## TELECOMMUNICATIONS ENGINEERING SCHOOL TECHNICAL UNIVERSITY OF CARTAGENA

Department of Information Technologies and Communications



## MASTER'S THESIS MASTER'S DEGREE IN TELECOMMUNICATIONS ENGINEERING

Investigations on Integral Equation Techniques Applied to the Analysis of Radiofrequency Circuits for Satellite Applications



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#### Introduction

The use of numerical techniques applied to the analysis of microwaves circuits is one of the most interesting issues in the telecommunications industry. By using these computational techniques, we can reduce the time invested in development. This allows that the required components in communication systems could be designed and analysed by a computer.

Among these methods, the integral equation technique [1] has proved to be powerful due to its possibilities to carry out an efficient analysis of some structures. This technique has been successfully employed in numerous scenarios: both evaluation of radiated electromagnetic fields by antennas in free-space, analysis of multilayered radiofrequency circuits and problems and circuits which involve the analysis of waveguides and cavities.

One of the numerical techniques that can be used to solve integral equations is the Method of Moments (MoM) [1]. On the other hand, the solution of this kind of electromagnetic problems in periodic structures requires the computation of periodic Green's functions as the kernel of the corresponding integral equations.

The difficulty of the implementation of the integral equation techniques arises from the fact that these periodic Green's functions in homogeneous media can be written either as spatial or spectral infinite series. These series can present singularities and can exhibit a slowly convergent behaviour. According to this, one of the most important challenge in the implementation of many integral equation techniques is the efficient and accurate computation of periodic Green's functions.

A number of techniques, either analytical or numerical, have been developed in the past to accelerate the convergence of the series involved in the evaluation of Green's functions. Among these techniques, we should mention Ewald's method [4]. As commented in [5], the original series that converges slowly can be split into two functions which exhibit Gaussian convergence. Nevertheless, these new series required the computation of special mathematical functions that can increase the total computational time.

Another technique employed to accelerate the convergence of slow series is Kummer's transformation [3,6]. This technique has been efficiently applied in [2] and consists of ex-

tracting the asymptotic behaviour to accelerate the original series and summing efficiently the retained terms.

In addition to the previous techniques, we should mention Veisoglu's transformation [7], Shanks's transformation [8] and the summation by parts algorithm [9], among other analytical and numerical methods [3]. Most publications that carry out a comparative study between the different analytical and numerical methods for the acceleration of these series [3,10] seem to indicate that Ewald's method is the best choice in most scenarios. That is probably due to its versatility and good compromise between accuracy and efficiency.

In the described context, the main aim of this work will be the review of the integral equation technique applied to the analysis of periodic structures.

Specifically, we will try to extend the formulation of 2-D Green's functions with 1-D periodicity reported in [11]. We also go into detail about the acceleration of the functions involved in parallel-plate waveguide problems.

As a continuation of the work developed in [11], some transformations will be carried out to 2-D Green's functions with 2-D periodicity. In particular, we will study Ewald's method and the spectral Kummer's transformation. In addition, we also review the acceleration of the Green's functions involved in cavity and rectangular waveguide problems.

By means of the developed software tool, we could compare the convergence and the computational time required by all the reported methods for both 2-D Green's functions with 1-D periodicity and 2-D Green's functions with 2-D periodicity. Thanks to that, results and conclusions about the efficiency of the applied techniques will be summarized.

Finally and attending to the second line of research of this project, some structures based on coaxial to microstrip transition will be analysed by using the software tool FEST3D. Hence, we will be able to achieve meaningful conclusions through comparing the analysis of the same structures carried out with FEST3D and with another commercial tool HFSS.

To conclude, we will report the most important reached conclusions and explain our future lines of investigation.

#### **Project Structure**

Chapter 1. The 2-D Green's Functions With 1-D Periodicity. This first chapter is the continuation of my Final Degree Project [11] in the study of the 2-D Green's functions with 1-D periodicity.

On the one hand, the formulation developed in [11] will be extended thanks to the acquired knowledge in the spectral Kummer's transformation. We will explain different approaches when we retain the asymptotic terms in Kummer's transformation and according to this, different ways of summing the retained terms.

On the other hand, we will show how to apply this technique to the functions involved in parallel-plate waveguide problems with the intention of reducing the computational time. This means a practical implementation of the theory that was outlined in [11].

Chapter 2. The 2-D Green's Functions With 2-D Periodicity. In this chapter, the formulation developed for the 2-D Green's functions with 1-D periodicity is extended to the computation of the double series involved in problems with 2-D periodicity.

Firstly, the formulation of both the spatial and spectral Green's functions is obtained. We also formulate the gradient of these Green's functions that can be useful in the integral equation technique for the evaluation of the electromagnetic scattering produced by dielectric or magnetic objects inside waveguides.

After that, Ewald's method and the spectral Kummer's transformation are applied to accelerate the convergence of these functions [2]. In the application of Kummer's transformation, we also distinguish between different approaches to retain the asymptotic terms. As a consequence, the extracted terms could be summed in different ways.

On the other hand, we will show a practical implementation of the outlined theory applying this technique to the Green's functions involved in cavity and waveguide problems with the intention of reducing the computational time.

Chapter 3. Numerical Results. In this chapter, the numerical results that have been obtained when we implement the methods described in Chapter 1 and Chapter 2 for the 2-D Green's functions with 1-D and 2-D periodicities are shown. These comparisons have been carried out with a software developed in Matlab.

In relation to the 2-D Green's functions with 1-D periodicity, the convergence of the new strategy of applying Kummer's transformation will be compared with the previous approach reported in [11].

Regarding the 2-D Green's functions with 2-D periodicity, the convergence of both Green's functions and their gradients for different scenarios will be shown. We compare these ones with the convergence in the case of applying the techniques that have been proposed in Chapter 2 (Ewald's method and Kummer's transformation). In the case of

Kummer's transformation, the advantages of using either approach in the retention of terms are justified.

Using this software, we will be able to compare the efficiency of the applied methods and to deduce outstanding conclusions.

Chapter 4. Using FEST3D to Analyse Microstrip Structures. This chapter is about the second line of investigation carried out in this project in collaboration with our external partners Marco Guglielmi and Vicente Boria at Universidad Politécnica de Valencia.

Here, the software tool FEST3D is used in order to analyse some structures based on a coaxial to microstrip transition. The aim of this chapter is to study the convergence parameters to obtain accurate simulated performances in comparison to the results obtained by the use of HFSS.

Chapter 5. General Conclusions and Future Lines of Research. In this last chapter, we will discuss the general conclusions of this master's thesis, its applications and usefulness and we will present the future research lines.

#### Chapter 1

# The 2-D Green's Functions With 1-D Periodicity

The Green's functions with 1-D periodicity was previously studied in my Final Degree Project [11]. In [11], we worked on the demonstration and the acceleration of the spatial and spectral Green's functions for the case of 1-D periodicity and their gradients.

Specifically, we applied Ewald's method and Kummer's transformation. Consequently, through programming we could compare the efficiency of the proposed techniques.

In this chapter, the formulation about the spectral Kummer's transformation developed in [11] is extended. Different approaches when we retain the asymptotic terms in Kummer's transformation are explained and according to this, different ways of adding the retained terms are studied.

It should be noted that this problem has a practical interest since the Green's functions for the proposed problem are the basis for the analysis, through the integral equation technique, of inductive obstacles in rectangular waveguide [12]. They are widely used in space applications and in devices with emerging technologies such as Substrate Integrated Waveguide (SIW) [13] and Substrate Integrated Non-Radiative Dielectric (SINRD) [14].

In fact, we apply the theoretical functions studies to the case of electromagnetic problems associated with the computation of Green's functions such as parallel-plate waveguides. We show how to accelerate the convergence of these functions with the intention of reducing the computational time.

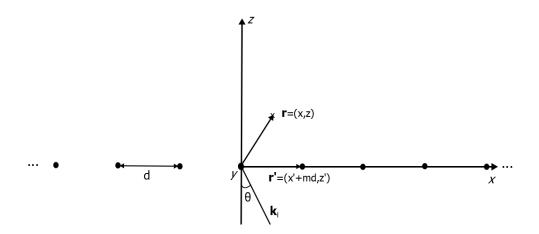


Figure 1.1: Physical configuration of an infinite distribution of line sources which are infinite and invariant on y-direction and are separated with a period d in x-direction.

#### 1.1 Revisited of the Spectral Kummer's Transformation

It is important to remember that the structure under discussion here is a one-dimensional array of line sources that are parallel to the z-axis and periodically located in a homogeneous medium along the x-direction (see Fig. 1.1).

