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ANALYTICAL POLE RESIDUE CALCULATION IN SPECTRAL METHOD OF MOMENTS FORMULATIONS FOR PERIODIC STRUCTURES

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Abstract—An analytical method for evaluating pole-residues in spectral method of moments (MoM) formulations is presented. Spectral integral formulations for periodic structures involve the inverse of the MoM matrix, which exhibits a periodic set of pole singularities, corresponding to the zeros of the matrix's determinant. So far, these singularities have not been extracted and the corresponding pole-residues were calculated directly from the differential or integral definitions of the residue. In this work, we consider an analytical expression for the solution to the MoM matrix equation, which enables the extraction of pole singularities and the analytical evaluation of pole-residues. We also present a comparison to previous methods.

1. INTRODUCTION

When applying the spectral domain method of moments (MoM) to periodic structures, one encounters periodic sets of pole singularities corresponding to the eigenmodes of the periodic structure [1–3]. In closed configurations, the solution can be expressed as a discrete sum of eigenmodes or mathematically as the sum of pole contributions, whereas in open configurations there is, in addition, a continuous

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spectrum of radiating modes, expressed mathematically by the branch-cut contributions [4]. Even when the pole contributions are only part of the solution, they can provide important physical information such as the power lost to surface waves [2]. This paper addresses the issue of calculating the pole contributions when the structure is excited by localized sources.

We consider spectral MoM formulations in which the field is expressed as a Sommerfeld integral, with the integrand calculated by solving numerically the MoM matrix equation, using iterative matrix inversion. The poles of this integrand correspond to zeros of the determinant of the MoM matrix [2], which location can only be found numerically using zero searching algorithms.

As is well known, evaluation of pole-residues in closed form is generally possible with the use of L'Hopital's rule whenever the singular expression is represented as a rational function [5–7]. Unfortunately, this is not the case in MoM formulations, where iterative matrix inversion is usually used (the exception is the trivial case of a single basis function, in which the matrix becomes a scalar [6, 7]). This is the reason why so-far the pole-residues in MoM formulations have been calculated by a numerical evaluation of the limit which constitutes the residue [2] or by numerical integration around the pole [8].

In this paper, a new approach is proposed in which the solution to the MoM matrix equation is expressed as a rational function using Laplace's formula [9], instead of using an iterative matrix inversion. This enables an analytical evaluation of pole-residues using L'Hopital's rule. We shall demonstrate that the proposed method is numerically stable, accurate, and its numerical cost is comparable to previous methods.

2. SPECTRAL INTEGRAL REPRESENTATION

For simplicity, we shall consider here only 2D configurations including periodic structures along the x axis with *aperiodic* excitation. An example is shown in Fig. 1, where an infinite metal strip grating is located over a grounded dielectric slab (GDS) and excited by a line source in the y direction.

The spectral integral is obtained by using the array scanning method (ASM) [2, 3]. In this approach, the MoM matrix equation is formulated for an auxiliary *periodic* problem in which the source is duplicated to form an infinite linear phased array with phase difference ϕ. First, the auxiliary periodic problem is solved using Floquet mode representation. The solution to the original aperiodic problem is then obtained by integrating over the 0th Floquet mode of the solution along

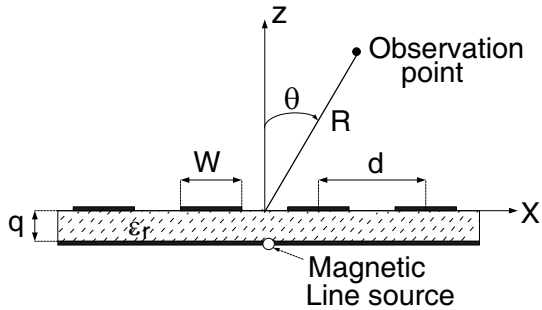

Figure 1. The geometry of a periodic structure excited by a magnetic line source in the y direction located at the ground plane (representing slot excitation). The structure consists of a metal strip grating over a grounded dielectric slab (GDS).

the entire real axis of ϕ.

