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Efficient quadrature for fast oscillating integral of paraxial optics

Abstract The study concerns the determination of quadrature for the integral solution of the paraxial wave equation. The difficulty in computation of the integral is associated with the rapid change of the integrand phase. The developed quadrature takes into account the fast oscillating character of the integrand. The presented method is an alternative to the commonly used methods based on the use of the Fourier transform. The determination of the quadrature is discussed on the example of the integral arisen in the theory of propagation and focusing on hard X-rays waves. Due to the generality of the presented quadrature, it may also be applied to issues related to standard optics and acoustics.

2010 Mathematics Subject Classification: 65D32, 65E05, 65Z05, 35Q60.

Key words and phrases: paraxial wave equation, quadrature, quick oscillating integrands, X-ray optics.

1. Introduction An efficient method of integrals calculation of fast oscillating functions is topical due to many applications in applied mathematics, physics and engineering. The integrals of this type are difficult to calculate using standard methods of numerical integration when the rate of oscillations of the integrands exceeds the number of quadrature points. The method for calculation of such integrals was for the first time suggested by Filon [5], and since then many various improvements have been submitted for the calculation of a generalized Fourier transform. For example, these are methods of Clenshaw - Curtis type [2], [4], Levin's method [19], [20], [21], methods of Levin type [23], Huybrechs and Vandewalle method [7], and also [30], [31], [22], [9], [10], [11], [33], [34].

Filon numerical quadrature for the integral $\int_{a}^{b} f(x) e^{i\omega g(x)} dx$ is based on approximation of the function f(x) by a polynomial p(x) using values of the function f(x) in nodes and the subsequent calculation of the integral

^{*} This publication is co-financed by the European Union as part of the European Social Fund within the project Center for Applications of Mathematics.

 $\int_{a}^{b} p(x) e^{\omega g(x)} dx \text{ instead of the integral } \int_{a}^{b} f(x) e^{i\omega g(x)} dx. \text{ Iserles [8], [9] analyzed the method convergence at various oscillation frequencies and he showed that the accuracy of quadrature formulas increases, when the oscillation frequency increases. Later Iserles and Nîrsett [10], [11] expanded the approach [8], [9], and also suggested a generalization of Filon's method for the integral <math>\int_{a}^{b} f(x) e^{i\omega g(x)} dx.$ They showed that with the growth of frequency ω , the error of approximation may be decreased. In both methods, in Filon's method and in the generalized Filon's method, the function f(x) is approximated by splines, which may be used for smooth enough functions, provided that the moments $\int_{a}^{b} x^{k} e^{i\omega g(x)} dx$ may be precisely calculated for first values of the parameter k [11].

Levin's method [19] is applicable to a wide class of the integrals

$$\int_{a}^{b} f(x) e^{i\omega g(x)} dx$$

without the explicit calculation of the moments. The initial problem of integration had been transformed to the problem solved by the collocation method, with the weight function satisfying a certain differential equation. Levin showed [20] that for ω large enough, accuracy increases with the increase of the function oscillation rate. Xiang showed that in case of a smooth enough function f(x) Filon's method is identical to Levin's method with the suitable polynomial interpolation [34].

In the present paper, the method of numerical computation of the integral (1) with a quickly oscillating integrand is considered. The integral (1) gives a solution to the paraxial wave equation (4) [35], [3], [6], [32], [26]. The problem has arisen due to scientific research and developments in modern technologies in the field of hard X-ray microscopy: it has many various practical uses. Therefore, in the beginning of the work some applications of the considered integral are shortly presented. The presented facts have technical character and illuminate the requirements of the developed method of the integral calculation. They also provide information about a class of functions, which is useful for consideration of the investigated problem. Nevertheless, this technical information can be omitted without the loss of understanding of mathematical aspects. The considered integral is two-dimensional, but the approach to calculation of quickly oscillating integrals is applicable to this kind of problems as well.