The periodic 2-D Green's function generated by this array of line sources is given by

$$G(\bar{r}, \bar{r}') = \frac{1}{4j} \sum_{m=-\infty}^{+\infty} H_0^{(2)}(kR_m) e^{-jk_{x0}md}$$
(1.1)

where  $k_{x0} = k \sin(\theta)$  is the phase per period imposed by the excitation plane wave and  $R_m$  is the spatial distance between the observation point and the line sources.

$$R_m = \sqrt{(x - x' - md)^2 + (z - z')^2}$$
 (1.2)

This is the spatial series representation. If the 1-D version of Poisson's formula is applied to (1.1), we obtain the spectral representation given by

$$\widetilde{G}(\bar{r}, \bar{r}') = \frac{1}{2d} \sum_{m=-\infty}^{+\infty} \frac{e^{-\gamma_m|z-z'|}}{\gamma_m} e^{-jk_{xm}(x-x')}$$
(1.3)

where  $k_{xm} = k_{x0} + \frac{2\pi m}{d} = k \sin(\theta) + \frac{2\pi m}{d}$  and  $\gamma_m = \sqrt{k_{xm}^2 - k^2}$ .

Both series are slowly convergent in most cases. For this reason, Kummer's transformation [6] is one of the techniques used to accelerate the convergence of these series. According to [3], this technique can be applied in the spectral or in the spatial domain. In this case, we retain the asymptotic terms of the spectral function (1.3), applying the spectral Kummer's transformation, as follows

$$\widetilde{G}_{k}(\bar{r}, \bar{r}') = \frac{1}{2d} \sum_{\substack{m = -\infty \\ m \neq 0}}^{+\infty} \left( \frac{e^{-\gamma_{m}|z - z'|}}{\gamma_{m}} - \widetilde{G}_{m} \right) e^{-jk_{xm}(x - x')} + \widetilde{G}_{0} + \frac{1}{2d} \sum_{\substack{m = -\infty \\ m \neq 0}}^{+\infty} \widetilde{G}_{m} e^{-jk_{xm}(x - x')}$$
(1.4)

where  $\widetilde{G}_0$  is the contribution of the term m=0 in which we do not apply the extraction. The asymptotic retained term  $\widetilde{G}_e(\bar{r},\bar{r}')$  has to be efficiently added.

$$\widetilde{G}_e(\bar{r}, \bar{r}') = \frac{1}{2d} \sum_{\substack{m = -\infty \\ m \neq 0}}^{+\infty} \widetilde{G}_m e^{-jk_{xm}(x - x')}$$

$$\tag{1.5}$$

The novel consideration is that  $G_m$  can be obtained by two different ways resulting in two different approaches of formulating the dynamic part. Consequently, two different ways of adding the retained part can be used. The advantages of each approach will be studied in Chapter 3, where we can see that the improvement of each approach is different.

It should be pointed out that in both strategies the exponential  $e^{-\gamma_m|z-z'|}$  is approximated by its first order expansion, so that, we use  $e^{-|k_{xm}||z-z'|}$ . This is because when the observation point is near the source (critical case),  $|z-z'| \to 0$  and the exponential become not very significant and its first order approximation is enough.

The first option, which is not the strategy explained previously in [11], is the following

$$\frac{1}{\gamma_m} = \frac{1}{\sqrt{k_{xm}^2 - k^2}} = \frac{1}{|k_{xm}| \sqrt{1 - \underbrace{\left(\frac{k}{k_{xm}}\right)^2}_{u}}}$$
(1.6)

Using Taylor expansion in u=0

$$\frac{1}{\sqrt{1-u}} = 1 + \frac{1}{2}u + \frac{3}{8}u^2 + \frac{5}{16}u^3 + \frac{35}{128}u^4 + \dots = \sum_{q=0}^{+\infty} \frac{\prod_{n=0}^{q-1}(2n+1)}{2^q \, q!} u^q \tag{1.7}$$

 $\widetilde{G}_m$  can be written as

$$\widetilde{G}_{m} = \frac{1}{|k_{xm}|} \left( 1 + \frac{1}{2} \left( \frac{k}{k_{xm}} \right)^{2} + \frac{3}{8} \left( \frac{k}{k_{xm}} \right)^{4} + \frac{5}{16} \left( \frac{k}{k_{xm}} \right)^{6} + \dots \right) e^{-|k_{xm}||z-z'|} \\
= \left( \frac{1}{|k_{xm}|} + \frac{k^{2}}{2|k_{xm}|^{3}} + \frac{3k^{4}}{8|k_{xm}|^{5}} + \frac{5k^{6}}{16|k_{xm}|^{7}} + \dots \right) e^{-|k_{xm}||z-z'|} \\
= \sum_{q=0}^{Q} \frac{\prod_{n=0}^{q-1} (2n+1)}{2^{q} q!} \frac{k^{2q}}{|k_{xm}|^{2q+1}} e^{-|k_{xm}||z-z'|} \tag{1.8}$$

where Q is the number of the retained terms that we use in the approximation of the asymptotic series  $\widetilde{G}_m$ .

It is important to note that  $\frac{1}{\gamma_m}$  is positive, so here the absolute value has been omitted because all these terms are positive due to its own absolutes values. Using this  $\widetilde{G}_m$  approach, the series  $\widetilde{G}_e(\bar{r},\bar{r}')$  that we have to efficiently sum is

$$\widetilde{G}_{e}(\overline{r}, \overline{r}') = \frac{1}{2d} \sum_{\substack{m = -\infty \\ m \neq 0}}^{+\infty} \left( \frac{1}{|k_{xm}|} + \frac{k^{2}}{2|k_{xm}|^{3}} + \frac{3k^{4}}{8|k_{xm}|^{5}} + \frac{5k^{6}}{16|k_{xm}|^{7}} + \dots \right) e^{-|k_{xm}||z-z'|} e^{-jk_{xm}(x-x')}$$

$$= \frac{e^{-jk_{x0}(x-x')}}{2d} \sum_{\substack{m = -\infty \\ m \neq 0}}^{+\infty} \left( \sum_{q=0}^{Q} \underbrace{\prod_{n=0}^{q-1} (2n+1)}_{f_{q}} \frac{k^{2q}}{|k_{xm}|^{2q+1}} \right) e^{-|k_{xm}||z-z'|} e^{-j\frac{2\pi m}{d}(x-x')} \tag{1.9}$$

In advance, we can realize that this approach will result in a better approximation of the spectral series and therefore in a faster convergence rate in comparison to the other one. The options that we propose to sum efficiently this series are:

- Option A.1: Sum by Ewald's method.
- Option A.2: Lerch transcendent.
- Option A.3: Summation by parts technique.

The formulation of each option will be developed in the subsections 1.1.1, 1.1.2 and 1.1.3, respectively.

The other approach to extract the asymptotic terms is shown in [11] and is based on

$$\frac{1}{\sqrt{k_{xm}^2 - k^2}} = \frac{1}{\sqrt{\left(k_{x0} + \frac{2\pi m}{d}\right)^2 - k^2}} = \frac{1}{\sqrt{k_{x0}^2 + 2\frac{2\pi m}{d}k_{x0} + \left(\frac{2\pi m}{d}\right)^2 - k^2}}$$

$$= \frac{1}{\left(\frac{2\pi m}{d}\right)\sqrt{1 + \underbrace{\frac{k_{x0}d}{\pi m} + \frac{k_{x0}^2 - k^2}{\left(\frac{2\pi m}{d}\right)^2}}_{u}}} \tag{1.10}$$

Carrying out the expansion using Taylor series when  $m \to \infty$  or, what is the same,  $u \to 0$ , we have the following approximation

$$\frac{1}{\sqrt{1+u}} = 1 - \frac{1}{2}u + \frac{3}{8}u^2 - \frac{5}{16}u^3 + \frac{35}{128}u^4 - \dots = \sum_{q=0}^{+\infty} \underbrace{\frac{(-1)^q \prod_{n=0}^{q-1} (2n+1)}{2^q q!}}_{f_q} u^q \quad (1.11)$$

and taking into account that the powers of u are

$$u = {1 \choose 0} \frac{k_{x0}d}{\pi m} + {1 \choose 1} \frac{(k_{x0}^2 - k^2)d^2}{(2\pi m)^2}$$
 (1.12a)

$$u^{2} = {2 \choose 0} \frac{k_{x0}^{2} d^{2}}{(\pi m)^{2}} + {2 \choose 1} \frac{k_{x0} d}{\pi m} \frac{(k_{x0}^{2} - k^{2}) d^{2}}{(2\pi m)^{2}} + {2 \choose 2} \frac{(k_{x0}^{2} - k^{2})^{2} d^{4}}{2^{4} (\pi m)^{4}}$$

$$= {2 \choose 0} \frac{k_{x0}^{2} d^{2}}{(\pi m)^{2}} + {2 \choose 1} \frac{k_{x0} (k_{x0}^{2} - k^{2}) d^{3}}{2^{2} (\pi m)^{3}} + {2 \choose 2} \frac{(k_{x0}^{2} - k^{2})^{2} d^{4}}{2^{4} (\pi m)^{4}}$$