The following can be applied to both magnetic and electric field integral equations (MFIE and EFIE). The EFIE is obtained by imposing a zero tangential electric field on the metal strips and is solved for the induced electric currents on the metal strips at $z = 0$. The MFIE is obtained by imposing the continuity of the tangential components of the magnetic fields across the slots at $z = 0$. In particular, by applying the equivalence theorem, the aperture is closed by a conductive sheet, and the continuity of the tangential component of the electric field is guaranteed by defining two unknown magnetic current densities (with opposite signs) on the opposite sides of the conductive sheet. In following part, we write for simplicity only the EFIE, keeping in mind that the MFIE is obtained by replacing the electric currents on the strips with the magnetic currents discussed above and replacing the Green function accordingly (will be used in Section 4). The incident field here is the electric/magnetic field due to the magnetic line source (slot excitation) at $z = -q$ for the EFIE/MFIE, respectively.

The electric field due to the *induced* currents in the auxiliary periodic problem can be written as a sum of Floquet modes [10]

$$\underline{E}^P(x, z; k_x) = \sum_{n=-\infty}^{\infty} \underline{\underline{\widetilde{G}}}(z; k_{xn})\underline{\widetilde{J}}_s(k_{xn})e^{-jk_{xn}x}, \tag{1}$$

where $k_{xn} = k_x + 2\pi n/d$ $(n = 0, \pm 1, \pm 2, \ldots)$ is the propagation constant in the x direction of the nth spatial harmonic, d is the period of the structure, $\underline{\widetilde{J}}_s(k_z)$ is the Fourier transform with respect to x of the

induced surface current at $z = 0$ in a single unit cell (the electric current on the strip or the magnetic current on the slot), and $\underline{\underline{\widetilde{G}}}$ is the dyadic *spectral* Green function for the background structure. In the example of Fig. 1, for the EFIE, $\underline{\underline{\widetilde{G}}}$ is the Green function for the electric field at $z = 0$ due to an electrical line current at $z = 0$ embedded in a GDS without the metal strips. For the MFIE, $\underline{\underline{\widetilde{G}}}$ is the Green function for the magnetic field at $z = 0$ due to a magnetic line current at $z = 0$ in a closed parallel plate wave-guide (recall that for the MFIE, the $z = 0$ plane is covered by a conductive sheet, as mentioned above). Similarly, the electric field due to the phased array of duplicated *sources* (in the example of Fig. 1, the magnetic line source at $z = -q$ should be duplicated) can be written in the form of (1) with the current and Green function replaced accordingly.

Next, the auxiliary problem is solved using the MoM. The induced current is expressed as a sum of N basis functions, their Fourier transforms denoted by $\left\{\widetilde{B}_r(k_x)\right\}$. Enforcing the boundary conditions using a set of weight functions with Fourier transforms $\left\{\widetilde{W}_p(k_x)\right\}$, results in a standard MoM matrix equation of the form $\mathbf{Z} \cdot \mathbf{A} = \mathbf{S}$ with $\mathbf{Z}$ denoting a known $N \times N$ matrix with four blocks (corresponding to the x and y components of the field). The elements of the block matrixes can be expressed in the following form [2, 10]

$$Z_{pr}(k_x) = \sum_{n=-M}^{M} \widetilde{W}_p(-k_{xn})\widetilde{G}(k_{xn})\widetilde{B}_r(k_x n) \quad p, r = 1, 2, \ldots N, \tag{2}$$

where $\widetilde{G}$ is one of the four components of $\underline{\underline{\widetilde{G}}}$, and M is the number of spatial harmonics employed in the numerical calculation. $\mathbf{A}$ is a column vector of size N, containing the coefficients of the basis-functions. $\mathbf{A}$ is determined by inverting the $\mathbf{Z}$ matrix, i.e., $\mathbf{A} = \mathbf{Z^{-1}S}$, using standard iterative numerical procedures for matrix inversion such as Gaussian elimination and etc. $\mathbf{S}$ is the "source vector" a known column vector of size N and its elements can be found in [2].