Within the paper, only the application of the integral to the problem of hard X-rays propagation and focusing is considered. However, the same equations describe any electromagnetic wave within the limits of the paraxial approach, and a quasi-monochromatic acoustic wave with a corresponding parity in scales (in order to address to acoustic problems, it is necessary to replace the speed of light with the sound speed). Therefore, the submitted method of calculation may be useful not only in hard X-ray optics, but also in standard optics and in acoustics.

2. Integral of the theory of propagation of electromagnetic waves within the paraxial approach Due to the nanotechnologies development and chemical and biological research [27], [18], [29], [25], [28], [12], [13], X-ray microscopy developed quickly during the last 15-20 years. The basic scheme of an X-ray microscope is presented in Fig. 1.



Figure 1: A schematic drawing of an X-ray microscope. The monochromatic beam of X-rays falls onto a system of lenses (for simplification only one lens is shown). The distribution of an electromagnetic field after the lenses (at x = 0) is given by A(0, y, z). The distribution of an electromagnetic field A(x, y, z) on the detector has to be calculated.

In order to obtain focusing of X-rays, roentgen waves propagate through a special system of lenses, subsequently the X-rays propagate in air, until reaching the detector, where an image is fixed. A solution of the electrodynamics problem describing the X-rays propagation between lenses and the detector is known and it is given by the integral [12], [16], [17], [14]

$$A(x, y, z) = \iint_{S} A(0, \xi, \eta) \ G(x, y, z, \zeta, \eta) \ d\xi \ d\eta.$$
(1)

Here the function $A(0, y, z) e^{ik_x x}$ describes spatial dependence of intensity of an electric field after the wave has passed through the system of X-ray refractive lenses. The function $A(x, y, z) e^{ik_x x}$ is intensity of the electric field on the image plain being located at the distance x from the last lens. y, zare coordinates along coordinate lines directed perpendicularly to the optical axis of the optical system. $\vec{k} = (k_x, 0, 0)$ means the X-rays wave vector, $k_x = \frac{\omega_0}{c}$, c denotes the speed of light and ω_0 is an electromagnetic wave angular frequency. $G(x, y, z, \zeta, \eta)$ is the so-called Kirchhoff propagator [12], [16], [17], [14]

$$G(x, y, z, \zeta, \eta) = -\frac{i}{\pi\lambda^2} * \exp\left(i * \frac{(y-\zeta)^2 + (z-\eta)^2}{\lambda^2}\right), \qquad \lambda^2 = \frac{2xc}{\omega_0}.$$
 (2)

The symbol S in (1) shows the integration domain. The integral (1) is computed over the cross section of the X-ray beam after the beam has passed through the system of lenses. It is possible to take a square of the side aas the integration domain S; the size a depends on parameters of an optical system and will be given below. When $x \to 0$ the propagator (2) turns into

$$G(x = 0, y, z, \zeta, \eta) = \delta(y - \zeta) \delta(z - \eta), \qquad (3)$$

where $\delta(y-\zeta)$ denotes the delta function.

The Kirchhoff propagator (2) is a solution of the paraxial wave equation [35], [3], [6], [32], [26]

$$\frac{\partial A}{\partial x} = \frac{i c}{2 \omega_0} \left(\frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \right) A. \tag{4}$$

It describes propagation of a monochromatic electromagnetic wave in vacuum within a paraxial approach. The solution (2) of equation (4) corresponds to the boundary condition (3).

The function A(0, y, z) is given by a solution of the problem of propagation of an electromagnetic wave through the system of lenses. We have some a priori information about the function A(0, y, z). For example, it is possible to show that, if lenses are ideal, then the function A(0, y, z) is twice differentiable with respect to y, z. Real lenses are nonideal. So, generally speaking, they are described by continuous, but not by necessarily differentiable functions. Thus, from the practical point of view, we take an interest in both cases, when A(0, y, z) is n-differentiable function and when A(0, y, z), is a continuous, but non-differentiable function.

