Computation of Gabor coefficients for objects with polygonal cross section

Citation for published version (APA):

Sun, L., Eijsvogel, S., Sepehripour, F., Dilz, R., & van Beurden, M. C. (2021). Computation of Gabor coefficients for objects with polygonal cross section. In *2021 International Conference on Electromagnetics in Advanced Applications, ICEAA 2021* (pp. 72-77). [9539818] Institute of Electrical and Electronics Engineers. <https://doi.org/10.1109/ICEAA52647.2021.9539818>

DOI:

[10.1109/ICEAA52647.2021.9539818](https://doi.org/10.1109/ICEAA52647.2021.9539818)

Document status and date:

Published: 21/09/2021

Document Version:

Accepted manuscript including changes made at the peer-review stage

Please check the document version of this publication:

- A submitted manuscript is the version of the article upon submission and before peer-review. There can be important differences between the submitted version and the official published version of record. People interested in the research are advised to contact the author for the final version of the publication, or visit the DOI to the publisher's website.
- The final author version and the galley proof are versions of the publication after peer review.
- The final published version features the final layout of the paper including the volume, issue and page numbers.

[Link to publication](#)

General rights

Copyright and moral rights for the publications made accessible in the public portal are retained by the authors and/or other copyright owners and it is a condition of accessing publications that users recognise and abide by the legal requirements associated with these rights.

- Users may download and print one copy of any publication from the public portal for the purpose of private study or research.
- You may not further distribute the material or use it for any profit-making activity or commercial gain
- You may freely distribute the URL identifying the publication in the public portal.

If the publication is distributed under the terms of Article 25fa of the Dutch Copyright Act, indicated by the "Taverne" license above, please follow below link for the End User Agreement:

www.tue.nl/taverne

Take down policy

If you believe that this document breaches copyright please contact us at:

openaccess@tue.nl

providing details and we will investigate your claim.

Computation of Gabor coefficients for objects with polygonal cross section

L. Sun, S. Eijsvogel, F. Sepehripour, R. J. Dilz and M. C. van Beurden

Department of Electrical Engineering

Eindhoven University of Technology

Eindhoven, Netherlands

M.C.v.Beurden@tue.nl

Abstract—The Gabor transformation connects the spectral and spatial domain in a recently developed spatial spectral Maxwell solver. A key step involves computing the Gabor coefficients of the characteristic function of dielectric scattering objects. Therefore, computing Gabor coefficients accurately and efficiently is significant in the further development of this Maxwell solver. We discuss a method to numerically calculate the integrals involved in computing the Gabor coefficients, based on Gauss's theorem and recurrence relations.

Index Terms—Maxwell solver, Gabor transformation, polygonal object, recurrence relation, Olver's algorithm

I. INTRODUCTION

In optical scatterometry and metrology for the production of integrated circuits, a fast and reliable Maxwell solver is key to reconstruct the geometry parameters of metrology targets on the wafer. This is because the key geometrical details of metrology targets that are relevant for process control are much smaller than the wavelength of the light that illuminates the target. The tendency in the semiconductor industry is to shrink the area occupied by the targets, which implies that the finiteness of the target becomes observable and the periodicity assumption of the target no longer suffices. This has led us to develop a Maxwell solver based on a volume integral equation that is capable of simulating finitely sized dielectric targets in a layered medium [1]. In this Maxwell solver, the fields are expressed in terms of Gabor frames, that allow for efficient transformations between the (continuous) spatial and (continuous) spectral domains. The spatial domain is employed for the field-material interactions and the spectral domain for an efficient convolution with the layered-medium Green function. The Gabor frame discretization is an effective tool in this Maxwell solver to transform between spatial and spectral domain. However, as a consequence, the efficient and accurate calculation of Gabor coefficients to describe scattering objects in this representation plays a key role in this process [1].

The 3D full-wave Maxwell solver employs a Gabor-frame discretization in the two directions parallel to the layer interfaces. A two-dimensional (2D) cross-section of a scattering object embedded in a multi-layered medium can be approximated adequately by a collection of polygons. To compute Gabor coefficients of geometrical objects that represent dielectric scatterers embedded in the layered medium, Gabor transformations of 2D characteristic functions, which represent

the 2D cross-sections of scattering objects, are required. These functions are equal to one on the support of a polygon and zero outside. One 2D integral is required for each Gabor coefficient in the geometrical representation of each polygon that represents part of a scattering object. Often, a large number of polygons is required, which leads to a vast number of two-dimensional integrals to be computed. In most cases the analytical solution of these integrals is hard to get due to the complicated structure of integrand and the support of the integration domain. Various numerical quadrature methods can be applied to acquire numerical approximations, such as quadrature rules based on interpolating functions. In real applications, these double integrals can occur billions of times, which brings a heavy computational burden to the preprocessing step of this type of Maxwell solver. Therefore, even a small improvement in this preprocessing step can bring a lot of benefits.