The scattered field due to the *induced* surface currents in the *original* problem can be expressed in the following form [2]

$$\underline{E}^{scat}(x, z) = \int_{-\infty}^{\infty} \mathbf{A}^T(k_x)\underline{\underline{\widetilde{G}}}(z, k_x)\underline{\widetilde{\mathbf{B}}}(k_x)e^{-jk_x x}dk_x \tag{3}$$

where the integrand includes *only the 0th Floquet mode*, and the vector $\underline{\widetilde{\mathbf{B}}}$ includes all basis functions. The spectral integral in (3) can be evaluated by deforming the integration contour in the complex k_x

plane and expressing (3) using the discrete eigenmodes of the periodic structure (pole-residues), and in open configurations (such as in Fig. 1), a set of continuous spectrums (periodic set of branch cuts) [11]. The continuous spectrum can be evaluated asymptotically in closed-form in the far-field zone, as in [11], or alternatively, one can eliminate the continuous spectrum by replacing $\underline{\underline{\widetilde{G}}}$ in (1) with the Green function proposed in [5].

We encounter two possible types of poles in (3): (a) poles of $\mathbf{A}$, representing modes of the periodic structure and their amplitudes are given by the corresponding pole-residues. (b) poles of $\underline{\underline{\widetilde{G}}}$, representing modes of the *background* structure, which in general differ from poles of type (a), and do not contribute.

3. POLE-RESIDUE CALCULATION

3.1. Previous Methods

If $\mathbf{A}$ in (3) is calculated via $\mathbf{A} = \mathbf{Z}^{-1}\mathbf{S}$, with the inverse calculated iteratively, one cannot use L'Hopitals rule in order to evaluate the pole-residues in (3), since $\mathbf{A}$ is not in the form of a rational function. One way of calculating the pole-residue is using the limit definition

$$\operatorname{Res}\{\underline{F}(k_x), k_{xp}\} \stackrel{\Delta}{=} \lim_{k_x \to k_{xp}} \underline{F}(k_x)\,(k_x - k_{xp}) \equiv \lim_{\Delta \to 0} \underline{F}(k_{xp} + \Delta)\,\Delta, \quad (4)$$

where $\underline{F}$ is the integrand in (3), k_{xp} is the pole location and $\Delta = k_x - k_{xp}$. Equation (4) is evaluated numerically as the limit of the following sequence

$$\operatorname{Res}\{\underline{F}(k_x), k_{xp}\} \stackrel{\Delta}{=} \underline{F}(k_{xp} + \Delta_m)(\Delta_m), \quad m = 1, 2, \ldots, \quad (5)$$

where Δ_m are increasingly smaller distances from the pole, which are reduced until convergence is obtained, i.e., the limit is reached.

A second way of evaluating the residue is by numerical integration around the pole

$$\operatorname{Res}\{\underline{F}(k), k_{xp}\} = \frac{1}{2\pi j} \oint_{C_p} \underline{F}(k_x) dk_x \approx \frac{1}{2\pi j} \sum_{m=1}^{IP} \underline{F}(k_{xm}) \Delta k_{xm}, \quad (6)$$

where k_{xm} is a point on the integration contour around the pole (in the counter clockwise direction) and Δk_{xm} is a segment on the integration path. IP denotes the number of integration points.

It should be noted that, the numerical cost of both these methods is $O(N^3)$ which is the cost of the matrix inversion. The number of iterations in the numerical limit method or the number of integration

points in the integral method are typically small, as the numerical example in Section 3 shows.

