B} in frequency space (with zeros on the main diagonal):

$$\mathbf{B}\mathbf{a} = \mathbf{b} \quad (12)$$

where

$$B_{ij} = \begin{cases} (1/c_j) \times 2j, & \text{if } i > j \text{ and the sum } i+j \text{ is odd,} \\ 0, & \text{otherwise.} \end{cases}$$

Here

$$0 \leq i, \quad j \leq n, \quad c_i = \begin{cases} 2, & i=0, \\ 1, & i>0. \end{cases}$$

Note. The matrix \mathbf{B} is upper triangular and contains zeros on the main diagonal.

Let us consider the relationship of differentiation matrices in the physical and phase spaces.

Theorem. Differentiation matrices in the physical and phase spaces are related by the relation $\mathbf{TB} = \mathbf{DT}$ where matrix \mathbf{T} is the Chebyshev transform, which maps the coefficients \mathbf{a} of a Chebyshev series into the values that series takes at \mathbf{x} .

Proof. Let us write down the expression for the derivative of a function, approximated by the Chebyshev polynomials in the physical space: $\mathbf{p}'(\mathbf{x}) = \mathbf{Dp}(\mathbf{x}) = \mathbf{DT}(\mathbf{x})\mathbf{a}$. In frequency space the same derivative will look like $\mathbf{p}' = \mathbf{Tb}$.

Taking into account that in the frequency space the vector $\mathbf{p}(\mathbf{x})$ can be represented as

$$\mathbf{p} = \mathbf{Ta}, \quad (13)$$

where matrix \mathbf{T} is the Chebyshev transform, which maps the coefficients \mathbf{a} of a Chebyshev series into the values the series takes at \mathbf{x} .

Chebyshev transform consists of $T_{ij} = T_i(x_j)$, $i, j=0, \dots, n$, where each column T_i , $i=0, \dots, n$ consists of Chebyshev polynomial with values at j th collocation point. The derivative in the frequency space is calculated in accordance with the expression

$$\mathbf{p}' = \mathbf{Tb} = \mathbf{Tb}. \quad (14)$$

From Eqs. (8) and (14) it follows

$$\mathbf{TB} = \mathbf{DT} \quad (15)$$

Consequence. The relationship between matrices \mathbf{B} and \mathbf{D} is carried out using elementary transformations $\mathbf{B} = \mathbf{T}^{-1}\mathbf{DT}$ and $\mathbf{D} = \mathbf{TBT}^{-1}$.

3. Regularization of the method of quadrature

In the case where the integration is set on the interval $x \in [a, b]$, then the transition to a standard domain $[-1, 1]$ of the Chebyshev polynomials of the first kind can be carried out by the change of

variables $x = \frac{b-a}{2}t + \frac{b+a}{2}$, $t \in [-1, 1]$. The derivative of the required function is calculated by the formula

$$p'(x) = \frac{2}{b-a} p'(t). \quad (16)$$

According to the introduced linear transformation the Gauss–Lobatto nodes $t_j = \cos\left(\frac{j\pi}{n}\right)$ in the original coordinates have the form

$$x_j = \frac{b-a}{2} \cos\left(\frac{j\pi}{n}\right) + \frac{b+a}{2}, \quad j=0, 1, \dots, n.$$

Vectors of the functions values and their derivatives at the Gauss–Lobatto nodes are calculated by the formulas

$$\begin{aligned} \mathbf{p} &= [p(x_0), p(x_1), \dots, p(x_n)]^T, \quad \mathbf{p}' = [p'(x_0), p'(x_1), \dots, p'(x_n)]^T, \\ \mathbf{f} &= [f(x_0), f(x_1), \dots, f(x_n)]^T, \quad \mathbf{g}' = [g'(x_0), g'(x_1), \dots, g'(x_n)]^T. \end{aligned} \quad (17)$$

Obviously, in accordance with the definition of the Chebyshev differentiation matrix, we can write \mathbf{p}' in vector-matrix form of (16) taking into account (8) and (10):

$$\mathbf{p}' = \frac{2}{b-a} \mathbf{Dp} \quad (18)$$

and the system (6) can now be written as

$$\frac{2}{b-a} \mathbf{Dp} + i \cdot \text{diag}(\omega \mathbf{g}') \mathbf{p} = \mathbf{f}, \quad (19)$$

or

$$(\mathbf{D} + i\omega \mathbf{A}) \mathbf{p} = \lambda \mathbf{f}, \quad (20)$$

where $\lambda = (b-a)/2$, $\mathbf{A} = \text{diag}(\lambda g'(x_0), \lambda g'(x_1), \dots, \lambda g'(x_n))$ is diagonal matrix. The solution of the system (20) contains $p(b)$ and $p(a)$, whereas the required integral is calculated using the formula (7).