One more feature of the problem is that we have no explicit representation of A(0, y, z). We know only the values of the function A(0, y, z) at the grid points (y_k, z_m) , $y_{k+1} = y_k + h$, $z_{m+1} = z_m + h$. That is, we have the matrix A_{km} of the values of A(0, y, z) in the points (y_k, z_m) of the grid Ω_h as an information about the function A(0, y, z); and we have to restore the function A(0, y, z) by means of suitable interpolation. Nevertheless, it is possible to vary the step h of the grid Ω_h in wide range, reducing or increasing the resolution. In this context, we can consider A(0, y, z) as a known function.

The integral (1) is difficult for numerical calculation with the application of the usual methods. In order to understand better the reason of complexity

of calculation of the integral, we consider a practical situation. In the X-ray microscopy, approximately 30 beryllium lenses are often used to get focusing of X-rays waves [18], [15], [14]. Thus, the focus of such an optical system is approximately equal to 0.3 meter; the frequencies of the used X-ray waves are about $\omega_0 \approx 10^{19} \frac{1}{s}$. Hence, in the focal point of the X-rays optical system of 30 berillium lenses, the parameter $\lambda \approx 5*10^{-6}m$. Due to lenses' forms, the stream of electromagnetic waves gradually fades closer to lenses' edges, and there is a concept of working area of lens being named the lens aperture [13], [18], [14]. For lenses, utilized in the X-ray optics, the lens aperture $d \approx 5*10^{-4}$ m, and consequently it is natural to take the square $S = \left[-\frac{d}{2}, \frac{d}{2}\right] \times \left[-\frac{d}{2}, \frac{d}{2}\right]$ as an integration domain in (1).

We see that $\left(\frac{d}{\lambda}\right)^2 \approx 10^4$, and due to this fact, we undoubtedly should consider the integrand in (1) as a fast oscillating function.

We can choose the aperture size d as a unit of measure of distance, and introduce new, dimensionless variables $y' = \frac{y}{d}$, $\xi' = \frac{\xi}{d}$. Then the integral (1) takes a standard form of a fast-oscillating integral: $\iint f(t) e^{i\omega g(t)} dS'$, where

 $\omega = \frac{d^2}{\lambda^2} \gg 1, \ t = (y', z'), \ \tau = (\xi', \eta'), \ g = (y' - \xi')^2 + (z' - \eta')^2 = |t - \tau|^2, \\ S' = [-0.5, 0.5] \times [-0.5, 0.5], \ dS' = d\xi' d\eta', \ f(y', z') = A(0, y'd, z'd).$ In our case the region of integration is a two-dimensional one. Further, we will not use this form of the fast-oscillating integral (1) because of many scientific and technological usages of the integral under consideration; we wish to keep, as close as possible, the connection of our consideration with real applications.

Usual quadrature formulas are based on splitting the given region of the integration S into small subdomains s_{ij} and the subsequent approximation of the integrand inside of small subdomains s_{ij} following the first few terms of Taylor series. One can easily show that the values of $G(x, y, z, \zeta, \eta)$ in the vicinity $(\xi_0 - \frac{h}{2}, \xi_0 + \frac{h}{2}) \times (\eta_0 - \frac{h}{2}, \eta_0 + \frac{h}{2})$ of any given point $(\xi_0, \eta_0) \in S$ can be well approximated with the help of the first few terms of Taylor series of $G(x, y, z, \zeta, \eta)$ in the point (ξ_0, η_0) , only if the step h satisfies restriction $h \ll \frac{\lambda^2}{d} \approx 5 * 10^{-8}$ m. If we know this upper restriction on the step h, we can easily estimate the minimum number of nodes N of quadrature along each coordinate axis: $N \gg 10^4$. In a two-dimensional case, the minimum number of nodes for calculation of integral (1) is estimated already as $N^2 \gg 10^8$. In practice, we need to calculate N integrals of the form (1) in a one-dimensional case, and N^2 integrals of such a kind in a two-dimensional case. Obviously, such quantity of calculations is a demanding task even for a powerful super-computer.