3.2. The Proposed Method

The solution to the MoM matrix equation can be brought into the form of a rational function by using Laplace's formula [9]

$$\mathbf{Z}^{-1}\left(k_x\right)=\frac{\mathbf{Z}^{\mathbf{A}}\left(k_x\right)}{\left|\mathbf{Z}\left(k_x\right)\right|}, \tag{7}$$

where $|\mathbf{Z}|$ and $\mathbf{Z}^{\mathbf{A}}$ are the determinant and adjugate of $\mathbf{Z}$, respectively. The elements of $\mathbf{Z}^{\mathbf{A}}$ are given by [9]

$$\left[\mathbf{Z}^{\mathbf{A}}\right]_{ij}=(-1)^{(i+j)}\left|\mathbf{M}_{ji}(\mathbf{Z})\right|, \tag{8}$$

with $\mathbf{M}_{ji}(\mathbf{Z})$ denoting the minor of the matrix $\mathbf{Z}$ obtained by removing the jth row and the ith column in $\mathbf{Z}$. The use of (7) enables to write the solution for the vector $\mathbf{A}$ in the following form

$$\mathbf{A}\left(k_x\right)=\frac{\mathbf{Z}^{\mathbf{A}}\left(k_x\right)\mathbf{S}\left(k_x\right)}{\left|\mathbf{Z}\left(k_x\right)\right|}. \tag{9}$$

Let k_{xp} be a pole of (9) for which $|\mathbf{Z}(k_{xp})|=0$, then the corresponding pole-residue can be calculated using L'Hopital's rule as

$$\operatorname{Res}\left\{\mathbf{A}\left(k_x\right),k_{xp}\right\}=\frac{\mathbf{Z}^{\mathbf{A}}\left(k_{xp}\right)\mathbf{S}\left(k_{xp}\right)}{\frac{\partial|\mathbf{Z}|}{\partial k_x}\left(k_{xp}\right)}. \tag{10}$$

The derivative of the determinant in (10) is calculated using Jacobi's Law [12]

$$\frac{\partial\left|\mathbf{Z}\right|}{\partial k_x}\left(k_{xp}\right)=tr\left\{\mathbf{Z}^{\mathbf{A}}\left(k_{xp}\right)\ \frac{\partial\mathbf{Z}}{\partial k_x}\left(k_{xp}\right)\right\}. \tag{11}$$

In (11), $tr\{\}$ denotes the trace of the matrix, and $\partial\mathbf{Z}/\partial k_x$ is the derivative of matrix $\mathbf{Z}$, which can be calculated numerically. Alternatively, if the weight and basis functions are given in closed form, the elements of $\partial\mathbf{Z}/\partial k_x$ can be calculated as

$$\begin{aligned}\frac{\partial}{\partial k_x}Z_{pr}(k_x) \;=\; & \sum_{n=-M}^{M}-\frac{\partial}{\partial k_x}\widetilde{W}_p(-k_{xn})\widetilde{G}(k_{xn})\widetilde{B}_r(k_{xn})\\ & +\sum_{n=-M}^{M}\widetilde{W}_p(-k_{xn})\frac{\partial}{\partial k_x}\widetilde{G}(k_{xn})\widetilde{B}_r(k_{xn})\\ & +\sum_{n=-M}^{M}\widetilde{W}_p(-k_{xn})\widetilde{G}(k_{xn})\frac{\partial}{\partial k_x}\widetilde{B}_r(k_{xn}).\end{aligned} \tag{12}$$