Theorem. Matrix of the system (20) $(\mathbf{D} + i\omega \mathbf{A})$ becomes singular only when at least one of the values $g'(x_k)$, $k=0, \dots, n$ becomes zero.

Proof. Suppose a diagonal matrix $\mathbf{A} = \text{diag}(\lambda g'(x_0), \lambda g'(x_1), \dots, \lambda g'(x_n))$ is composed of non-zero elements. Then for matrix \mathbf{B} , defined by (12), $\det(\mathbf{B} + i\omega \mathbf{A}) = \det(i\omega \mathbf{A})$, and thus

$$\det(\mathbf{D} + i\omega \mathbf{A}) = \det(\mathbf{T}(\mathbf{B} + i\omega \mathbf{A})\mathbf{T}^{-1}) = \det(\mathbf{B} + i\omega \mathbf{A}) \neq 0,$$

because the matrix \mathbf{T} is non-singular.

Let us write down Eq. (20) in the case of finding a solution in frequency space, taking into account that $\mathbf{D} = \mathbf{TBT}^{-1}$, and $\mathbf{p} = \mathbf{Ta}$:

$$\mathbf{TBa} + i\omega \mathbf{ATa} = \lambda \mathbf{f}. \quad (21)$$

Note. Both matrices $\mathbf{B} + i\omega \mathbf{A}$ and $\mathbf{D} + i\omega \mathbf{A}$ are degenerate (or not degenerate) simultaneously.

That equation is still valid for an arbitrary set of different grid points.

Here, in order to reduce formulas the following designations are used: $T_{ij} = T_i(x_j)$ and $\lambda_i = \lambda \omega g'(x_i)$. The solution to this system of linear algebraic equations for the coefficients of the n th degree Chebyshev series $\mathbf{a} = (a_0, a_1, \dots, a_n)$ over the basis functions allows to determine the approximate value of the integral using Eq. (7).

The method proposed by the authors modifies the Levin method to the case of the existence of stationary points of the phase function, when the Levin method cannot be applied directly to calculate the desired integrals. This is explained by the fact that in the numerical implementation of the Levin algorithm, the resulting system of linear algebraic equations, whose solution gives us the opportunity to eventually compute the integral, is degenerate or almost degenerate (with very small eigenvalues close to zero). Of course, one can apply the Tikhonov regularization method or TSVD to obtain an approximate solution of the resulting system of linear algebraic equations, but this in itself will introduce into the solution some

Table 1
Dependence of the residual amount on the number of approximating polynomials.

Nodes n	Residual. Algorithm without regularization		Residual. Algorithm with regularization (5, 0i)	
	Re	Im	Re (Regularization)	Im (Regularization)
30	4.03221E–06	2.13053E–06	3.60128E–06	6.75707E–06
40	4.42854E–09	3.2344E–10	2.22451E–09	4.7457E–10
50	4.82014E–12	5.28999E–12	8.80185E–13	1.00364E–13
60	5.9508E–14	9.76996E–15	0	0
65	9.76996E–15	0	0	0

additional errors that will later affect the accuracy of the integral calculation.

The approach of the authors is to use a fairly simple method of simultaneous transformation of the amplitude and phase functions (with the integrand remaining unchanged) in order to get rid of the stationary points of the phase function and, consequently, to overcome the degeneracy of the system of linear algebraic equations of the Levin method. In this case, it is possible to use the simple and effective Levin method for calculating integrals in the case of the initial presence of stationary points.