For calculation of the integral (1), the technique based on Fourier transformation is recommended in the literature on X-ray optics [24]. Namely, at first step, the integration domain S in (1) is extended up to all R^2 -plane, and the function A(0, y, z) is redefined with zero outside the initial region of the integration S. In order to obtain the solution A(x, y, z) given by the integral (1), first we need to use the convolution theorem (the Fourier transform of a convolution is equal to the pointwise product of the Fourier transforms) and then, utilize the inverse Fourier transform [24], [1]. In this way, we can replace the initial integral with an integral of the Fourier transforms of the initial functions:

$$A(x, y, z) = \iint_{R^2} A(0, \xi, \eta) G(x, y, z, \zeta, \eta) d\xi d\eta =$$

$$= \iint_{R^2_k} \tilde{A}(0, k_y, k_z) \tilde{G}(x, y, z, k_y, k_z) dk_y dk_z$$
(5)

The last integral in the right part (5) is essentially better for the numerical integration in comparison to (1). An effective calculation of integral (1) is prevented by presence of small λ^2 in the exponent denominator in (2). The Fourier transform $\tilde{G}(x, y, z, k_y, k_z)$ of the propagator $G(x, y, z, \zeta, \eta)$ has the following form:

$$\tilde{G}(x, y, z, k_y, k_z) = \frac{1}{2\pi} e^{-\frac{i\lambda^2}{4} \left(k_y^2 + k_z^2\right)} e^{-i(k_y y + k_z z)}$$
(6)

and the small multiplier λ^2 is contained already in the exponent numerator, instead of the denominator, and the problem disappears. Therefore, the usage of the Fourier transformation essentially simplifies calculations, and the integral is successfully computed. However, such a technique of the integral calculation has certain defects:

- Redefinition of A(0, y, z) up to all R^2 -plane leads to the redundancy of computer calculations as a result.
- The function $\tilde{G}(x, y, z, k_y, k_z)$ does not vanish when $k_y^2 + k_z^2 \to \infty$. Therefore, the requirement that the function $A(0, k_y, k_z)$ should tend to zero faster than $\frac{1}{k_y^2 + k_z^2}$ when $k_y^2 + k_z^2 \to \infty$ is a necessary condition for existence of the integral in the right-hand part of (5). We know that the rate of the decrease of the Fourier transform when $k_y^2 + k_z^2 \to \infty$ is inseparably linked to smoothness of an initial function. Thus, at least twice differentiability of the function A(0, y, z) with respect to variables y, z is necessary for the existence of the integral in right-hand side of (5). However, in general, we can not suppose that the function A(0, y, z) possesses such smoothness.
- The integration region cannot be boundless in numerical computations, and we must take the finite subdomain $S_k \in R_k^2$ instead of R_k^2 , and also, we apply the discrete Fourier transformation instead of the continuous one. It brings an additional error. The suitable domain of the integration S_k should be chosen experimentally in accordance with results of a few test simulations.

• It is known that the Fourier-approximation of any function by a finite Fourier series smoothes the initial function. At present, the problem of influence of minor defects of refracting X-ray lenses on the image is topical. The smoothing effect of the finite Fourier series can significantly reduce influence of defects and can essentially complicate research of influence of lenses defects.

Thus, the suggestion of some other ways of computation of the integral (1) eliminating at least some of the listed imperfections would be desirable.