$$(1.12b)$$

$$u^{3} = \binom{3}{0} \frac{k_{x0}^{3} d^{3}}{(\pi m)^{3}} + \binom{3}{1} \frac{k_{x0}^{2} d^{2}}{(\pi m)^{2}} \frac{(k_{x0}^{2} - k^{2}) d^{2}}{(2\pi m)^{2}} + \binom{3}{2} \frac{k_{x0} d}{(\pi m)} \frac{(k_{x0}^{2} - k^{2})^{2} d^{4}}{2^{4} (\pi m)^{4}} + \binom{3}{3} \frac{(k_{x0}^{2} - k^{2})^{3} d^{6}}{2^{6} (\pi m)^{6}}$$

$$= \binom{3}{0} \frac{k_{x0}^{3} d^{3}}{(\pi m)^{3}} + \binom{3}{1} \frac{k_{x0}^{2} (k_{x0}^{2} - k^{2}) d^{4}}{2^{2} (\pi m)^{4}} + \binom{3}{2} \frac{k_{x0} (k_{x0}^{2} - k^{2})^{2} d^{5}}{2^{4} (\pi m)^{5}} + \binom{3}{3} \frac{(k_{x0}^{2} - k^{2})^{3} d^{6}}{2^{6} (\pi m)^{6}}$$

$$(1.12c)$$

$$u^{4} = \binom{4}{0} \frac{k_{x0}^{4} d^{4}}{(\pi m)^{4}} + \binom{4}{1} \frac{k_{x0}^{3} d^{3}}{(\pi m)^{3}} \frac{(k_{x0}^{2} - k^{2}) d^{2}}{(2\pi m)^{2}} + \binom{4}{2} \frac{k_{x0}^{2} d^{2}}{(\pi m)^{2}} \frac{(k_{x0}^{2} - k^{2})^{2} d^{4}}{2^{4} (\pi m)^{4}}$$

$$+ \binom{4}{3} \frac{k_{x0} d}{(\pi m)} \frac{(k_{x0}^{2} - k^{2})^{3} d^{6}}{2^{6} (\pi m)^{6}} + \binom{4}{4} \frac{(k_{x0}^{2} - k^{2})^{4} d^{8}}{2^{8} (\pi m)^{8}}$$

$$= \binom{4}{0} \frac{k_{x0}^{4} d^{4}}{(\pi m)^{4}} + \binom{4}{1} \frac{k_{x0}^{3} (k_{x0}^{2} - k^{2}) d^{5}}{2^{2} (\pi m)^{5}} + \binom{4}{2} \frac{k_{x0}^{2} (k_{x0}^{2} - k^{2})^{2} d^{6}}{2^{4} (\pi m)^{6}}$$

$$+ \binom{4}{3} \frac{k_{x0} (k_{x0}^{2} - k^{2})^{3} d^{7}}{2^{6} (\pi m)^{7}} + \binom{4}{4} \frac{(k_{x0}^{2} - k^{2})^{4} d^{8}}{2^{8} (\pi m)^{8}}$$

$$(1.12d)$$

In general, the powers of u can be expressed as

$$u^{q} = \sum_{a=0}^{q} {q \choose a} \frac{k_{x0}^{(q-a)} (k_{x0}^{2} - k^{2})^{a}}{2^{2a}} \left(\frac{d}{\pi m}\right)^{q+a}$$
(1.13)

therefore,  $\frac{1}{\gamma_m}$  can be approximated by Q terms as

$$\frac{1}{\gamma_m} \approx \left| \sum_{q=0}^{Q} \sum_{a=0}^{q} {q \choose a} \frac{k_{x0}^{(q-a)} (k_{x0}^2 - k^2)^a}{2^{2a+1}} \left( \frac{d}{\pi m} \right)^{q+a+1} f_q \right|$$
 (1.14)

and finally  $\widetilde{G}_m(\bar{r}, \bar{r}')$  is

$$\widetilde{G}_{m}(\bar{r}, \bar{r}') = \left| \frac{d}{2\pi m} - \frac{k_{x0}d^{2}}{(2\pi m)^{2}} + \frac{(k^{2} - k_{x0}^{2})d^{3}}{2(2\pi m)^{3}} + \dots \right| e^{-\left|\frac{2\pi m}{d} + k_{x0}\right||z - z'|}$$

$$= \left| \sum_{q=0}^{Q} \sum_{q=0}^{q} {q \choose a} \frac{k_{x0}^{(q-a)} (k_{x0}^{2} - k^{2})^{a}}{2^{2a+1}} \left(\frac{d}{\pi m}\right)^{q+a+1} f_{q} \right| e^{-\left|\frac{2\pi m}{d} + k_{x0}\right||z - z'|} \tag{1.15}$$

Using this  $\widetilde{G}_m$  approach, the series  $\widetilde{G}_e(\bar{r},\bar{r}')$  that we have to efficiently sum is

$$\widetilde{G}_{e}(\overline{r}, \overline{r}') = \frac{1}{2d} \sum_{\substack{m = -\infty \\ m \neq 0}}^{+\infty} \left| \frac{d}{2\pi m} - \frac{k_{x0}d^{2}}{(2\pi m)^{2}} + \frac{(k^{2} - k_{x0}^{2})d^{3}}{2(2\pi m)^{3}} + \dots \right| e^{-\left|\frac{2\pi m}{d} + k_{x0}\right||z - z'|} e^{-jk_{xm}(x - x')}$$

$$= \frac{1}{2d} \sum_{\substack{m = -\infty \\ m \neq 0}}^{+\infty} \left| \sum_{q = 0}^{Q} \sum_{a = 0}^{q} {q \choose a} \frac{k_{x0}^{(q - a)}(k_{x0}^{2} - k^{2})^{a}}{2^{2a + 1}} \left( \frac{d}{\pi m} \right)^{q + a + 1} f_{q} \right| e^{-\left|\frac{2\pi m}{d} + k_{x0}\right||z - z'|} e^{-jk_{xm}(x - x')} \tag{1.16}$$

On the other hand, if we are interested in grouping the terms respect to the powers of m, we can proceed as follows

$$m \to \begin{pmatrix} 1 \\ 0 \end{pmatrix} \frac{k_{x0}d}{\pi m}$$
 (1.17a)

$$m^2 \to {2 \choose 0} \frac{k_{x0}^2 d^2}{(\pi m)^2} + {1 \choose 1} \frac{(k_{x0}^2 - k^2) d^2}{2^2 (\pi m)^2}$$
 (1.17b)

$$m^3 \to \binom{3}{0} \frac{k_{x0}^3 d^3}{(\pi m)^3} + \binom{2}{1} \frac{k_{x0}(k_{x0}^2 - k^2)d^3}{2^2(\pi m)^3}$$
 (1.17c)

$$m^4 \to {4 \choose 0} \frac{k_{x0}^4 d^4}{(\pi m)^4} + {3 \choose 1} \frac{k_{x0}^2 (k_{x0}^2 - k^2) d^4}{2^2 (\pi m)^4} + {2 \choose 2} \frac{(k_{x0}^2 - k^2)^2 d^4}{2^4 (\pi m)^4}$$
 (1.17d)

$$m^{5} \to \begin{pmatrix} 5 \\ 0 \end{pmatrix} \frac{k_{x0}^{5} d^{5}}{(\pi m)^{5}} + \begin{pmatrix} 4 \\ 1 \end{pmatrix} \frac{k_{x0}^{3} (k_{x0}^{2} - k^{2}) d^{5}}{2^{2} (\pi m)^{5}} + \begin{pmatrix} 3 \\ 2 \end{pmatrix} \frac{k_{x0} (k_{x0}^{2} - k^{2})^{2} d^{5}}{2^{4} (\pi m)^{5}}$$
(1.17e)

Now, if we define  $t = \lfloor \frac{q}{2} \rfloor$ , we can write the powers of m as

$$m^q \to \frac{d^q}{(\pi m)^q} \sum_{a=0}^t \frac{k_{x0}^{(q-2a)} (k_{x0}^2 - k^2)^a}{2^{2a}} {q-a \choose a}$$
 (1.18)

where each term goes with its factor  $f_q$ 

$$m^q \to \frac{d^q}{(\pi m)^q} \sum_{a=0}^t \frac{k_{x0}^{(q-2a)} (k_{x0}^2 - k^2)^a}{2^{2a}} {q-a \choose a} f_{q-a}$$
 (1.19)

The use of this leads to the following Q-th order approximation of  $\frac{1}{\gamma_m}$ 

$$\frac{1}{\gamma_m} \approx \left| \frac{d}{2\pi m} \left( \sum_{q=0}^{Q} \frac{d^q}{(\pi m)^q} \sum_{a=0}^{t} \frac{k_{x0}^{(q-2a)} (k_{x0}^2 - k^2)^a}{2^{2a}} {q-a \choose a} f_{q-a} \right) \right| 
= \left| \sum_{q=0}^{Q} \frac{d^{q+1}}{(\pi m)^{q+1}} \sum_{a=0}^{t} \frac{k_{x0}^{(q-2a)} (k_{x0}^2 - k^2)^a}{2^{2a+1}} {q-a \choose a} f_{q-a} \right|$$
(1.20)

and finally  $\widetilde{G}_m(\bar{r}, \bar{r}')$  is

$$\widetilde{G}_{m}(\overline{r}, \overline{r}') = \left| \frac{d}{2\pi m} - \frac{k_{x0}d^{2}}{(2\pi m)^{2}} + \frac{(k^{2} - k_{x0}^{2})d^{3}}{2(2\pi m)^{3}} + \dots \right| e^{-\left|\frac{2\pi m}{d} + k_{x0}\right||z - z'|} \\
= \left| \sum_{q=0}^{Q} \frac{d^{q+1}}{(\pi m)^{q+1}} \sum_{a=0}^{t} \frac{k_{x0}^{(q-2a)} (k_{x0}^{2} - k^{2})^{a}}{2^{2a+1}} {q - a \choose a} f_{q-a} \right| e^{-\left|\frac{2\pi m}{d} + k_{x0}\right||z - z'|}$$
(1.21)