Inspired by the idea exploited in the local normal-vector field formulation in [2], we then transform a double integral into a sequence of line integrals by solving two ordinary differential equations and applying Gauss's theorem. Rather than computing the double integral, these line integrals can either be computed numerically via various quadrature rules or be developed further analytically in the form of recurrence relations. We discuss several examples and perform benchmarking to show how these two methods compare in terms of accuracy, numerical stability, and computation time.

In Section II, we give the statement of the problem and define the pertaining integrals needed to compute the Gabor coefficients of characteristic functions. Section III discusses a way to calculate the 1D line integrals based on a recurrence relation. In Section IV, we give two numerical examples to show how the methods work on rectangular and triangular cross sections. Finally, we draw conclusions in Section V.

II. STATEMENT OF THE PROBLEM

A. 2D Gabor transform

For any $f(x, y) \in L^2(\mathbb{R}^2)$, we have its Gabor frame expansion

$$f(x, y) = \sum_{\mathbf{m}, \mathbf{n}} f_{\mathbf{m}, \mathbf{n}} g_{\mathbf{m}, \mathbf{n}}(x, y), \quad (1)$$

in which $g_{\mathbf{m}, \mathbf{n}}(x, y)$ is a Gabor frame function and $f_{\mathbf{m}, \mathbf{n}}$ is a Gabor coefficient, and $\mathbf{m} = (m_x, m_y)$ and $\mathbf{n} = (n_x, n_y)$.

The Gabor frame functions (2D) are defined as:

$$g_{\mathbf{m},\mathbf{n}}(x, y) = g_{m_x, n_x}(x, \alpha_x X, \beta_x K_x) g_{m_y, n_y}(y, \alpha_y Y, \beta_y K_y), \quad (2)$$

where

$$g_{m,n}(x, X, K) = g_X(x - mX) e^{jnKx}, \quad (3)$$

where $g_X(x) = 2^{1/4} \exp[-\pi(x/X)^2]$ is Gaussian window function. Further, $m_x, m_y, n_x, n_y \in \mathbb{Z}$, $\alpha_x, \alpha_y, \beta_x, \beta_y$ are oversampling parameters ($\alpha_x \beta_x = \alpha_y \beta_y = q/p$), and X, Y are spacing parameters of the window functions of the Gabor frame that satisfy $X = \frac{2\pi}{K_x}$ and $Y = \frac{2\pi}{K_y}$.

Gabor coefficients are defined via the 2D Gabor transformation:

$$f_{\mathbf{m},\mathbf{n}} = \iint_{\mathbb{R}^2} f(x, y) \eta_{\mathbf{m},\mathbf{n}}^*(x, y) dx dy, \quad (4)$$

where $\eta_{\mathbf{m},\mathbf{n}}(x, y)$ is the 2D dual window function, obtained by multiplying its counterparts in one-dimensional (1D). From [3], the 1D dual window can be represented again by the original Gabor frame expansion:

$$\begin{aligned} \eta_{m,n}(x) &= \eta(x - m\alpha X) e^{jn\beta Kx} \\ &= \sum_{l,k} \left(\gamma_{l,k} g_X(x - (m+l)\alpha X) e^{-jk m \alpha \beta Kx + j(k+n)\beta Kx} \right), \end{aligned} \quad (5)$$

where $\gamma_{l,k}$ are Gabor coefficients. With this representation, the integral in (4) can be rewritten as a linear combination of integrals of the form:

$$\begin{aligned} I_{\mathbf{m}+\mathbf{l},\mathbf{n}+\mathbf{k}} &= \iint_{\mathbb{R}^2} f(x, y) \exp \left\{ -\pi \left[\frac{x}{X} - (m_x + l_x) \alpha_x \right]^2 \right\} \\ &\quad \cdot \exp \left\{ -j(k_x + n_x) \beta_x K_x x \right\} \\ &\quad \cdot \exp \left\{ -\pi \left[\frac{y}{Y} - (m_y + l_y) \alpha_y \right]^2 \right\} \\ &\quad \cdot \exp \left\{ -j(n_y + k_y) \beta_y K_y y \right\} dx dy. \end{aligned} \quad (6)$$

This type of integral has to be computed many times.