Instead of the possible method of regularization or the method of penalty functions of a general form, the authors propose an “analog” of the exact penalty function method, in which the operands are perturbed, but the final solution remains unperturbed. Namely, the proposed simultaneous transformation of the amplitude and phase functions is equivalent to the spectral shift to the region of positive eigenvalues of the matrix of a system of linear algebraic equations with a simultaneous change of the right-hand side.

In order to deliberately avoid the singularity of the matrix $\mathbf{TB} + i\omega\mathbf{AT}$ of the system (21) even in the case of stationary points, we modify the integrand, multiplying and dividing it by the same function $\exp(iCx)$, where C is a complex number. Then the integral (1) takes the form

$$\int_a^b f(x)e^{-iCx} e^{i(Cx+\omega g(x))} dx. \quad (22)$$

Multiplying and dividing by a function $\exp(iCx)$ does not lead to the appearance of a singularity and the value of the integrand does not change [27].

Regularization theorem. In case $\text{Re}(C) > -\omega|g'(x)|$ the matrix $\tilde{\mathbf{M}} = \mathbf{TB} + i\omega\tilde{\mathbf{A}}\mathbf{T}$ is non-degenerate and there exists the unique solution of the system (23).

Proof. Introducing the notations $\tilde{f}(x) = f(x)e^{-iCx}$ and $\tilde{g}(x) = C(x) + \omega g(x)$, we get a new equation for new unknown coefficients $\tilde{\mathbf{a}}$, similar to Eq. (21):

$$\mathbf{TB}\tilde{\mathbf{a}} + i\omega\tilde{\mathbf{A}}\mathbf{T}\tilde{\mathbf{a}} = \lambda\tilde{\mathbf{f}}. \quad (23)$$

Choosing the constant C in (22) in such a way that the inequality $\text{Re}(C) > -\omega|g'(x)|$, $x \in [a, b]$ is true, allows to ensure all diagonal elements of the matrix of the linear algebraic equations system (23) being nonzero, and guarantees the existence and uniqueness of the system solution.

The proposed simultaneous transformation of the amplitude and phase functions is equivalent to the spectral shift to the region of positive eigenvalues of the matrix of a system of linear algebraic equations with a simultaneous change of the right-hand side. The solution of the system itself may change, but the functional $p(b) - p(a)$ is transformed into $\tilde{p}(b) - \tilde{p}(a)$, which remains unchanged.

Ensuring sustainability is much more difficult due to the structure of the system (23), in which the elements with maximum absolute values are concentrated in the far right column of the matrix — see formula (12). However, using this regularization method allows to improve the properties of the system (taking

into account the number of approximation points), and to increase (in absolute value) the diagonal elements by choosing constant C , thus ensuring the predominance of the leading elements on the diagonal.

4. Numerical results illustrating the method

Example 1. Let us calculate quite simple integral $\int_0^\pi x^2 \exp(i \sin(4x)) dx$ with the phase function $\sin(4x)$, which has 4 stationary points in the interval $[0, \pi]$.

The exact value of the integral, calculated using the Maple CAS with an accuracy up to 20 significant digits is: 7.9313270043818201811, -2.2039905892931603323 . The constant C for the regularized algorithm is selected using only one criterion: $\text{Re}C > -\omega|g'(x)|$, $x \in [a, b]$, $C = (5, 0i)$.

Results of calculating the integral value depending on the number of grid nodes are shown in Table 1.

Example 2. Consider the calculation of the integral with a stationary point $x = 0$

$$I(x) = \int_{-1}^1 e^{i\omega x^4} dx, \quad (24)$$

when $\omega = -100$. Here the amplitude function is a constant $f(x) = 1$, the phase function is four times differentiable function and the first three of its derivatives vanish at the point $x = 0$. The exact numerical value of the integral calculated using one of the packages for symbolic computation is the following

$$I(x_{\text{exact}}) = (0.5270586802656407 - i \cdot 0.2150847721248018).$$

Calculations carried out using the proposed algorithm lead to the following result. The graph shows the deviation of the obtained solutions from the exact solution depending on the number of approximation points for the derivative of the function and the value of the “regularization” parameter C (logarithmic scale).