Using this  $\widetilde{G}_m$  approach, the series  $\widetilde{G}_e(\bar{r},\bar{r}')$  that we have to efficiently sum is

$$\widetilde{G}_{e}(\bar{r}, \bar{r}') = \frac{1}{2d} \sum_{\substack{m=-\infty\\m\neq 0}}^{+\infty} \left| \frac{d}{2\pi m} - \frac{k_{x0}d^{2}}{(2\pi m)^{2}} + \frac{(k^{2} - k_{x0}^{2})d^{3}}{2(2\pi m)^{3}} + \dots \right| e^{-\left|\frac{2\pi m}{d} + k_{x0}\right||z-z'|} e^{-jk_{xm}(x-x')}$$

$$= \frac{1}{2d} \sum_{\substack{m=-\infty\\m\neq 0}}^{+\infty} \left| \sum_{q=0}^{Q} \frac{d^{q+1}}{(\pi m)^{q+1}} \sum_{a=0}^{t} \frac{k_{x0}^{(q-2a)}(k_{x0}^{2} - k^{2})^{a}}{2^{2a+1}} {q-a \choose a} f_{q-a} \right| e^{-\left|\frac{2\pi m}{d} + k_{x0}\right||z-z'|} e^{-jk_{xm}(x-x')} \tag{1.22}$$

It is important to note that  $\frac{1}{\gamma_m}$  is positive so here we have to use the absolute value because not all these terms are positive. In advance, we can realize that this approach will result in a worse approximation of the spectral series and for this reason in a slower convergence rate in comparison with the previous one. However, the advantage here is that the remaining series is quasi-static, so that, it would be better in the case of problems that require a frequency sweep, such as those corresponding to the analysis of practical microwave devices like filters.

The options that we propose to sum efficiently this series are:

- Option B.1: Sum by Ewald's method.
- Option B.2: Polylogarithmic functions.

• Option B.3: Summation by parts technique.

The formulation of each option will be detailed in the subsections 1.1.4, 1.1.5 and 1.1.6, respectively.

To summarize, in the option A we are assuming that  $(k_{x0} + \frac{2\pi m}{d})$  is more significant than k, in the approximation of  $\frac{1}{\gamma_m}$  but in the option B we are assuming that not only is  $(\frac{2\pi m}{d})$  more important than k but also than  $k_{x0}$ . For this reason, the approximation A is more complete than B and therefore the improvement resulted through the option A would be better. On the contrary, it has the disadvantage of containing the frequency in the term  $k_{x0}$ . Depending on the problem to be solved, we can choose which to use.

In the following subsections, we explain how to sum efficiently the remaining part of the Kummer's series  $\widetilde{G}_e(\bar{r}, \bar{r}')$  using both approaches. Whenever possible, we will try to explain the methods in a general way for the extraction of Q asymptotic terms.

#### 1.1.1 Option A.1. Approach of $k_{xm}$ : Sum by Ewald's Method.

The first alternative to sum the asymptotic retained terms obtained by the application of this first approach of Kummer's transformation is using the corresponding terms in Ewald's method. This can be considered a combination of both techniques. By using this proposed Kummer-Ewald technique we are able to choose the effort that we want to invest in each technique.

We first start with the connection between the first asymptotic term in the spectral domain and the first asymptotic term in Ewald's method. Then, we extract the second term and we show how to sum it by using Ewald's method.

• Extraction of one term.

In this case, the  $\widetilde{G}_e(\bar{r},\bar{r}')$  series that we have to efficiently sum is

$$\widetilde{G}_e(\bar{r}, \bar{r}') = \frac{1}{2d} \sum_{\substack{m = -\infty \\ m \neq 0}}^{+\infty} \frac{e^{-|k_{xm}||z - z'|}}{|k_{xm}|} e^{-jk_{xm}(x - x')}$$
(1.23)

The idea is to identify this series with an approximation of the spectral one and then use Ewald's transformation to sum the asymptotic term.

$$\widetilde{G}_{e}(\bar{r}, \bar{r}') = \frac{1}{2d} \sum_{\substack{m = -\infty \\ m \neq 0}}^{+\infty} \frac{e^{-|k_{xm}||z-z'|}}{|k_{xm}|} e^{-jk_{xm}(x-x')}$$

$$= \underbrace{\frac{1}{2d} \sum_{m = -\infty}^{+\infty} \frac{e^{-|k_{xm}||z-z'|}}{|k_{xm}|} e^{-jk_{xm}(x-x')}}_{G} - \underbrace{\frac{1}{2d} \frac{e^{-|k_{x0}||z-z'|}}{|k_{x0}|} e^{-jk_{x0}(x-x')}}_{G} (1.24)$$

Using this notation,  $\widetilde{G}_e(\bar{r}, \bar{r}')$  is

$$\widetilde{G}_e(\bar{r}, \bar{r}') = S - \frac{1}{2d} \frac{e^{-|k_{x0}||z-z'|}}{|k_{r0}|} e^{-jk_{x0}(x-x')}$$
 (1.25)

Taking into account that the spectral Green's function is

$$\widetilde{G}(\bar{r}, \bar{r}') = \frac{1}{2d} \sum_{m=-\infty}^{+\infty} \frac{e^{-\gamma_m |z-z'|}}{\gamma_m} e^{-jk_{xm}(x-x')}$$
(1.26)

we can obtain its approximation when  $m \to \infty$  as

$$\widetilde{G}(\bar{r}, \bar{r}')\big|_{m \to \infty} = \frac{1}{2d} \sum_{m = -\infty}^{+\infty} \frac{e^{-\gamma_m |z - z'|}}{\gamma_m} e^{-jk_{xm}(x - x')} \bigg|_{m \to \infty} 
= \frac{1}{2d} \sum_{m = -\infty}^{+\infty} \frac{e^{-|k_{xm}||z - z'|}}{|k_{xm}|} e^{-jk_{xm}(x - x')}$$
(1.27)

Now, the series S obtained in the retained first term (1.25) can be identified with this approximation of the spectral formulation  $\widetilde{G}(\bar{r},\bar{r}')\big|_{m\to\infty}$  and since

$$\widetilde{G}(\bar{r}, \bar{r}')\big|_{m \to \infty} = G_{Ewald}(\bar{r}, \bar{r}')\big|_{m \to \infty} = \left[G_{spectral}(\bar{r}, \bar{r}') + G_{spatial}(\bar{r}, \bar{r}')\right]\big|_{m \to \infty}$$
(1.28)

we can sum S by means of Ewald's transformation by the use of the approximation of the Ewald's method components when  $m \to \infty$ . Remembering that the spectral Ewald's method component  $G_{spectral}(\bar{r}, \bar{r}')$  is [5,11]

$$G_{spectral}(\bar{r}, \bar{r}') = \frac{1}{4d} \sum_{p=-\infty}^{+\infty} \frac{e^{-jk_{xp}(x-x')}}{jk_{zp}} \times \left[ e^{jk_{zp}|z-z'|} \operatorname{erfc}\left(|z-z'|\varepsilon + \frac{jk_{zp}}{2\varepsilon}\right) + e^{-jk_{zp}|z-z'|} \operatorname{erfc}\left(-|z-z'|\varepsilon + \frac{jk_{zp}}{2\varepsilon}\right) \right]$$

$$(1.29)$$

where  $k_{zp}^2 = k^2 - k_{xp}^2$ . The approximation of  $G_{spectral}(\bar{r}, \bar{r}')$  is given by

$$G_{spectral}(\bar{r}, \bar{r}')\big|_{m \to \infty} = \frac{1}{4d} \sum_{p=-\infty}^{+\infty} \frac{e^{-jk_{xp}(x-x')}}{jk_{zp}}$$

$$\times \left[ e^{jk_{zp}|z-z'|} \operatorname{erfc}\left(|z-z'|\varepsilon + \frac{jk_{zp}}{2\varepsilon}\right) + e^{-jk_{zp}|z-z'|} \operatorname{erfc}\left(-|z-z'|\varepsilon + \frac{jk_{zp}}{2\varepsilon}\right) \right] \Big|_{m \to \infty}$$

$$= \frac{1}{4d} \sum_{p=-\infty}^{+\infty} \frac{e^{-jk_{xp}(x-x')}}{|k_{xp}|}$$