We are interested in the Gabor coefficients for the characteristic function of a scattering object that coincides with a 2D domain D . The characteristic function $s(x, y)$ is then given by:

$$s(x, y) = \begin{cases} 1, & (x, y) \in D \\ 0, & (x, y) \in \mathbb{R}^2 \setminus D \end{cases}, \quad (7)$$

and the Gabor coefficients of this characteristic function can then be expressed in terms of the integrals defined in Eq. (6), where the domain of integration can now be restricted to the support D of $s(x, y)$.

B. A special case where analytical solution is available

In the case of a rectangular object that is aligned with the x and y direction, i.e., when integral domain D in (7) is an aligned rectangle, the double integral $I_{\mathbf{m}+\mathbf{l},\mathbf{n}+\mathbf{k}}$ defined in (12) is analytically integrable because the integrand is separable in its x and y arguments.

$$\begin{aligned} I_{\mathbf{m}+\mathbf{l},\mathbf{n}+\mathbf{k}} &= \int_{x_1}^{x_2} e^{-\pi \left[\frac{x}{X} - \alpha_x(m_x + l_x) \right]^2} e^{-j(n_x + k_x) \beta_x K_x x} dx \\ &\quad \cdot \int_{y_1}^{y_2} e^{-\pi \left[\frac{y}{Y} - \alpha_y(m_y + l_y) \right]^2} e^{-j(n_y + k_y) \beta_y K_y y} dy \\ &= P_1 \cdot P_2 \cdot P_3, \end{aligned} \quad (8)$$

where

$$P_1 = \frac{XY}{4} e^{-\pi \beta_x(n_x + k_x)[\beta_x(n_x + k_x) + 2i\alpha_x(m_x + l_x)]} e^{-\pi \beta_y(n_y + k_y)[\beta_y(n_y + k_y) + 2i\alpha_y(m_y + l_y)]}, \quad (9)$$

$$\begin{aligned} P_2 &= \operatorname{erf} \left[-\frac{\sqrt{\pi}}{X} (\alpha_x X(m_x + l_x) - x_1) + i\beta_x \sqrt{\pi} (n_x + k_x) \right] \\ &\quad - \operatorname{erf} \left[-\frac{\sqrt{\pi}}{X} (\alpha_x X(m_x + l_x) - x_2) + i\beta_x \sqrt{\pi} (n_x + k_x) \right], \end{aligned} \quad (10)$$

and

$$\begin{aligned} P_3 &= \operatorname{erf} \left[-\frac{\sqrt{\pi}}{Y} (\alpha_y Y(m_y + l_y) - y_1) + i\beta_y \sqrt{\pi} (n_y + k_y) \right] \\ &\quad - \operatorname{erf} \left[-\frac{\sqrt{\pi}}{Y} (\alpha_y Y(m_y + l_y) - y_2) + i\beta_y \sqrt{\pi} (n_y + k_y) \right]. \end{aligned} \quad (11)$$

When the integration domain D is not a rectangle, the double integral $I_{\mathbf{m}+\mathbf{l},\mathbf{n}+\mathbf{k}}$ in (12) cannot be decomposed into a product of two integrals to obtain an analytical solution. Therefore, numerical integration is required to evaluate $I_{\mathbf{m}+\mathbf{l},\mathbf{n}+\mathbf{k}}$.

C. Gauss's theorem

Based on Gauss's theorem we can rewrite the integral type $I_{\mathbf{m}+\mathbf{l},\mathbf{n}+\mathbf{k}}$ as a contour integral over functions $P(x, y)$ and $Q(x, y)$, owing to the finite support of $s(x, y)$, i.e.

$$\begin{aligned} I_{\mathbf{m}+\mathbf{l},\mathbf{n}+\mathbf{k}} &= \iint_D \frac{\partial}{\partial x} P(x, y) + \frac{\partial}{\partial y} Q(x, y) dx dy \\ &= \oint_{\partial D} -Q(x, y) dx + P(x, y) dy. \end{aligned} \quad (12)$$