3. Efficient quadrature based on the idea of Filon's method. It is natural to employ the idea of Filon's method for the calculation of an integral (1). We split the integration region S into small subareas s_{km} : $S = \bigcup_{\substack{(k,m) \ (k,m)}} s_{km}$. Let the point (ζ_k, η_m) be the centre of the domain $s_{km} = [\zeta_k - \frac{h}{2}, \zeta_k + \frac{h}{2}] \times [\eta_m - \frac{h}{2}, \eta_m + \frac{h}{2}]$. It is easy to show that the Gauss function in $G(x, y, z, \zeta, \eta)$ is well approximated by an exponent function within any small area of the integration s_{km}

$$e^{i*\frac{(y-\zeta)^2+(z-\eta)^2}{\lambda^2}} \approx e^{i*\frac{(y-\zeta_k)^2+(z-\eta_m)^2+2(y-\zeta_k)(\zeta_k-\zeta)+2(z-\eta_m)(\eta_m-\eta)}{\lambda^2}},$$

(ζ,η) $\in s_{km}$ (y,z) $\in \mathbb{R}^2$, (7)

provided that the grid step h satisfies the condition $\frac{h}{\lambda} \ll 1$. Therefore, in order to obtain A(x, y, z), we will apply splines constructed on the basis of the exponent functions. By using the condition $\frac{h}{\lambda} \ll 1$, we can obtain a useful estimate: $N \gg 100$ grid points for each space dimension is necessary to perform the calculation in the area with the diameter $d \approx 5 * 10^{-4}$ m. If high accuracy is not required, we can take only N = 1000 along each dimension. It is 10^2 times less than the previous estimation in case of one dimension, and 10^4 times less in case of two dimensions. The advantage is essential.

During the derivation of quadrature, we will take into account that the function A(0, y, z) may be fast oscillating as well. In the X-ray optics, the function A(0, y, z) is calculated by means of solving the equation describing the propagation of an electromagnetic wave through a system of lenses [17], [15]:

$$\frac{\partial A}{\partial x} - b(x, y, z) A = \frac{i c}{2 \omega_0} \left(\frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \right) A, \tag{8}$$

where b(x, y, z) is a complex function depending on a lens material and its form. The function b(x, y, z) is equal to zero at the points, in which the electromagnetic wave propagates through air, and $b(x, y, z) = \frac{i\omega_0}{2c} \left[1 - \frac{1}{n^2}\right] d(x, y, z)$ at the points corresponding to a lens material. Here d(x, y, z) describes the lens form. $n = 1 - \delta + i\beta$ is a complex factor of refraction for a lens material. The imaginary part of n defines the attenuation of an electromagnetic wave in a lens material. The right part of the equation (8) is comparatively small [13], [17], [15]. By neglecting this small right-hand term, we obtain a relation for the function A(0, y, z), after the X-rays waves have propagated through the system of N_L lenses [13], [17], [15]:

$$A(0, y, z) \sim e^{i\phi(y, z)}, \qquad \phi(y, z) = \frac{(y^2 + z^2)}{l^2}$$
 (9)

where $l^{-2} = \frac{\omega_0 \delta}{c} N_L \frac{1}{R}$, R is a radius of curvature of a parabolic lenses and N_L denotes the number of lenses. When we use many lenses, the frequency is high and the curvature of lenses is small (for example, $R = 50 \mu m$), the denominator l^2 will be small. For the optical system of 30 beryllium lenses $l \approx 7 * 10^{-6}$ m. That is, l is comparable with λ .

Taking into account the above consideration, it is the expedient to the interpolate $A(0,\xi,\eta)$ by means of the complex exponent function in the vicinity $\left(y_k - \frac{h}{2}, y_k + \frac{h}{2}\right) \times \left(z_m - \frac{h}{2}, z_m + \frac{h}{2}\right)$ of the point (y_k, z_m) :

$$A(0,\xi,\eta) \approx A_{k,m} * e^{i\psi_{km}(\xi,\eta)}, \quad \psi_{km} = [\alpha_{km}(\xi - y_k) + \beta_{km}(\eta - z_m)], \quad (10)$$

$$\alpha_{km} = \frac{1}{2ih} \ln \frac{A_{k+1,m}}{A_{k-1,m}}, \qquad \beta_{km} = \frac{1}{2ih} \ln \frac{A_{k,m+1}}{A_{k,m-1}},$$