$$\times \left[ e^{|k_{xp}||z-z'|} \operatorname{erfc}\left(|z-z'|\varepsilon + \frac{|k_{xp}|}{2\varepsilon}\right) + e^{-|k_{xp}||z-z'|} \operatorname{erfc}\left(-|z-z'|\varepsilon + \frac{|k_{xp}|}{2\varepsilon}\right) \right]$$

$$(1.30)$$

We separate the term p = 0 because we are not interested in summing it directly

$$\frac{1}{4d} \sum_{p=-\infty}^{+\infty} \frac{e^{-jk_{xp}(x-x')}}{|k_{xp}|} \times \left[ e^{|k_{xp}||z-z'|} \operatorname{erfc} \left( |z-z'|\varepsilon + \frac{|k_{xp}|}{2\varepsilon} \right) + e^{-|k_{xp}||z-z'|} \right] \\
\operatorname{erfc} \left( -|z-z'|\varepsilon + \frac{|k_{xp}|}{2\varepsilon} \right) \\
= \frac{1}{4d} \sum_{\substack{p=-\infty \\ p\neq 0}}^{+\infty} \frac{e^{-jk_{xp}(x-x')}}{|k_{xp}|} \times \left[ e^{|k_{xp}||z-z'|} \operatorname{erfc} \left( |z-z'|\varepsilon + \frac{|k_{xp}|}{2\varepsilon} \right) + e^{-|k_{xp}||z-z'|} \right] \\
\operatorname{erfc} \left( -|z-z'|\varepsilon + \frac{|k_{xp}|}{2\varepsilon} \right) \\
+ e^{-|k_{x0}||z-z'|} \operatorname{erfc} \left( -|z-z'|\varepsilon + \frac{|k_{x0}|}{2\varepsilon} \right) \\
+ e^{-|k_{x0}||z-z'|} \operatorname{erfc} \left( -|z-z'|\varepsilon + \frac{|k_{x0}|}{2\varepsilon} \right) \right]$$
(1.31)

On the other hand, recalling that the spatial Ewald's method component  $G_{spatial}(\bar{r}, \bar{r}')$  is [5, 11]

$$G_{spatial}(\bar{r}, \bar{r}') = \frac{1}{4\pi} \sum_{m=-\infty}^{+\infty} e^{-jk_{x0}md} \sum_{q=0}^{+\infty} \left(\frac{k}{2\varepsilon}\right)^{2q} \frac{1}{q!} E_{q+1}(R_m^2 \varepsilon^2)$$
 (1.32)

and taking into account that the approximation when  $m \to \infty$  in the spectral domain corresponds to  $k \to 0$  in the spatial domain, the limit of  $G_{spatial}(\bar{r}, \bar{r}')$  when  $k \to 0$ 

is given by

$$\lim_{k \to 0} G_{spatial}(\bar{r}, \bar{r}') = \lim_{k \to 0} \left\{ \frac{1}{4\pi} \sum_{m = -\infty}^{+\infty} e^{-jk_{x0}md} \sum_{q = 0}^{+\infty} \left(\frac{k}{2\varepsilon}\right)^{2q} \frac{1}{q!} \operatorname{E}_{q+1}(R_m^2 \varepsilon^2) \right\}$$

$$= \frac{1}{4\pi} \sum_{m = -\infty}^{+\infty} e^{-jk_{x0}md} \operatorname{E}_1(R_m^2 \varepsilon^2)$$
(1.33)

The found approximations of Ewald's method components can be used to sum the series S

$$S = \frac{1}{4d} \sum_{\substack{p = -\infty \\ p \neq 0}}^{+\infty} \frac{e^{-jk_{xp}(x-x')}}{|k_{xp}|} \times \left[ e^{|k_{xp}||z-z'|} \operatorname{erfc} \left( |z-z'|\varepsilon + \frac{|k_{xp}|}{2\varepsilon} \right) + e^{-|k_{xp}||z-z'|} \right]$$

$$\operatorname{erfc} \left( -|z-z'|\varepsilon + \frac{|k_{xp}|}{2\varepsilon} \right) + \frac{1}{4d} \frac{e^{-jk_{x0}(x-x')}}{|k_{x0}|} \times \left[ e^{|k_{x0}||z-z'|} \operatorname{erfc} \left( |z-z'|\varepsilon + \frac{|k_{x0}|}{2\varepsilon} \right) \right]$$

$$+ e^{-|k_{x0}||z-z'|} \operatorname{erfc} \left( -|z-z'|\varepsilon + \frac{|k_{x0}|}{2\varepsilon} \right) + \frac{1}{4\pi} \sum_{m=-\infty}^{+\infty} e^{-jk_{x0}md} \operatorname{E}_{1}(R_{m}^{2}\varepsilon^{2})$$

$$(1.34)$$

and using this transformation of S, we can rewrite  $\widetilde{G}_e(\bar{r}, \bar{r}')$  as follows

$$\widetilde{G}_{e}(\overline{r}, \overline{r}') = S - \frac{1}{2d} \frac{e^{-|k_{x0}||z-z'|}}{|k_{x0}|} e^{-jk_{x0}(x-x')} = \frac{1}{4d} \sum_{\substack{p=-\infty\\p\neq 0}}^{+\infty} \frac{e^{-jk_{xp}(x-x')}}{|k_{xp}|} \\
\times \left[ e^{|k_{xp}||z-z'|} \operatorname{erfc}\left(|z-z'|\varepsilon + \frac{|k_{xp}|}{2\varepsilon}\right) + e^{-|k_{xp}||z-z'|} \operatorname{erfc}\left(-|z-z'|\varepsilon + \frac{|k_{xp}|}{2\varepsilon}\right) \right] \\
+ \frac{1}{4d} \frac{e^{-jk_{x0}(x-x')}}{|k_{x0}|} \\
\times \left[ e^{|k_{x0}||z-z'|} \operatorname{erfc}\left(|z-z'|\varepsilon + \frac{|k_{x0}|}{2\varepsilon}\right) + e^{-|k_{x0}||z-z'|} \operatorname{erfc}\left(-|z-z'|\varepsilon + \frac{|k_{x0}|}{2\varepsilon}\right) \right] \\
+ \frac{1}{4\pi} \sum_{m=-\infty}^{+\infty} e^{-jk_{x0}md} \operatorname{E}_{1}(R_{m}^{2}\varepsilon^{2}) - \frac{1}{2d} \frac{e^{-|k_{x0}||z-z'|}}{|k_{x0}|} e^{-jk_{x0}(x-x')} \tag{1.35}$$

Regrouping terms and summing together the residual terms in m=0 and p=0, the first asymptotic series  $\widetilde{G}_e(\bar{r},\bar{r}')$  can be expressed as

$$\widetilde{G}_{e}(\bar{r}, \bar{r}') = \frac{1}{4d} \sum_{\substack{p = -\infty \\ p \neq 0}}^{+\infty} \frac{e^{-jk_{xp}(x-x')}}{|k_{xp}|} \times \left[ e^{|k_{xp}||z-z'|} \operatorname{erfc}\left(|z-z'|\varepsilon + \frac{|k_{xp}|}{2\varepsilon}\right) + e^{-|k_{xp}||z-z'|} \operatorname{erfc}\left(-|z-z'|\varepsilon + \frac{|k_{xp}|}{2\varepsilon}\right) \right] + \frac{1}{4\pi} \sum_{m=-\infty}^{+\infty} e^{-jk_{x0}md} \operatorname{E}_{1}(R_{m}^{2}\varepsilon^{2}) + \frac{1}{2d} \frac{e^{-jk_{x0}(x-x')}}{|k_{x0}|} \left[ \frac{1}{2} \left( e^{|k_{x0}||z-z'|} \operatorname{erfc}\left(|z-z'|\varepsilon + \frac{|k_{x0}|}{2\varepsilon}\right) + e^{-|k_{x0}||z-z'|} \operatorname{erfc}\left(-|z-z'|\varepsilon + \frac{|k_{x0}|}{2\varepsilon}\right) \right) - e^{-|k_{x0}||z-z'|} \right]$$
(1.36)

where the last term T contains the residual value when m=0

$$T = \frac{1}{2d} \frac{e^{-jk_{x0}(x-x')}}{|k_{x0}|} \left[ \frac{1}{2} \left( e^{|k_{x0}||z-z'|} \operatorname{erfc} \left( |z-z'|\varepsilon + \frac{|k_{x0}|}{2\varepsilon} \right) + e^{-|k_{x0}||z-z'|} \operatorname{erfc} \left( -|z-z'|\varepsilon + \frac{|k_{x0}|}{2\varepsilon} \right) \right) - e^{-|k_{x0}||z-z'|} \right]$$
(1.37)

Despite there is no problem with T when  $k_{x0} \neq 0$ , we have to use its limit when  $k_{x0} = 0$ .

$$\lim_{k_{x0}\to 0} T = \lim_{k_{x0}\to 0} \left\{ \frac{1}{2d} \frac{e^{-jk_{x0}(x-x')}}{|k_{x0}|} \left[ \frac{1}{2} \left( e^{|k_{x0}||z-z'|} \operatorname{erfc} \left( |z-z'|\varepsilon + \frac{|k_{x0}|}{2\varepsilon} \right) + e^{-|k_{x0}||z-z'|} \operatorname{erfc} \left( -|z-z'|\varepsilon + \frac{|k_{x0}|}{2\varepsilon} \right) \right) - e^{-|k_{x0}||z-z'|} \right] \right\}$$

$$= \frac{|z-z'|}{2d} - \frac{e^{-|z-z'|^2\varepsilon^2}}{2\varepsilon d\sqrt{\pi}} - \frac{|z-z'|\operatorname{erf}(|z-z'|\varepsilon)}{2d} \tag{1.38}$$

#### • Extraction of two terms.

In this part, we try to apply this procedure to the extraction of one more term in order to accelerate even more the convergence of the spectral 2-D Green's function with 1-D periodicity.