Functions $P(x, y)$ and $Q(x, y)$ are given by

$$\begin{aligned} P(x, y) &= h_1(y, \mathbf{p}_2) \cdot \operatorname{erf}[h_2(x, \mathbf{p}_3)], \\ Q(x, y) &= h_1(x, \mathbf{p}_1) \cdot \operatorname{erf}[h_2(y, \mathbf{p}_4)], \end{aligned}$$

where

$$\begin{aligned} h_1(x, \mathbf{p}_1) &= \frac{Y}{4} \exp \left\{ -\frac{\pi}{X^2} (x - \alpha_x(m_x + l_1)X)^2 \right. \\ &\quad \left. - \pi \beta_y^2 (n_y + k_y)^2 - j \left(\beta_x K_x (n_x + k_x) x \right. \right. \\ &\quad \left. \left. + 2\pi \alpha_y \beta_y (m_y + l_y) (n_y + k_y) \right) \right\}, \end{aligned} \quad (13)$$

$$\begin{aligned} h_1(y, \mathbf{p}_2) &= \frac{X}{4} \exp \left\{ -\frac{\pi}{Y^2} (y - \alpha_y(m_y + l_y)Y)^2 \right. \\ &\quad \left. - \pi \beta_x^2 (n_x + k_x)^2 - j \left(\beta_y K_y (n_y + k_y) y \right. \right. \\ &\quad \left. \left. + 2\pi \alpha_x \beta_x (m_x + l_x) (n_x + k_x) \right) \right\}, \end{aligned} \quad (14)$$

$$h_2(x, \mathbf{p}_3) = \sqrt{\pi} \left(\frac{x}{X} - \alpha_x(m_x + l_x) \right) + j\sqrt{\pi}\beta_x(n_x + k_x), \quad (15)$$

$$h_2(y, \mathbf{p}_4) = \sqrt{\pi} \left(\frac{y}{Y} - \alpha_y(m_y + l_y) \right) + j\sqrt{\pi}\beta_y(n_y + k_y), \quad (16)$$

and vectors

$$\begin{aligned} \mathbf{p}_1 &= (X, Y, \alpha_x, \alpha_y, m_x + l_x, n_x + k_x, m_y + l_y, n_y + k_y), \\ \mathbf{p}_2 &= (Y, X, \alpha_y, \alpha_x, m_y + l_y, n_y + k_y, m_x + l_x, n_x + k_x), \\ \mathbf{p}_3 &= (X, \alpha_x, m_x + l_x, n_x + k_x), \\ \mathbf{p}_4 &= (Y, \alpha_y, m_y + l_y, n_y + k_y), \end{aligned}$$

contain independent parameters. Essentially, $P(x, y)$ and $Q(x, y)$ are the same function with different variable and parameter notations.

D. Parametrization for polygonal object

Suppose the scattering object is an M -sided polygon, and along the i -th edge of the polygon (for $i = 1, 2, \dots, M$ counterclockwise), we apply the following parametrization:

$$\begin{cases} \frac{x_i(t)}{X} = c_{i1}t + d_{i1}, \\ \frac{y_i(t)}{Y} = c_{i2}t + d_{i2}, \end{cases} \quad (17)$$

where $t \in [0, 1]$. After substituting (17) in (12) we get

$$I_{\mathbf{m}+\mathbf{l}, \mathbf{n}+\mathbf{k}} = \sum_{i=1}^M [I(\mathbf{c}_i) + I(\mathbf{d}_i)], \quad (18)$$

and the representations of $I(\mathbf{c}_i)$ and $I(\mathbf{d}_i)$ are:

$$I(\mathbf{c}_i) = c_0^i \int_0^1 \exp(-c_1^i t^2 + c_2^i t) \operatorname{erf}(c_3^i t + c_4^i) dt, \quad (19)$$

$$I(\mathbf{d}_i) = d_0^i \int_0^1 \exp(-d_1^i t^2 + d_2^i t) \operatorname{erf}(d_3^i t + d_4^i) dt, \quad (20)$$

where vectors

$$\begin{aligned} \mathbf{c}_i &= (c_0^i, c_1^i, c_2^i, c_3^i, c_4^i), \\ \mathbf{d}_i &= (d_0^i, d_1^i, d_2^i, d_3^i, d_4^i), \end{aligned}$$

denote the boundary-related parameters, which satisfy $c_0^i, d_0^i, c_2^i, d_2^i, c_4^i, d_4^i \in \mathbb{C}$, $c_1^i, d_1^i, c_3^i, d_3^i \in \mathbb{R}$, $c_1^i, d_1^i \geq 0$.

III. RECURRENCE RELATION AND OLVER'S ALGORITHM

We are not aware of any method to find a general solution for (19) analytically, due to the product of the Gaussian function and the complex error function $\operatorname{erf}(z)$ in the integrand. Numerical integration is possible but slow. To avoid a numerical sampling of the integral, we use a Taylor series expansion to replace the complex error function $\operatorname{erf}(z)$.