The calculation of $\mathbf{Z^A}$ in (10)–(11) from its definition in (8) requires calculation of N^2 determinants of minor matrixes of size $N-1$. If the determinants are calculated using matrix decomposition such as LU factorization (costing $O((N-1)^3)$), then the overall numerical cost of calculating $\mathbf{Z^A}$ is $O(N^5)$. Therefore, at first glance, the proposed approach is numerically more expensive than calculating $\mathbf{Z}^{-1}$ using Gaussian elimination with only $O(N^3)$ operations. However, there is a more efficient method for calculating $\mathbf{Z^A}$, presented in [13], which costs only $O(N^3)$. According to this method, $\mathbf{Z^A}$ is calculated as $\mathbf{Z^A}(k_x) = \mathbf{Z}^{-1}(k_x)\,|\mathbf{Z}(k_x)|$ (see (7)). Surprisingly, although $\mathbf{Z}$ is ill-conditioned near a pole and $\mathbf{Z}^{-1}$ is calculated with a large error, multiplication by $|\mathbf{Z}(k_{xp})|$ cancels this error and $\mathbf{Z^A}$ can be calculated with a very good accuracy (see [13], for more details). A fast calculation of $\mathbf{Z^A}$ is enabled by using singular value decomposition (SVD), $\mathbf{Z} = \mathbf{U\Sigma V^T}$, where $\mathbf{U}$ and $\mathbf{V}$ are $N \times N$ *orthogonal* matrixes and $\mathbf{\Sigma}$ is a *diagonal* $N \times N$ matrix. We can now calculate $\mathbf{Z^A}$ as

$$\begin{aligned}\mathbf{Z^A} &= \mathbf{Z}^{-1}\,|\mathbf{Z}| = \mathbf{V\Sigma^{-1}U^T}\left|\mathbf{U\Sigma V^T}\right| \\ &= \mathbf{V\Sigma^{-1}U^T}\,|\mathbf{U}|\,|\mathbf{\Sigma}|\left|\mathbf{V^T}\right| = \mathbf{V\Sigma^{-1}U^T}\prod_{i=1}^{N}\Sigma_{ii},\end{aligned} \tag{13}$$

where $|\mathbf{U}| = \left|\mathbf{V^T}\right| = \pm 1$ (see [13] for details on how to determine the sign) and Σ_{ii} are the diagonal elements of $\mathbf{\Sigma}$. $\mathbf{V\Sigma^{-1}U^T}$ is calculated using only one matrix multiplication, since calculating $\mathbf{\Sigma^{-1}}$ and multiplying it by $\mathbf{U^T}$ is straightforward ($\mathbf{\Sigma}$ is diagonal). The costs of matrix multiplication and the SVD are $O(N^3)$, so this is also the overall cost of calculating $\mathbf{Z^A}$, which is the same as $\mathbf{Z^{-1}}$ using Gaussian elimination. It is also possible to use other matrix decompositions for $\mathbf{Z}$, which are also discussed in [13].

4. NUMERICAL EXAMPLE

4.1. Numerical Details

Next, we present a numerical example, which demonstrates the advantage of using the proposed method (see (10)–(11)) or the integral method (see (6)) over using the numerical limit method in (5). In this example, we calculate the pole-residues corresponding to surface waves. We used the structure in Fig. 1, which is excited by a magnetic line source in the y direction (TM to z case) located at the ground plane. The slot and the strip widths are $w = 0.5d$, the substrate height is $q = 0.6d$ and the dielectric constant of the slab is $\varepsilon_r = 15$. A magnetic-field integral equation (MFIE) was used for H_y [1] (the $\mathbf{Z}$

matrix is replaced by the $\mathbf{Y}$ matrix but the structures of both matrixes is exactly the same).

Four basis functions were required in the MoM solution to obtain a relative error less than 0.01%. Standard weighted Chebyshev polynomials [10] were chosen as basis and weight functions (Galerkin's method). The locations of the poles k_{xpn} were found by searching the zeros of $|\mathbf{Y}|$ using Muller's algorithm [14]. The results presented next were calculated using only the poles corresponding to the first 11 spatial harmonics ($n = -5 \div 5$). The pole-residues decrease considerably for higher harmonics and can be neglected. The current choice of 11 spatial harmonics produces a relative error of less than 0.01%.