In [11], the spectral series was reported by a mathematical development based on the Sommerfeld identity. To carry out this approach, we need to go into detail about the spectral proof by the same procedure as the components of Ewald's method. This is because we are going to identify the corresponding terms in both developments in

order to sum the asymptotic spectral terms through Ewald's method. This can be consider a way to sum efficiently the non-analytical retained part.

For this purpose, the start from the spatial series (1.1) given by

$$G(\bar{r}, \bar{r}') = \sum_{m=-\infty}^{\infty} e^{-jk_{x0}md} \frac{1}{4j} H_0^{(2)}(kR_m)$$
(1.39)

and we use the Sommerfeld identity for 2-D cylindrical radiated fields

$$\frac{1}{4j}H_0^{(2)}(kR_m) = \frac{1}{2\pi} \int_0^\infty \frac{e^{-R_m^2 s^2 + \frac{k^2}{4s^2}}}{s} ds$$
 (1.40)

where s is the complex variable of integration. On the other hand, 1-D Poisson's formula is given by

$$\sum_{m=-\infty}^{+\infty} f(md) = \frac{1}{d} \sum_{m=-\infty}^{+\infty} \tilde{f}\left(\frac{2\pi m}{d}\right)$$
 (1.41)

where  $\tilde{f}(k_x)$  is the Fourier transform of  $f(\xi)$ , that is

$$\tilde{f}(k_x) = \int_{-\infty}^{+\infty} f(\xi)e^{-jk_x\xi} d\xi \tag{1.42}$$

If we start from (1.40) and we identify terms, we can write f(md) as

$$f(md) = \frac{1}{2\pi} e^{-jk_{x0}md} \int_0^\infty \frac{e^{-R_m^2 s^2 + \frac{k^2}{4s^2}}}{s} ds$$
 (1.43)

where we can replace  $R_m$  as

$$f(md) = \frac{1}{2\pi} e^{-jk_{x0}md} \int_0^\infty \frac{e^{-[(z-z')^2 + (x-x'-md)^2]s^2 + \frac{k^2}{4s^2}}}{s} ds$$
 (1.44)

According to this,  $f(\xi)$  is written as follows

$$f(\xi) = \frac{1}{2\pi} e^{-jk_{x0}\xi} \int_0^\infty \frac{e^{-[(z-z')^2 + (x-x'-\xi)^2]s^2 + \frac{k^2}{4s^2}}}{s} ds$$
 (1.45)

Using the equation given in (1.42),  $\tilde{f}(k_x)$  can be expressed as

$$\tilde{f}(k_x) = \int_{-\infty}^{\infty} \frac{1}{2\pi} e^{-jk_{x0}\xi} \int_{0}^{\infty} \frac{e^{-[(z-z')^2 + (x-x'-\xi)^2]s^2 + \frac{k^2}{4s^2}}}{s} ds \, e^{-jk_x\xi} d\xi \tag{1.46}$$

Thus, if  $k_x$  is  $k_x = \frac{2\pi m}{d}$ , the previous equation remains

$$\tilde{f}\left(\frac{2\pi m}{d}\right) = \int_{-\infty}^{\infty} \frac{1}{2\pi} e^{-jk_{x0}\xi} \int_{0}^{\infty} \frac{e^{-[(z-z')^2 + (x-x'-\xi)^2]s^2 + \frac{k^2}{4s^2}}}{s} ds \, e^{-j(\frac{2\pi m}{d})\xi} d\xi \quad (1.47)$$

grouping terms

$$\tilde{f}\left(\frac{2\pi m}{d}\right) = \frac{1}{2\pi} \int_{-\infty}^{\infty} d\xi \int_{0}^{\infty} ds \frac{1}{s} e^{-[(z-z')^{2} + (x-x'-\xi)^{2}]s^{2} + \frac{k^{2}}{4s^{2}}} e^{-j(\frac{2\pi m}{d} + k_{x0})\xi}$$
(1.48)

If we name  $k_{xm}$  as  $k_{xm} = k_{x0} + \frac{2\pi m}{d}$ , we can rewrite the previous equation as

$$\tilde{f}\left(\frac{2\pi m}{d}\right) = \frac{1}{2\pi} \int_{-\infty}^{\infty} d\xi \int_{0}^{\infty} ds \frac{1}{s} e^{-[(z-z')^2 + (x-x'-\xi)^2]s^2 + \frac{k^2}{4s^2}} e^{-jk_{xm}\xi}$$
(1.49)

Now, we try to find the following relation

$$\int_{-\infty}^{+\infty} e^{-a\xi^2 + b\xi} d\xi = \sqrt{\frac{\pi}{a}} e^{\frac{b^2}{4a}}$$
 (1.50)

For this purpose, we define I as the integral part of (1.49) which depends on  $\xi$  and we proceed as follows

$$I = \int_{-\infty}^{+\infty} e^{-[(z-z')^2 + (x-x'-\xi)^2]s^2 + \frac{k^2}{4s^2}} e^{-jk_{xm}\xi} d\xi$$

$$= \int_{-\infty}^{+\infty} e^{-[(z-z')^2 + (x-x'-\xi)^2]s^2 + \frac{k^2}{4s^2} - jk_{xm}\xi} d\xi$$

$$= \int_{-\infty}^{+\infty} e^{-(z-z')^2 s^2 - (x-x')^2 s^2 + 2(x-x')\xi s^2 - \xi^2 s^2 + \frac{k^2}{4s^2} - jk_{xm}\xi} d\xi$$

$$= \int_{-\infty}^{+\infty} e^{-(z-z')^2 s^2 - (x-x')^2 s^2 + \frac{k^2}{4s^2}} e^{-\xi^2 s^2 + \xi(2s^2(x-x') - jk_{xm})} d\xi$$

$$= \int_{-\infty}^{+\infty} e^{-(z-z')^2 s^2 - (x-x')^2 s^2 + \frac{k^2}{4s^2}} e^{-\xi^2 s^2 + \xi(2s^2(x-x') - jk_{xm})} d\xi$$
(1.51)

Now, we apply the relation given in (1.50) by identifying  $a = s^2$  and  $b = 2(x - x')s^2 - jk_{xm}$ , where  $\frac{b^2}{4a}$  is

$$\frac{b^2}{4a} = \frac{(2s^2(x-x')-jk_{xm})^2}{4s^2} 
= \frac{4s^4(x-x')^2 - 4s^2(x-x')jk_{xm} - k_{xm}^2}{4s^2} 
= s^2(x-x')^2 - (x-x')jk_{xm} - \frac{k_{xm}^2}{4s^2}$$
(1.52)

Consequently,

$$\int_{-\infty}^{+\infty} e^{-\xi^2 s^2 + \xi(2s^2(x-x') - jk_{xm})} d\xi = \sqrt{\frac{\pi}{s^2}} e^{s^2(x-x')^2 - (x-x')jk_{xm} - \frac{k_{xm}^2}{4s^2}}$$
(1.53)

The equation (1.53) leads to the following transformation in (1.49)

$$\tilde{f}\left(\frac{2\pi m}{d}\right) = \frac{1}{2\pi} \int_{0}^{\infty} ds \frac{1}{s} e^{-(z-z')^{2}s^{2} - (x-x')^{2}s^{2} + \frac{k^{2}}{4s^{2}}} \sqrt{\frac{\pi}{a}} e^{s^{2}(x-x')^{2} - (x-x')jk_{xm} - \frac{k_{xm}^{2}}{4s^{2}}} 
= \frac{1}{2\sqrt{\pi}} e^{-(x-x')jk_{xm}} \int_{0}^{\infty} ds \frac{1}{s^{2}} e^{-(z-z')^{2}s^{2} - (x-x')^{2}s^{2} + (x-x')^{2}s^{2} + \frac{k^{2}}{4s^{2}} - \frac{k_{xm}^{2}}{4s^{2}}} 
= \frac{1}{2\sqrt{\pi}} e^{-(x-x')jk_{xm}} \int_{0}^{\infty} ds \frac{e^{-(z-z')^{2}s^{2}} e^{-\frac{k_{xm}^{2}-k^{2}}{4s^{2}}}}{s^{2}}$$
(1.54)