$$A_{k,m} = A(0, y_k, z_m).$$

When we calculate the factors α_{km} , β_{km} , we need to take into account that ln is a multivalued function. The standard computer programs for the complex logarithm always give the logarithm a phase from the interval $(-\pi, \pi)$, while in our problem the logarithm phase can change significantly and we need to choose the correct branches of the logarithm. When h is small enough, we can easily avoid the problem of many-valuedness of the complex ln. To this end, we can apply the asymptotic series to $\ln \frac{A_{k+1,m}}{A_{k-1,m}}$, $\ln \frac{A_{k,m+1}}{A_{k,m-1}}$. For example:

$$\ln \frac{A_{k+1,m}}{A_{k-1,m}} = \frac{A_{k+1,m} - A_{k-1,m}}{A_{k,m}} \\ \times \left(1 - \frac{A_{k+1,m} - 2A_{k,m} + A_{k-1,m}}{2A_{k,m}} + O\left(\Delta A\right)^2 \right), \quad (11)$$

where $\Delta A = \max_{(k,m)} \left\{ \left| \frac{A_{k+1,m} - A_{k,m}}{A_{k,m}} \right|, \left| \frac{A_{k+1,m} - A_{k,m}}{A_{k+1,m}} \right| \right\}$. A similar formula is valid for $\ln \frac{A_{k,m+1}}{A_{k,m-1}}$. Usage of equality (11) solves the problem of choice of the correct branches of the logarithm.

We use the formula (7) in order to obtain the approximation of the propagator (2) in vicinity of the point (y_k, z_m) . Then we multiply approximations of $A(0, \xi, \eta)$ and $G(x, y, z, \zeta, \eta)$ and we integrate the result over the areas $s_{km} = \left[y_k - \frac{h}{2}, y_k + \frac{h}{2}\right] \times \left[z_m - \frac{h}{2}, z_m + \frac{h}{2}\right], -\frac{M}{2} \le m \le \frac{M}{2}, -\frac{M}{2} \le k \le \frac{M}{2}.$ We add up all the results of the integration, and in this way we obtain an approximate value B(x, y, z) of the searched integral

$$A(x, y, z) \approx B(x, y, z) = -\sum_{k, m = -\frac{M}{2}}^{\frac{M}{2}} \frac{i}{\pi \lambda^2} A_{km} * K_{km} * L_{km}, \qquad (12)$$

where

$$K_{km} = \begin{cases} \frac{2e^{i*\frac{(y-y_k)^2}{\lambda^2}}}{\tilde{\alpha}_{km}} \sin\left[\tilde{\alpha}_{km}\frac{h}{2}\right], & \left|\tilde{\alpha}_{km}\frac{h}{2}\right| > 0.1\\ e^{i*\frac{(y-y_k)^2}{\lambda^2}}h\left(1 - \frac{h^2}{24}\left(\tilde{\alpha}_{km}\right)^2\right), \left|\tilde{\alpha}_{km}\frac{h}{2}\right| \le 0.1 \end{cases}$$
(13)

with $\tilde{\alpha}_{km} = \alpha_{km} + \frac{2(y-y_k)}{\lambda^2}$,

$$L_{km} = \begin{cases} \frac{2e^{i*\frac{(z-z_m)^2}{\lambda^2}}}{\tilde{\beta}_{km}} \sin\left[\tilde{\beta}_{km}\frac{h}{2}\right], & \left|\tilde{\beta}_{km}\frac{h}{2}\right| > 0.1\\ e^{i*\frac{(z-z_m)^2}{\lambda^2}}h\left(1 - \frac{h^2}{24}\left(\tilde{\beta}_{km}\right)^2\right), \left|\tilde{\beta}_{km}\frac{h}{2}\right| < 0.1 \end{cases}$$
(14)

and $\tilde{\beta}_{km} = \beta_{km} + \frac{2(z-z_m)}{\lambda^2}$. During the derivation of formulas (13), (14), we have taken into account uncertainties $\frac{0}{0}$, which arise when $h \to 0$. In order to obtain a good result for a very small h, we have used the expansion of the function sin in the Taylor series taking into account up to cubic terms. We see that procedures of the calculation of the partial integrals for various subareas s_{km} can vary. This follows the fact that the oscillation frequency of the integrand is changeable and strongly depends on position of the points in the area S. The quadrature is adapted to changing behavior of the integrand.