The SW power was calculated in a similar fashion to [2], using the proposed residue calculation method (Eqs. (10)–(12)) and compared to the numerical limit calculation of the residue (Eq. (5)). Using the general form of (3) for the magnetic field H_y due to the induced currents, the SW power is calculated as [2]

$$P_{sw} = \frac{1}{|\partial\beta/\partial\omega|}\frac{\mu_0}{2}\sum_{n=-5}^{5}\int_{-q}^{\infty}\left|\mathrm{Res}\left\{\mathbf{A}^T(k_x)\widetilde{G_{yy}}(z,k_x)\widetilde{\mathbf{B}_y}(k_x),\ k_{xpn}\right\}\right|^2 dz, \tag{14}$$

where β is the propagation constant of the surface wave, μ_0 is the permeability constant for the dielectric material and $\widetilde{G_{yy}}$ is the Green function for the magnetic field at $z = 0$ due to the *induced* magnetic currents (see discussion after (1)). We have also used in (14) the fact that the Floquet modes are orthogonal to each other.

4.2. Results

Next, two cases are presented for the computation of the surface wave (SW) power. In the first case, shown in Fig. 2, the pole locations were calculated with a relative accuracy of $\varepsilon = 10^{-15}$ and both methods were compared, showing a good agreement. In the "numerical limit" method, the relative distance from the pole, $\delta(\ll 1)$, defined by $\delta = \Delta_m/k_{xp}$ (see notation after (5)), was reduced until the convergence criteria was met. The difference between the two methods can be seen in the enlarged segment shown in Fig. 2. The results for $\delta = 10^{-8}$ (dashed line), $\delta = 10^{-9}$ (dotted line) and $\delta = 10^{-10}$ (dashed-dotted line) demonstrate that while the proposed method calculates the residue with a single calculation, the numerical limit method requires repeated calculations until the required relative error is obtained.

In the second case, shown in Fig. 3, the accuracy of the pole locations was reduced by multiplying the previously found pole

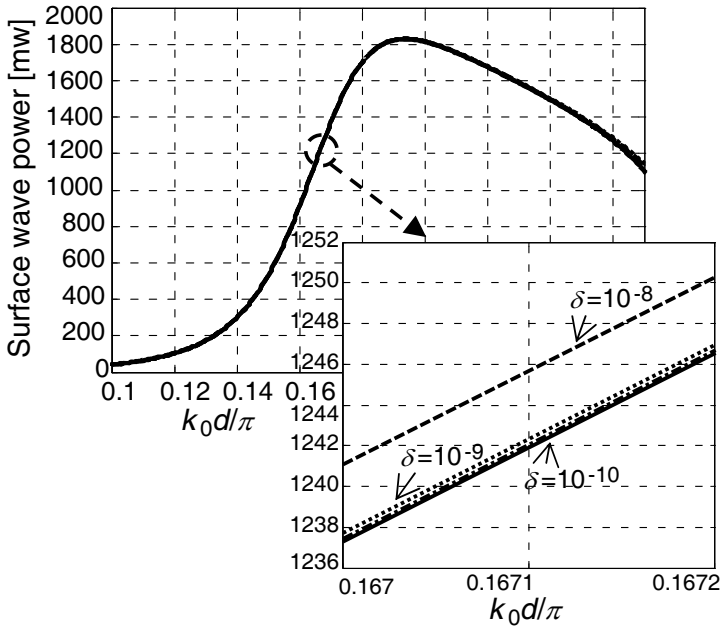

Figure 2. SW Power vs. frequency. Comparison between the proposed method and the numerical limit method for different values of δ with pole location accuracy of 10^{-15}. Legend: solid line-proposed method; dashed line-num. limit with $\delta = 10^{-8}$; doted line-num. limit with $\delta = 10^{-9}$; dashed-doted line-num. limit with $\delta = 10^{-10}$.