A. Taylor series expansion

Notice that the product of a Gaussian function and polynomial is analytically integrable, so we consider the Taylor series of a complex error function first.

We have

$$\operatorname{erf}(z) = \frac{2}{\sqrt{\pi}} \sum_{n=0}^{\infty} \frac{(-1)^n}{(2n+1)n!} z^{2n+1}, \quad (21)$$

and for $\forall z \in \mathbb{C}$ this Taylor series converges to $\operatorname{erf}(z)$ since it is an entire function [4].

In practice we need to truncate this infinite series after a finite number of terms to approximate $\operatorname{erf}(z)$. Hence for a given $N \in \mathbb{N}$, we can represent $\operatorname{erf}(z)$ as:

$$\begin{aligned} \operatorname{erf}(z) &= \frac{2}{\sqrt{\pi}} \left[\sum_{n=0}^{N-1} \frac{(-1)^n z^{2n+1}}{(2n+1)n!} + \sum_{n=N}^{\infty} \frac{(-1)^n z^{2n+1}}{(2n+1)n!} \right] \\ &\triangleq P_{2N}(z) + R_{2N}(z). \end{aligned} \quad (22)$$

Notice that $P_{2N}(z)$ is actually equivalent to the first $2N$ items in the original Taylor series of $\operatorname{erf}(z)$ in (21). For a given $\varepsilon > 0$, this truncation number N can be determined correspondingly.

B. Recurrence relation

Recalling (19) and omitting the boundary notation i , we have:

$$I_\alpha = c_0 \int_0^1 e^{-c_1 t^2 + c_2 t} \operatorname{erf}(c_3 t + c_4) dt, \quad (23)$$

where $c_0, c_2, c_4 \in \mathbb{C}$, $c_1, c_3 \in \mathbb{R}$, $c_1 \geq 0$. Together with (22) we have

$$\begin{aligned} I_\beta &= c_0 \int_0^1 e^{-c_1 x^2 + c_2 x} P_{2N}(c_3 x + c_4) dx \\ &= \frac{2c_0}{\sqrt{\pi}} \sum_{n=0}^{N-1} \frac{(-1)^n}{(2n+1)n!} \int_0^1 e^{-c_1 x^2 + c_2 x} (c_3 x + c_4)^{2n+1} dx \\ &= \frac{2c_0 e^{c_7}}{\sqrt{\pi} c_3} \sum_{n=0}^{N-1} \frac{(-1)^n}{(2n+1)n!} \int_{c_4}^{c_3+c_4} e^{-c_5 y^2 + c_6 y} y^{2n+1} dy, \end{aligned} \quad (24)$$

where $y = c_3 x + c_4$ and when $c_3 \neq 0$ we have

$$c_5 = \frac{c_1}{c_3^2}, \quad (25)$$

$$c_6 = \frac{2c_1 c_4}{c_3^2} + \frac{c_2}{c_3}, \quad (26)$$

$$c_7 = -\frac{c_1 c_4^2}{c_3^2} - \frac{c_2 c_4}{c_3}. \quad (27)$$

We note that if $c_3 = 0$, the integral in (23) has a closed-form expression, see Section IV-A. For fixed c_1, c_2 , the difference between I_α and I_β is also bounded, and therefore I_β is an approximation of original integral I_α .

To ease the following analysis, we define the sequence

$$p_m = \frac{1 - (-1)^m}{2} = \begin{cases} 1, & m \text{ is odd,} \\ 0, & m \text{ is even.} \end{cases} \quad (28)$$

Therefore, if we let $m = 2n + 1$, then $n = \frac{1}{2}(m - 1)$, $0 \leq n \leq N - 1$, and we have:

$$\begin{aligned} I_\beta &= \frac{2c_0 e^{c_7}}{\sqrt{\pi} c_3} \sum_{m=0}^{2N-1} \frac{(-1)^{\frac{m-1}{2}}}{m(\frac{m-1}{2})!} p_m \int_{c_4}^{c_3+c_4} e^{-c_5 y^2 + c_6 y} y^m dy \\ &= \frac{2c_0 e^{c_7}}{\sqrt{\pi} c_3} \sum_{m=0}^{2N-1} \frac{(-1)^{\frac{m-1}{2}} [1 - (-1)^m]}{2m(\frac{m-1}{2})!} \\ &\quad \cdot \int_{c_4}^{c_3+c_4} e^{-c_5 y^2 + c_6 y} y^m dy \\ &\triangleq \frac{2c_0 e^{c_7}}{\sqrt{\pi} c_3} \sum_{m=0}^{2N-1} d_m I_m, \end{aligned} \quad (29)$$

where

$$d_m = \frac{(-1)^{\frac{m-1}{2}}}{m} \cdot \frac{[1 - (-1)^m]}{2}, \quad (30)$$

$$I_m = \frac{1}{(\frac{m-1}{2})!} \int_{c_4}^{c_3+c_4} e^{-c_5 y^2 + c_6 y} y^m dy. \quad (31)$$