Fig. 2 shows an example of the calculation of $|A(x, y, z)|^2$ obtained with the help of the formula (12) at distances x = 0.135 m and x = 0.255 m and for space step $h = 1.51 * 10^{-7}$ m. The focal spot of such an optical system is located approximately at x = 0.275 m, and we observe the focusing effect with the change of distance. The smaller the distance x from the system of lenses, the smaller is the value of lambda. For small values of the lambda make that the function becomes quickly an oscillating function. This indicates that in order to evaluate well the value of the function for small distances x, the sufficiently low value of h must be chosen; but for larger distances x, it is possible to use larger values of h.

THEOREM 3.1 If $A(0, y, z) \in C^n(S)$, $1 \le n \le 2$, then $|A(x, y, z) - B(x, y, z)| \le Ch^n$ at x > 0, where C is some constant depending on x and on A(0, y, z).



Figure 2: Examples of computation of $|A(x, y, z)|^2$ at the distances x = 0.135 m and x = 0.255 m, obtained for the function A(0, y, z), which corresponds to X-rays after the system of 30 beryllium lenses.

PROOF If one uses Taylor's theorem, one can write both the function A (with the Peano form of the remainder) and the Gaussian function in the following form:

$$A(0,\xi,\eta) = A_{k,m} e^{i\psi_{km}(\xi,\eta) + H_{k,m}(\xi,\eta)O(h)},$$
(15)

$$e^{i\frac{(y-\zeta)^2+(z-\eta)^2}{\lambda^2}} = e^{i\frac{(y-\zeta_k)^2+(z-\eta_m)^2+2(y-\zeta_k)(\zeta_k-\zeta)+2(z-\eta_m)(\eta_m-\eta)}{\lambda^2}} + O(h^2), \quad (16)$$
$$(\zeta,\eta) \in s_{km}, \quad x > 0,$$

where $\lim_{(\zeta,\eta)\to(\zeta_k,\eta_m)} H_{n,m}(\xi,\eta) = 0$. We have

$$A(x, y, z) = \iint_{S} A(0, \xi, \eta) \ G(x, y, z, \zeta, \eta) \ d\xi \ d\eta = B(x, y, z) + \sum_{k,m=-\frac{M}{2}}^{\frac{M}{2}} D_{km} F_{km},$$
$$D_{km} = -\frac{i}{\pi \lambda^2} A_{km} e^{i \frac{(y-\zeta_k)^2 + (z-\eta_m)^2}{\lambda^2}},$$
$$F_{km} = \iint_{s_{km}} e^{i \frac{2(y-\zeta_k)(\zeta_k-\zeta) + 2(z-\eta_m)(\eta_m-\eta)}{\lambda^2}} e^{i\psi_{km}(\xi,\eta)} (H_{n,m}(\xi, \eta) \ O(h) + O(h^2)) d\xi d\eta$$

The estimations are valid

$$|D_{km}| \le \frac{|A_{km}|}{\pi\lambda^2} \le D_{max}, \qquad D_{max} = \frac{1}{\pi\lambda^2} \sup_{(\xi,\eta)\in S} \{|A(0,\xi,\eta)|\},\$$

$$|F_{km}| \le F_{max} = \max_{k,m} \{ \sup_{(\xi,\eta) \in s_{km}} \{ |H_{k,m}(\xi,\eta)| \} \} O(h) + O(h^2) \to 0 \text{ at } h \to 0.$$