In the knowledge that the previous integral can be solved using [15] as

$$\int_{0}^{\infty} \frac{e^{-as^2} e^{-\frac{b}{s^2}}}{s^2} ds = \frac{\sqrt{\pi}}{2\sqrt{b}} e^{-2\sqrt{a}\sqrt{b}}$$
 (1.55)

where in this case  $a=(z-z')^2$  and  $b=\frac{k_{xm}^2-k^2}{4}$ , (1.54) remains

$$\tilde{f}\left(\frac{2\pi m}{d}\right) = \frac{1}{2\sqrt{\pi}}e^{-jk_{xm}(x-x')}\frac{2\sqrt{\pi}e^{-\sqrt{k_{xm}^2-k^2}|z-z'|}}{2\sqrt{k_{xm}^2-k^2}}$$
(1.56)

If we define  $\gamma_m$  as  $\gamma_m = \sqrt{k_{xm}^2 - k^2}$ ,  $\widetilde{G}(\bar{r}, \bar{r}')$  is given by

$$\widetilde{G}(\bar{r}, \bar{r}') = \frac{1}{2d} \sum_{m=-\infty}^{+\infty} \frac{e^{-\gamma_m |z-z'|}}{\gamma_m} e^{-jk_{xm}(x-x')}$$
(1.57)

As can be seen, the obtained spectral representation is the same as the one presented in [11] by the other procedure and previously reported in (1.3).

Once we have addressed this spectral proof, we can apply Kummer's transformation by the extraction of two terms in the spectral Green's function. The first term can be obtained by using the previous first order approximation but when we are interested in extracting more than one term, we have to analyse what happens in higher orders when  $m \to \infty$  in the spectral series and in the Ewald's method components. For this

aim, the strategy here is to obtain the retained terms by using the Taylor expansion in these proofs.

The starting point of the development done previously is

$$G(\bar{r}, \bar{r}') = \frac{1}{2\pi} \sum_{m=-\infty}^{+\infty} e^{-jk_{x0}md} \int_0^\infty \frac{e^{-R_m^2 s^2 + \frac{k^2}{4s^2}}}{s} ds$$
 (1.58)

and the starting point of the proofs done in [11] of the Ewald's components is

$$G_{spectral}(\bar{r}, \bar{r}') = \frac{1}{2\pi} \sum_{m=-\infty}^{+\infty} e^{-jk_{x0}md} \int_{0}^{\varepsilon} \frac{e^{-R_{m}^{2}s^{2} + \frac{k^{2}}{4s^{2}}}}{s} ds$$
 (1.59)

$$G_{spatial}(\bar{r}, \bar{r}') = \frac{1}{2\pi} \sum_{m=-\infty}^{+\infty} e^{-jk_{x0}md} \int_{\varepsilon}^{\infty} \frac{e^{-R_{m}^{2}s^{2} + \frac{k^{2}}{4s^{2}}}}{s} ds$$
 (1.60)

All of these components start in the spatial domain, where  $m \to \infty$  is  $k \to 0$ . So we have to calculate the limit of these integrals when  $k \to 0$ . Using the following Taylor expansion when  $u \to 0$ 

$$e^{u} = \sum_{n=0}^{+\infty} \frac{u^{n}}{n!} \tag{1.61}$$

we can rewrite the exponential of k in the previous proofs as

$$e^{\frac{k^2}{4s^2}} = \sum_{n=0}^{+\infty} \frac{\left(\frac{k^2}{4s^2}\right)^n}{n!} = 1 + \frac{k^2}{4s^2} + \dots$$
 (1.62)

It can be noted that the first term of the expansion corresponds to the development done when we extract only the first term because it corresponds to the first order approximation of these components. The idea is to use the second order Taylor expansion of  $e^{\frac{k^2}{4s^2}}$  in the equations (1.58), (1.59) and (1.60). This will allow us to use the two order expansion of Ewald's method components to sum the two order expansion of the spectral series.

Using this expansion in the equation (1.54) of the spectral development,  $\tilde{f}\left(\frac{2\pi m}{d}\right)$  remains

$$\tilde{f}\left(\frac{2\pi m}{d}\right) = \frac{1}{2\sqrt{\pi}}e^{-(x-x')jk_{xm}} \int_0^\infty \frac{e^{-(z-z')^2s^2}e^{-\frac{k_{xm}^2}{4s^2}}}{s^2} \left(1 + \frac{k^2}{4s^2}\right) ds$$

$$= \underbrace{\frac{1}{2\sqrt{\pi}}e^{-(x-x')jk_{xm}} \int_0^\infty \frac{e^{-(z-z')^2s^2}e^{-\frac{k_{xm}^2}{4s^2}}}{s^2}}_{S_1} + \underbrace{\frac{1}{2\sqrt{\pi}}e^{-(x-x')jk_{xm}} \int_0^\infty \frac{e^{-(z-z')^2s^2}e^{-\frac{k_{xm}^2}{4s^2}}}{s^2} \frac{k^2}{4s^2} ds}_{S_2}}_{S_2}$$

$$(1.63)$$

In the knowledge that the previous integrals can be solved using [15] as

$$\int_0^\infty \frac{e^{-as^2 - \frac{b}{s^2}}}{s^2} ds = \frac{\sqrt{\pi}}{2\sqrt{b}} e^{-2\sqrt{a}\sqrt{b}}$$
 (1.64a)

$$\int_0^\infty \frac{e^{-as^2 - \frac{b}{s^2}}}{s^4} ds = \frac{\sqrt{\pi} (1 + 2\sqrt{a}\sqrt{b})}{4b^{3/2}} e^{-2\sqrt{a}\sqrt{b}}$$
(1.64b)

where in this case  $a = (z - z')^2$  and  $b = \frac{k_{xm}^2}{4}$ , the series  $S_1$  remains

$$S_{1} = \frac{1}{2\sqrt{\pi}} e^{-jk_{xm}(x-x')} \int_{0}^{\infty} \frac{e^{-(z-z')^{2}s^{2}} e^{-\frac{k_{xm}^{2}}{4s^{2}}}}{s^{2}} \frac{1}{2\sqrt{\pi}} e^{-jk_{xm}(x-x')}$$

$$\frac{2\sqrt{\pi} e^{-\sqrt{|k_{xm}|^{2}}|z-z'|}}{2\sqrt{|k_{xm}|^{2}}} = \frac{1}{2} \frac{e^{-|k_{xm}||z-z'|}}{|k_{xm}|} e^{-jk_{xm}(x-x')}$$
(1.65)

and series  $S_2$  remains

$$S_{2} = \frac{1}{2\sqrt{\pi}} \frac{k^{2}}{4} e^{-jk_{xm}(x-x')} \int_{0}^{\infty} \frac{e^{-(z-z')^{2}s^{2}} e^{-\frac{k_{xm}^{2}}{4s^{2}}}}{s^{4}}$$

$$= \frac{1}{2\sqrt{\pi}} e^{-jk_{xm}(x-x')} \frac{\sqrt{\pi} k^{2} 2^{3} (1+|z-z'||k_{xm}|)}{4^{2}|k_{xm}|^{3}} e^{-\sqrt{|k_{xm}|^{2}}|z-z'|}$$

$$= \frac{1}{2} e^{-jk_{xm}(x-x')} \left(\frac{k^{2}}{2|k_{xm}|^{3}} + \frac{k^{2}|z-z'|}{2|k_{xm}|^{2}}\right) e^{-|k_{xm}||z-z'|}$$

$$(1.66)$$

Using this, we can write the asymptotic spectral series with the expansion of two terms as

$$\widetilde{G}_{e'}(\bar{r}, \bar{r}') = \frac{1}{2d} \sum_{m=-\infty}^{+\infty} \left( \frac{1}{|k_{xm}|} + \frac{k^2}{2|k_{xm}|^3} + \frac{k^2|z - z'|}{2|k_{xm}|^2} \right) e^{-|k_{xm}||z - z'|} e^{-jk_{xm}(x - x')}$$
(1.67)