At the zero value of the regularization parameter C the deviation from the exact solution essentially depends on the position of one (central) of the grid points with respect to a stationary point ($x = 0$) of the phase function. Depending on whether the grid point coincides with a stationary point the solution can deviate from the exact one by several orders. For example, at $N = 210$ and the value $C = (0, 0i)$ $\Delta I = 2.4128 \cdot 10^{-14}$, and at $N = 211$ and the same value of C , the deviation from the exact value $\Delta I = 2.60076 \cdot 10^{-9}$ is by 5 orders of magnitude greater.

With the increase of the real part of the parameter C the solution becomes smoother and less sharply varies depending on the number of approximation points. In addition, the speed of convergence is greatly increased, and the accuracy limit (of the order 10^{-15}) is achieved with fewer grid points (see Fig. 1).

Example 3. Consider an example that demonstrates the existence of a large number of stationary points (in the interval $[-1/2, 0]$ all the points are stationary) (Fig. 2).

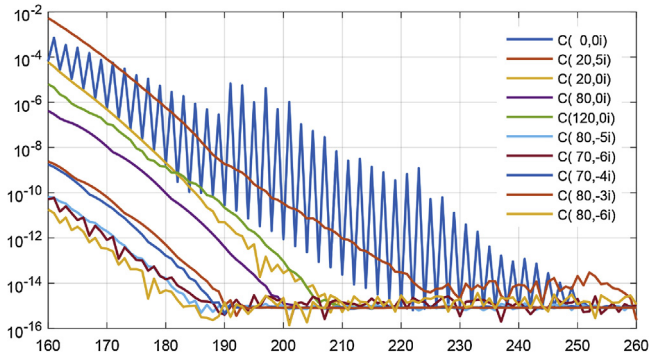


Fig. 1. Graphs of absolute deviations of the solutions $\Delta I = \|I_{\text{exact}} - I_{\text{calculated}}(N, C)\|$.

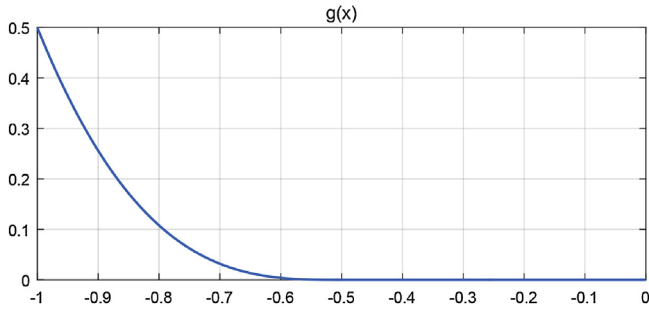


Fig. 2. Graph of the phase function $g(x)$.

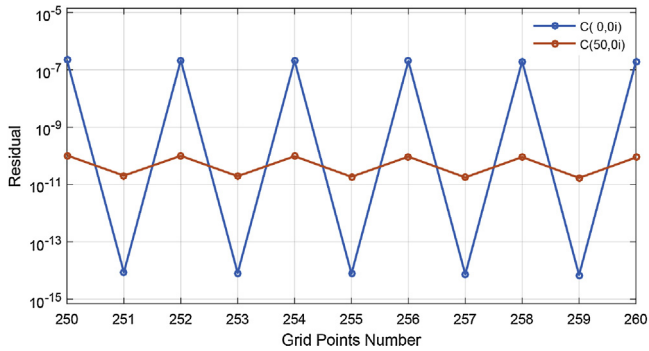


Fig. 3. Graph of the residual when changing the number of approximation points from 250 to 260: Blue line — without regularization, orange line — at the complex parameter $C = (50, 0i)$. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of the article.)

$$\int_{-1}^0 f(x) \exp(i\omega g(x)) dx, \quad (25)$$

$$\text{where } f(x) = 1, \omega = 100, g(x) = \begin{cases} \left(x + \frac{1}{2}\right)^4, & x \in \left[-1, -\frac{1}{2}\right] \\ 0, & x \in \left[-\frac{1}{2}, 0\right]. \end{cases}$$

The exact numerical value of the integral calculated using one of the packages for symbolic computation $I(x_{\text{exact}}) = (0.5270586802656407 - i \cdot 0.2150847721248018)$.