Therefore, $|A(x,y,z) - B(x,y,z)| \leq D_{max}F_{max}(M+1)^2h^2 = D_{max}F_{max}S \rightarrow 0 \text{ at}$ $h \rightarrow 0.$

REMARK 3.2 The method (12) is applicable for computations in case of the non-differentiable $A(0, y, z) \in C(S)$ as well, if the following technique is used. For any $A(0, y, z) \in L_1(S)$, the property $A(0, y, z) = A_0(0, y, z) + A_1(0, y, z)$ is valid, where $A_0(0, y, z) \in C^{\infty}(S)$, $A_1(0, y, z) \in L_1(S)$. For example,

$$A_{0}(0, y, z) = \frac{1}{\pi\varepsilon} \iint_{s} A(0, \xi, \eta) e^{-\frac{(y-\xi)^{2}+(z-\eta)^{2}}{\varepsilon^{2}}} d\xi d\eta,$$
(17)
$$A_{1}(0, y, z) = A(0, y, z) - A_{0}(0, y, z).$$

The function $A_0(0, y, z)$ satisfies the conditions of Theorem 3.1, and we can use $A_0(0, y, z)$ for the calculations under formula (12). The function $A_1(0, y, z)$ can be made arbitrarily small due to the choice of small enough ε , and it can be neglected. In practical calculations, the averaging is applied, in which the integral in (17) is replaced with the approximated integral sum.

4. Main results and discussion. Using ideas of Filon's type methods, we have constructed a quadrature for calculation of the integral (1).

The method is of the second order of accuracy, if the subintegral function is twice differentiable, and has the lower rate of convergence and, if the integrand possesses worse differentiability properties. The constructed method automatically turns into usual quadrature of the rectangles method, when h is small enough. This property is useful, because the rectangles method is applicable even in case of functions with bad differentiability properties (for example, if the function A(0, y, z) is non-differentiable, but is a piecewise continuous function). Therefore, it allows making calculations for the function A(0, y, z) without good differentiable properties within the limits of the proposed method, but by applying a supercomputer. In this sense, the method is a robust one; it well adapts to features of the situation and is good for carrying out scientific and technological research.

The method has a minor disadvantage as the admissible step h in the quadrature formula depends on x and step $h \to 0$ when $x \to 0$ (the inequality $h \ll \lambda$ should be satisfied). However, this disadvantage reveals itself only for very small x, and is unimportant from the practical point of view.

Acknowledgement. The authors are greatful to Leble S.B. and Kohn V.G. for helpful discussion and advices.

The work is supported by Ministry of Education and Science of the Russian Federation (Contracts a 14.Y26.31.0002 and 02.G25.31.0086)

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Wydajna kwadratura dla całkowania szybko oscylujących funkcji optyki rentgenowskiej

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Streszczenie Praca jest poświęcona wyznaczaniu kwardratury dla rozwiązań całkowych równania przewodnictwa cieplnego z zespolonym potencjałem. Trudność w wyznaczaniu tego typu całek jest związana z szybkimi oscylacjami funkcji całkowanej. Prezentowana metoda jest alternatywą dla powszechnie stosowanej metody opartej o zastosowanie transformacji Fouriera. Specyzowanie kwadratury jest przedyskutowane na przykładzie całek występujących przy badaniu teorii propagacji i skupiania promieniowania rentgenowskiego. Dzięki ogólności prezentowanej kwadratury, może być ona także zastosowana do zagadnień związanych z optyką i akustyką.

Klasyfikacja tematyczna AMS (2010): 65D32; 65E05; 65Z05; 35Q60.

Słowa kluczowe: równanie przewodnictwa cieplnego z zespolonym potencjałem, kwadratura, całkowanie szybko oscylującej funkcji, optyka rentgenowska.



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Communicated by: Wojciech Mitkowski

(Received: 18th of January 2015; revised: 10th of December 2015)