With integration by parts applied to (31), we find that the sequence I_m satisfies the following second-order inhomogeneous linear recurrence relation:

$$I_{m-1} + \frac{c_6(\frac{m-1}{2})!}{2(\frac{m}{2})!} I_m - c_5 I_{m+1} = \frac{1}{2(\frac{m}{2})!} (\gamma_m - \xi_m), \quad (32)$$

where

$$\gamma_m = c_0 e^{-c_5(c_3+c_4)^2 + c_6(c_3+c_4)} (c_3 + c_4)^m, \quad (33)$$

$$\xi_m = c_0 e^{-c_5 c_4^2 + c_6 c_4} c_4^m. \quad (34)$$

Once (32) is solved with two initial conditions, we obtain an approximation of I_α without numerical quadrature.

C. Olver's algorithm

It is well known that computing the minimal solution of a second-order difference equation, or three-term recurrence relation, directly from given initial values y_0, y_1 is an unstable procedure, see e.g. [5], [6]. F. W. J. Olver proposed a classic and stable algorithm for second-order inhomogeneous linear difference equations [7] in this form:

$$\begin{aligned} a_r y_{r-1} - b_r y_r + c_r y_{r+1} &= d_r, \\ y_0 &= k, \quad y_1 = m, \end{aligned} \quad (35)$$

where $a_r, b_r, c_r, d_r \in \mathbb{C}$ are given sequences, $r \in \mathbb{N}$ and $k, m \in \mathbb{C}$ are given constants.

The main idea of Olver's algorithm is to transfer the initial value problem to an equivalent boundary value problem (BVP). To do this, Olver abandoned the initial condition $y_1 = m$ and replaced it by another boundary condition $y_N = p$, which is obtained based on the asymptotic property of the minimal solution y_r , for sufficiently large N . In most cases (also in our case later on), $y_N = 0$. The solution of the well-conditioned BVP is $y_r^{(N)}$, Olver also proved that $y_r^{(N)}$ converges to the required solution y_r of the original initial value problem as $N \rightarrow \infty$. This linear BVP can be solved

efficiently by either Gaussian elimination or LU decomposition [8]. Therefore, for sufficient large N , $y_r^{(N)}$ will be an approximate solution of the difference equation (35). Olver's algorithm can also prevent unstable error propagation when solving higher-order inhomogeneous difference equations [9].

Back to problem (32) and comparing with (35), we have

$$a_r I_{r-1} - b_r I_r + c_r I_{r+1} = d_r, \quad (36)$$

where

$$a_r = 1, \quad b_r = -\frac{c_6(\frac{m-1}{2})!}{2(\frac{m}{2})!}, \quad (37)$$

$$c_r = -c_5, \quad d_r = \frac{1}{2(\frac{m}{2})!} (\gamma_m - \xi_m). \quad (38)$$

Hence the system (32) can be solved stably via Olver's algorithm.

IV. NUMERICAL EXPERIMENTS

Generally, every M -sided polygon can be decomposed into a combination of rectangles and right-angled triangles, so in this section we try to reconstruct these two fundamental objects with the method proposed in the preceding sections.

A. Rectangular object

In the first experiment we consider a support function $s_1(x, y)$ defined on a rectangular domain with coordinates $A(-\frac{1}{2}, -\frac{1}{2}), B(\frac{1}{2}, -\frac{1}{2}), C(\frac{1}{2}, \frac{1}{2}), D(-\frac{1}{2}, \frac{1}{2})$.

The Gabor parameters are given by: $-5 \leq m_i, n_i, k_i, l_i \leq 5$ and $m_i, n_i, k_i, l_i \in \mathbb{Z}$ where $i = x, y$.

$$X = Y = 1, K_x = K_y = 2\pi. \quad (39)$$

$$\alpha_x = \alpha_y = \beta_x = \beta_y = \sqrt{\frac{2}{3}}. \quad (40)$$

From Section II-B we recall that an analytical solution exists for (12) that can be used as a reference to check the method of the recurrence relation for the calculation of the Gabor coefficients.