locations by a factor of $(1 + 10^{-10})$. One can see that the "numerical limit" method fails to converge to the correct solution. This behavior is expected from (5), since the multiplication by Δ_m, which includes the inaccurate postulated pole location, introduces a zero and in addition, the pole in the integrand $\underline{F}$ is not canceled. Depending on the relative distance from the pole δ, the "numerical limit" method can converge to zero or diverge as a result of the pole. In the example of Fig. 3, it is clear that the solution converges towards zero. On the other hand, by comparing Figs. 2 and 3, it is seen that decreasing the accuracy of the pole location has not affected the proposed method. We note that despite the fact that the results of the numerical limit method for $\delta = 10^{-8}$ (Fig. 3) are similar to the proposed method results, there can be no indication that this is indeed the correct result without comparing it to the proposed method, since the results diverge when decreasing δ.

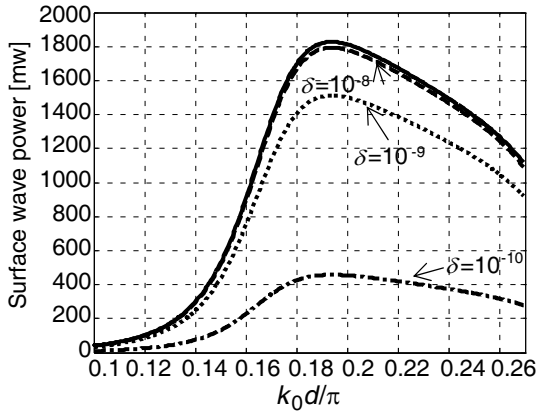

Figure 3. Re-calculation of the results of Fig. 2 with reduced pole location accuracy of 10^{-10}. Comparison of the proposed method to the numerical limit method with different values of δ. Legend: solid line-proposed method; dashed line-num. limit with $\delta = 10^{-8}$; doted line-num. limit with $\delta = 10^{-9}$; dashed-doted line-num. limit with $\delta = 10^{-10}$.

It should be noted that, the surface wave power presented here has no physical significance since the current of the source is constant for all frequencies. The surface wave power should be divided by the total radiated power at each frequency to give the correct indication of the surface wave power. However, since our purpose was only to demonstrate the numerical stability of the pole residue calculation, we did not make this calculation.

The integral method for calculating the residue was also checked. It was found that this method produces the same results as the proposed method in both cases of Figs. 2 and 3. When integrating around the pole one should choose an integration contour, which is larger than the "uncertainty region" in which the pole can lie. Considering the dimensionless spectral space $\xi = k_x/k$, the radius of the "uncertainty region" can be roughly approximated by $R = \varepsilon\xi_{xp}$ (where ε is the relative error in the pole location required in the pole searching algorithm and ξ_{xp} is the found pole location). The number of sampling points along this contour is typically small since the spectral period is proportional to $(kd)^{-1}$, which is much larger than the contour length $C \approx 2\pi R = 2\pi\varepsilon$. In this example $\varepsilon = 10^{-15}$ and only 10 points were needed. The overall cost of this method in this case is $10\times\ O(N^3)$. In "large" problems where $kd \gg \varepsilon^{-1}$ the spectral period is smaller than the contour length and the number of integration points increases with kd for a fixed accuracy ε.

5. CONCLUSION

So far, the evaluation of pole-residues in MoM solutions was done by approximating numerically the limit, which defines the residue, or by numerical integration around the pole. In this work, it has been found that the numerical limit method inherits a large sensitivity to the accuracy of the pole location and in some cases can produce unstable results. The integral method on the other hand is stable and accurate.

We presented here another method for calculating pole-residues. However, as opposed to previous method, this method is based on an analytical extraction of the pole singularity and can be used to validate the results, which are sometimes problematic due to the singularity presence, as seen in the case of the numerical limit method.

In the proposed method, one uses Laplace's formula to express the singular integrand as a rational function, enabling the use of L'Hopital rule and leading to a closed form evaluation of the residue. It was shown that the numerical cost of the proposed method is comparable to previous methods.

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