Calculations carried out using the proposed algorithm lead to the following result (see Figs. 3 and 4). With an odd number of approximation points the accuracy limit is practically achieved. In the case when the singular point ($x = -1/2$) falls into the set of approximation points, the deviation of the obtained solution from the exact solution is minimal: $\Delta I \approx 1.5 \cdot 10^{-15}$. With an even number of points, the singularity point ($x = 1/2$) does not fall into the set of approximation points. In the case of changing the number of approximation points from 250 to 260, with the regularization

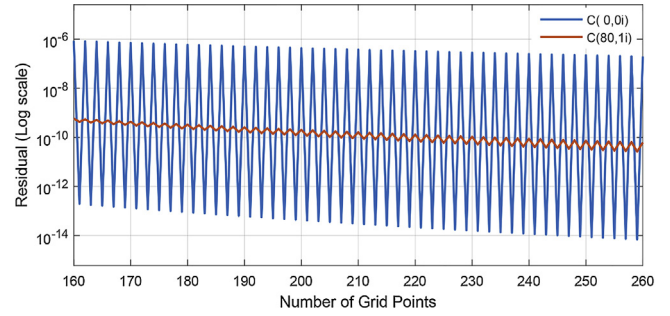


Fig. 4. Graph of the residual when changing the number of approximation points from 160 to 260: Blue line — without regularization, orange line — at the complex parameter $C = (50, 0i)$. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of the article.)

parameter $C = (50, 0i)$, the residual is increased by several orders of magnitude $\Delta I \approx 2.5 \cdot 10^{-7}$ (see Fig. 3).

In the case of changing the number of approximation points from 160 to 260, the regularization with the parameter $C = (50, 0i)$ ensures greater stability of the solution depending on the number of approximation points (see Fig. 4).

5. Conclusion

The article describes the new regularized algorithm for computing integrals of rapidly oscillating functions allowing effectively and accurately determine the required value in the presence of stationary points. In the case where the phase function has stationary points (its derivative vanishes on the interval of integration) the calculation of the corresponding integral is still a sufficiently difficult task even for the Levin method due to the degeneracy of the resulting system of linear equations. The basic idea of regularization, described in the article, is the simultaneous modification of the amplitude and phase functions, which does not change the integrand, but eliminates the degeneracy of the phase function in the interval of integration. Practically, this means a transition from calculating $\int_a^b f(x) e^{i\omega g(x)} dx$ to the integration of the new integrand $f(x) e^{-iCx} e^{i(Cx + \omega g(x))}$, where the constant C is chosen from the condition $\text{Re}(C) > -\omega |g'(x)|$, $x \in [a, b]$.

The numerical examples in the article show significant increase in integration accuracy when using regularization even in the absence of the stationary points. Properties of linear algebraic system are improved with increasing (by selecting constant C) of the diagonal elements of the matrix, providing the predominance of the leading elements on the diagonal.

A similar approach can be extended to the integrals in infinite limits using other (non-Chebyshev functions of the first kind) basis functions.

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References

- [1] A. Iserles, *Highly Oscillatory Problems*, Cambridge University Press, Cambridge, 2009.
- [2] A.G. Galstyan, O. Chuluunbaatar, Y.V. Popov, B. Piraux, Effects of nonzero photon momentum in $(g, 2e)$ processes, *Phys. Rev. A* 85 (2012), 023418-1-5.
- [3] A. Galstyan, O. Chuluunbaatar, A. Hamido, Y.V. Popov, F. Mota-Furtado, P.F. O'Mahony, N. Janssens, F. Catoire, B. Piraux, Reformulation of the strong-field approximation for light-matter interactions, *Phys. Rev. A* 93 (2016), 023422-1-14.