Based on the parametrization step (17) of this rectangular object's boundary, it is easy to notice that along each side we have either $c_0 = 0$ or $c_3 = 0$ in (19). I_α vanishes when $c_0 = 0$, and when $c_3 = 0$, I_α is integrable:

$$\begin{aligned} I_\alpha &= c_0 \int_0^1 e^{-c_1 t^2 + c_2 t} \operatorname{erf}(c_4) dt \\ &= \frac{c_0 \sqrt{\pi}}{2\sqrt{c_1}} \operatorname{erf}(c_4) e^{\frac{c_2^2}{4c_1}} \left[\operatorname{erf}\left(\frac{2c_1 - c_2}{2\sqrt{c_1}}\right) + \operatorname{erf}\left(\frac{c_2}{2\sqrt{c_1}}\right) \right]. \end{aligned} \quad (41)$$

Therefore, in the rectangular case the Gabor coefficients calculated based on the line integration are the same as the analytical solutions for the double integral.

Figure 1 shows the reconstructed characteristic function defined on the rectangular domain.

Fig. 1. Reconstructed characteristic function for a rectangular object, via computed Gabor coefficients. The original characteristic function $f_1(x, y)$ was supported on a rectangle with vertex coordinates $A(-\frac{1}{2}, -\frac{1}{2})$, $B(\frac{1}{2}, -\frac{1}{2})$, $C(\frac{1}{2}, \frac{1}{2})$, $D(-\frac{1}{2}, \frac{1}{2})$. Oversampling parameter $q = 2$, $p = 3$, spacing of the window function $X = Y = 1$, spacial shift $-5 \leq m_x, m_y \leq 5$, spectral shift $-5 \leq n_x, n_y \leq 5$.

B. Triangular object

In the second experiment we consider a characteristic function $f_2(x, y)$ defined on a triangular domain with vertex coordinates $A(-\frac{1}{2}, -\frac{1}{2})$, $B(\frac{1}{2}, -\frac{1}{2})$, $C(\frac{1}{2}, \frac{1}{2})$. We keep the same Gabor parameter setting as in the previous experiment.

In this triangular case the double integral in (6) is not analytically integrable and the line integral (12) along the sloped boundary is non-trivial. Therefore, this is a good benchmark to test the proposed method in a non-trivial case. In this experiment we use direct numerical quadrature on (12) as a reference.

Figure 2 shows the reconstructed characteristic function for the triangular object.

Fig. 2. Reconstructed characteristic function for a triangular object based on recurrence relation and Olver's algorithm. The original characteristic function $f_2(x, y)$ was supported on a triangle with vertex coordinates $A(-\frac{1}{2}, -\frac{1}{2})$, $B(\frac{1}{2}, -\frac{1}{2})$, $C(\frac{1}{2}, \frac{1}{2})$. Same parameters were used as in Fig. 1.

The original support function defined on a triangular domain can be reconstructed successfully with the proposed method based on the recurrence relation and Olver's algorithm. However, 4.66% of the total calculated Gabor coefficients have

an absolute error larger than 10^{-4} compared to the numerical reference.

There are two reasons why the proposed approximate integral I_β has large errors at some points.

Firstly, the real part and imaginary part of $\text{erf}(z)$ itself can get very large when z is far from the origin and complex-valued. Convergence of the Taylor series around the origin is poor compared to the increase of $\text{erf}(z)$. Therefore, thousands of terms are required to reach the qualified approximation, which results in difficulties when solving the recurrence relation. However, to make sure there exists a recurrence relation in the truncated series, one must use the Taylor series around the origin to approximate $\text{erf}(z)$, since there is no known explicit representation for n -th derivative of $\text{erf}(z)$. Even so, at some points the error can still be large along some directions, for example in the current case for the triangle it can be larger than 10^{-4} .

Secondly, the absolute value of the integrals I_m can be very large before vanishing eventually, which means a high working precision is required to represent them accurately in the propagation through the backward substitution process in the recurrence relation. Furthermore, the coefficient sequence d_m in (30) is alternating. Hence, one must set a high working precision to avoid loss of significant figures and due to cancellation errors. A high working precision results in an increase in computation time.

Figure 3 displays the absolute value of I_m with parameter setting: $m_x + l_x = 1$, $m_y + l_y = 21$, $n_x + k_x = 18$, $n_y + k_y = 19$, and the maximum of $|I_m|$ reaches a level of 10^{360} .

Fig. 3. In this specific example, we have $N = 1250$, i.e., 2500 integrals I_m were calculated based on Olver's algorithm to approximate $\text{erf}(z)$. The error in the approximation is 1.10652×10^{-129} .

Based on this sequence I_m , we obtained an approximate integral I_β and therefore one Gabor coefficient. Note that a total of 1166886 integrals were computed to reconstruct Figure 2 and we obtain a difference $I_\alpha - I_\beta = -1.09719 \times 10^{-129} - 1.4339 \times 10^{-130}j$.

V. CONCLUSION AND OUTLOOK

The complex error function $\text{erf}(z)$ and the Faddeeva function (also known as the plasma dispersion function) $w(z) = e^{-z^2} \text{erfc}(-iz)$ are connected by elementary relations [10], and

both of them can be evaluated in different ways such as a Padé rational approximation [11], a rational Chebyshev approximation by Schonfelder [12], continued fractions [13] and also what we used here Taylor series expansion [4]. In this paper we selected a Taylor-series expansion to approximate the complex error function $\text{erf}(z)$, and then approximated the target integral I_α that occurs in the calculation of Gabor coefficients. The main reason for choosing a Taylor-series expansion is that it can yield a second-order inhomogeneous recurrence relation, which is beneficial in computing Gabor coefficients because calculating abundant integrals is not necessary anymore, as long as this recurrence relation can be solved stably with two initial conditions. Olver's algorithm was used to complete this means for computing Gabor coefficients. As applications for this proposed method, two characteristic functions defined on rectangular domain and triangular domain were reconstructed. In the triangular case, we observed that 4.66% of the Gabor coefficients have an error larger than the set threshold of 10^{-4} and two reasons were given for this outcome.

In future research, other expansions are expected to better approximate the complex error function within the integral I_α , with which the new basis function sets either yield much faster convergence (and therefore coefficients would vanish dramatically and the approximated integral can be evaluated even term by term), or relatively faster convergence but at meantime still generate a recurrence relation.

ACKNOWLEDGMENT

This work was funded by NWO-TTW as part of the HTSM program under project number 16184 and as part of the NWO-TTW perspective program under project number P16-08.

L. Sun is grateful to B. P. de Hon and J. M. L. Maubach from TU Eindhoven and S. Chevillard from the French Institute for Research in Computer Science and Automation for their suggestions and comments.

REFERENCES

- [1] R. J. Dilz, *A spatial spectral domain integral equation solver for electromagnetic scattering in dielectric layered media*. Technische Universiteit Eindhoven, 2017.
- [2] M. C. van Beurden and I. D. Setija, "Local normal vector field formulation for periodic scattering problems formulated in the spectral domain," *JOSA A*, vol. 34, no. 2, pp. 224–233, 2017.
- [3] M. J. Bastiaans, *Gabor's expansion and the Zak transform for continuous-time and discrete-time signals: critical sampling and rational oversampling*. Citeseer, 1995.
- [4] S. Chevillard, "The functions erf and erfc computed with arbitrary precision," *Rapport de recherche RR2009-04, laboratoire de l'informatique du parallélisme (LIP)*, vol. 46, p. 29, 2009.
- [5] W. Gautschi, "Computational aspects of three-term recurrence relations," *SIAM review*, vol. 9, no. 1, pp. 24–82, 1967.
- [6] J. Wimp, *Computation with recurrence relations*. Pitman, 1984.
- [7] F. W. J. Olver, "Numerical solution of second-order linear difference equations," *Journal of Research of the National Bureau of Standards - B. Mathematics and Mathematical Physics*, vol. 71B, no. 2,3, 1967.
- [8] J. Cash, "A note on olver's algorithm for the solution of second-order linear difference equations," *Mathematics of Computation*, vol. 35, no. 151, pp. 767–772, 1980.
- [9] —, "An extension of olver's method for the numerical solution of linear recurrence relations," *Mathematics of Computation*, vol. 32, no. 142, pp. 497–510, 1978.

- [10] G. P. Poppe and C. M. Wijers, "More efficient computation of the complex error function," *ACM Transactions on Mathematical Software (TOMS)*, vol. 16, no. 1, pp. 38–46, 1990.
- [11] W. J. Cody, "Rational chebyshev approximations for the error function," *Mathematics of Computation*, vol. 23, no. 107, pp. 631–637, 1969.
- [12] J. Schonfelder, "Chebyshev expansions for the error and related functions," *Mathematics of Computation*, vol. 32, no. 144, pp. 1232–1240, 1978.
- [13] W. Gautschi, "Efficient computation of the complex error function," *SIAM Journal on Numerical Analysis*, vol. 7, no. 1, pp. 187–198, 1970.