- [4] A. Galstyan, Y.V. Popov, F. Mota-Furtado, P.F. O'Mahony, N. Janssens, S. Jenkins, O. Chuluunbaatar, B. Piraux, Modelling laser-atom interactions in the strong field regime, *Eur. Phys. J. D* 71 (2017), 97–111.
- [5] P.S. Vinitsky, Y.V. Popov, O. Chuluunbaatar, Fast proton-hydrogen charge exchange reaction at small scattering angles, *Phys. Rev. A* 71 (2005), 012706–1–9.
- [6] F.W. Byron Jr., C.J. Joachain, Multiple ionization processes in helium, *Phys. Rev.* 164 (1967) 1.
- [7] O. Chuluunbaatar, B.B. Joulakian, I.V. Puzynin, K. Tsokhuu, S.I. Vinitsky, Modified two-center continuum wave function: application to the dissociative double ionization of H_2 by electron impact, *J. Phys. B* 41 (2008), 015204–1–6.
- [8] A. Iserles, On the global error of discretization methods for highly-oscillatory ordinary differential equations, *BIT* 42 (2002) 561–599.
- [9] M. Hochbruck, C. Lubich, On Magnus integrators for time-dependent Schrödinger equations, *SIAM J. Numer. Anal.* 41 (3) (2003) 945–963.
- [10] B.N. Khoromskij, S. Sauter, A. Veit, Fast quadrature techniques for retarded potentials based on TT/QT tensor approximation, *Comput. Methods Appl. Math.* 11 (3) (2011) 342–362.
- [11] A. Iserles, S. Nørsett, From high oscillation to rapid approximation. I: Modified Fourier expansions, *IMA J. Numer. Anal.* 28 (2008) 862–887.
- [12] V. Khoromskaia, B.N. Khoromskij, Grid-based lattice summation of electrostatic potentials by assembled rank-structured tensor approximation, *Comp. Phys. Commun.* 185 (1) (2014) 3162–3174.
- [13] V. Khoromskaia, B.N. Khoromskij, Tensor approach to linearized Hartree–Fock equation for lattice-type and periodic systems, in: *MPI MIS preprint* 62, 2014, pp. 62.
- [14] B.N. Khoromskij, Tensor numerical methods for multidimensional PDEs: basic theory and initial applications, *ESAIM: Proc. Surv.* 48 (2014) 1–28, Edited by N. Champagnat, T. Lelièvre, A. Nouy.
- [15] S. Xiang, W. Gui, P. Mo, Numerical quadrature for Bessel transformations, *Appl. Numer. Math.* 58 (9) (2008) 1247–1261.
- [16] A. Iserles, D. Levin, Asymptotic expansion and quadrature of composite highly oscillatory integrals, *Math. Comp.* 80 (2011) 279–296.
- [17] J. Li, X. Wang, T. Wang, S. Xiao, An improved Levin quadrature method for highly oscillatory integrals, *Appl. Numer. Math.* 60 (2010) 833–842.
- [18] S. Olver, D. Huybrechts, Chapter 2: Highly oscillatory quadrature, in: *Highly Oscillatory Problems: Computation, Theory and Applications*, Cambridge University Press, Cambridge, 2008.
- [19] L. Ying, Fast evaluation of canonical oscillatory integrals, *Appl. Math. Inf. Sci.* (2012) 245–251.
- [20] O. Sheehan, *Fast, Numerically Stable Computation of Oscillatory Integrals with Stationary Points*, Oxford University Computing Laboratory, Oxford, United Kingdom, 2009.
- [21] D. Levin, Fast integration of rapidly oscillatory functions, *J. Comput. Appl. Math.* 67 (1996) 95–101.
- [22] G. Evans, J. Webster, A comparison of some methods for the evaluation of highly oscillatory integrals, *J. Comput. Appl. Math.* 112 (1999) 55–69.
- [23] L. Filon, On a quadrature formula for trigonometric integrals, *Proceedings of the Royal Society of Edinburgh* vol. 49 (1928) 38–47.
- [24] A. Iserles, On the numerical quadrature of highly-oscillatory integrals. I: Fourier transforms, *IMA J. Numer. Anal.* 24 (2004) 1110–1123.
- [25] J. Mason, D. Handscomb, *Chebyshev Polynomials*, Chapman and Hall/CRC, 2002.
- [26] B. Fornberg, *A Practical Guide to Pseudospectral Methods*, Cambridge University Press, Cambridge, 1996.
- [27] K. Lovetskiy, L. Sevastianov, N. Nikolaev, Regularized computation of oscillatory integrals with stationary points, *Procedia Comput. Sci.* 108 (2017) 998–1007.



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