Now, we can apply Kummer's transformation to the spectral Green's function as follows

$$\widetilde{G}_{k}(\bar{r}, \bar{r}') = \frac{1}{2d} \sum_{\substack{m = -\infty \\ m \neq 0}}^{+\infty} \left[ \frac{e^{-\gamma_{m}|z - z'|}}{\gamma_{m}} - \left( \frac{1}{|k_{xm}|} + \frac{k^{2}}{2|k_{xm}|^{3}} + \frac{k^{2}|z - z'|}{2|k_{xm}|^{2}} \right) \right] e^{-jk_{xm}(x - x')} + \widetilde{G}_{0} + \widetilde{G}_{e}(\bar{r}, \bar{r}')$$
(1.68)

where  $\widetilde{G}_0$  is the spectral series in m=0 and  $\widetilde{G}_e(\bar{r},\bar{r}')$  is the asymptotic retained part. In this case, the remaining series is

$$\widetilde{G}_{e}(\overline{r}, \overline{r}') = \frac{1}{2d} \sum_{\substack{m = -\infty \\ m \neq 0}}^{+\infty} \left( \frac{1}{|k_{xm}|} + \frac{k^{2}}{2|k_{xm}|^{3}} + \frac{k^{2}|z - z'|}{2|k_{xm}|^{2}} \right) e^{-|k_{xm}||z - z'|} e^{-jk_{xm}(x - x')}$$

$$= \underbrace{\frac{1}{2d} \sum_{m = -\infty}^{+\infty} \left( \frac{1}{|k_{xm}|} + \frac{k^{2}}{2|k_{xm}|^{3}} + \frac{k^{2}|z - z'|}{2|k_{xm}|^{2}} \right) e^{-|k_{xm}||z - z'|} e^{-jk_{xm}(x - x')}}_{\widetilde{G}_{e'}(\overline{r}, \overline{r}')}$$

$$- \underbrace{\frac{1}{2d} \left( \frac{1}{|k_{x0}|} + \frac{k^{2}}{2|k_{x0}|^{3}} + \frac{k^{2}|z - z'|}{2|k_{x0}|^{2}} \right) e^{-|k_{x0}||z - z'|} e^{-jk_{x0}(x - x')}}_{(1.69)}$$

where  $\widetilde{G}_{e'}(\bar{r}, \bar{r}')$  is the same as the series obtained in (1.67) when we calculate the asymptotic expansion in the spectral series. Accordingly,

$$\widetilde{G}_{e}(\bar{r}, \bar{r}') = \widetilde{G}_{e'}(\bar{r}, \bar{r}') - \frac{1}{2d} \left( \frac{1}{|k_{x0}|} + \frac{k^{2}}{2|k_{x0}|^{3}} + \frac{k^{2}|z - z'|}{2|k_{x0}|^{2}} \right) e^{-|k_{x0}||z - z'|} e^{-jk_{x0}(x - x')}$$
(1.70)

As mentioned before,  $\widetilde{G}_{e'}(\bar{r}, \bar{r}')$  is the approximation of the spectral series when  $m \to +\infty$ . The idea is to sum this series using Ewald's method. Through this proposed Kummer-Ewald transformation, the asymptotic retained part  $\widetilde{G}_{e'}(\bar{r}, \bar{r}')$  can be efficiently calculated by using the rapidly convergent components of Ewald's

method as follows

$$\widetilde{G}_{e'}(\bar{r}, \bar{r}') = \widetilde{G}(\bar{r}, \bar{r}')\big|_{m \to +\infty} = G_{Ewald}(\bar{r}, \bar{r}')\big|_{m \to +\infty} 
= \left[G_{spectral}(\bar{r}, \bar{r}') + G_{spatial}(\bar{r}, \bar{r}')\right]\big|_{m \to +\infty}$$
(1.71)

The proof of spectral component of Ewald's method has been reported in [5, 11]. In this development we have to use the expansion of the exponential that depends on k when  $k \to 0$ , as we have done in the spectral asymptotic expansion. For this purpose, we start from

$$\tilde{f}\left(\frac{2\pi m}{d}\right) = \frac{1}{2\sqrt{\pi}}e^{-(x-x')jk_{xm}} \int_0^\varepsilon ds \frac{e^{-(z-z')^2s^2}e^{-\frac{k_{xm}^2-k^2}{4s^2}}}{s^2}$$
(1.72)

and we replace  $e^{\frac{k^2}{4s^2}}$  by  $1 + \frac{k^2}{4s^2}$ 

$$\tilde{f}\left(\frac{2\pi m}{d}\right) = \frac{1}{2\sqrt{\pi}} e^{-jk_{xm}(x-x')} \int_0^{\varepsilon} ds \frac{e^{-(z-z')^2 s^2} e^{-\frac{k_{xm}^2}{4s^2}}}{s^2} \\
= \underbrace{\frac{1}{2\sqrt{\pi}} e^{-jk_{xm}(x-x')} \int_0^{\varepsilon} \frac{e^{-(z-z')^2 s^2} e^{-\frac{k_{xm}^2}{4s^2}}}{s^2}}_{S_1} \\
+ \underbrace{\frac{1}{2\sqrt{\pi}} e^{-jk_{xm}(x-x')} \int_0^{\varepsilon} \frac{e^{-(z-z')^2 s^2} e^{-\frac{k_{xm}^2}{4s^2}}}{s^2} \frac{k^2}{4s^2} ds}_{S_2}$$
(1.73)

In the knowledge that the previous integrals can be solved by means of [15] as

$$\int_{0}^{\varepsilon} \frac{e^{-as^{2} - \frac{b}{s^{2}}}}{s^{2}} ds = \frac{\sqrt{\pi}}{4\sqrt{b}} \left[ \operatorname{erfc} \left( \frac{\sqrt{b}}{\varepsilon} + \sqrt{a\varepsilon} \right) e^{2\sqrt{a}\sqrt{b}} \right. \\
+ e^{-2\sqrt{a}\sqrt{b}} \operatorname{erfc} \left( \frac{\sqrt{b}}{\varepsilon} - \sqrt{a\varepsilon} \right) \right] = \frac{e^{-2\sqrt{a}\sqrt{b}}\sqrt{\pi}}{4 b^{3/2}} + \frac{e^{-\frac{(\sqrt{b} + \sqrt{a\varepsilon^{2}})^{2}}{\varepsilon^{2}}}}{8 \varepsilon b^{3/2}} \\
\left[ 4 \sqrt{b} e^{2\sqrt{a}\sqrt{b}} - \varepsilon e^{\frac{b}{\varepsilon^{2}} + a\varepsilon^{2}} \sqrt{\pi} + 2 \sqrt{a}\sqrt{b} \varepsilon \sqrt{\pi} e^{\frac{b}{\varepsilon^{2}} + a\varepsilon^{2}} + \varepsilon e^{\frac{b}{\varepsilon^{2}} + a\varepsilon^{2}} e^{4\sqrt{a}\sqrt{b}} \sqrt{\pi} \right. \\
\left. - 2 \sqrt{a}\sqrt{b} \varepsilon e^{\frac{b}{\varepsilon^{2}} + a\varepsilon^{2}} e^{4\sqrt{a}\sqrt{b}} \sqrt{\pi} - (1 + 2 \sqrt{a}\sqrt{b}) \varepsilon e^{\frac{b}{\varepsilon^{2}} + a\varepsilon^{2}} \sqrt{\pi} \operatorname{erf} \left( \frac{\sqrt{b}}{\varepsilon} - \sqrt{a\varepsilon} \right) \right. \\
+ \left. (-1 + 2 \sqrt{a}\sqrt{b}) \varepsilon e^{\frac{b}{\varepsilon^{2}} + a\varepsilon^{2}} e^{4\sqrt{a}\sqrt{b}} \sqrt{\pi} \operatorname{erf} \left( \frac{\sqrt{b}}{\varepsilon} + \sqrt{a\varepsilon} \right) \right]$$

$$(1.74)$$

where in this case  $a=(z-z')^2$  and  $b=\frac{k_{xm}^2}{4}$  ,  $S_1$  remains

$$S_{1} = \frac{1}{4} \frac{e^{-jk_{xm}(x-x')}}{|k_{xm}|} \times \left[ e^{|k_{xm}||z-z'|} \operatorname{erfc}\left(|z-z'|\varepsilon + \frac{|k_{xm}|}{2\varepsilon}\right) + e^{-|k_{xm}||z-z'|} \right]$$

$$\operatorname{erfc}\left(-|z-z'|\varepsilon + \frac{|k_{xm}|}{2\varepsilon}\right)$$

$$(1.75)$$

and series  $S_2$  remains

$$S_{2} = \frac{1}{4}e^{-jk_{xp}(x-x')}\frac{k^{2}}{2}\left[\frac{2e^{-|k_{xm}||z-z'|}}{|k_{xm}|^{3}} + \frac{2e^{-\frac{|k_{xm}|^{2}}{4\varepsilon^{2}} - |z-z'|^{2}\varepsilon^{2}}}{\sqrt{\pi}\varepsilon|k_{xm}|^{2}} + e^{-|k_{xm}||z-z'|}\left(\frac{-1 - \operatorname{erf}\left(\frac{|k_{xm}|}{2\varepsilon} - |z-z'|\varepsilon\right)}{|k_{xm}|^{3}} + \frac{|z-z'|\left(1 - \operatorname{erf}\left(\frac{|k_{xm}|}{2\varepsilon} - |z-z'|\varepsilon\right)\right)}{|k_{xm}|^{2}}\right) + e^{|k_{xm}||z-z'|}\left(\frac{1 - \operatorname{erf}\left(\frac{|k_{xm}|}{2\varepsilon} + |z-z'|\varepsilon\right)}{|k_{xm}|^{3}} + \frac{|z-z'|\left(-1 + \operatorname{erf}\left(\frac{|k_{xm}|}{2\varepsilon} - |z-z'|\varepsilon\right)\right)}{|k_{xm}|^{2}}\right)\right]$$

$$(1.76)$$

Using this, we can write the asymptotic spectral component using the expansion of two terms as

$$G_{spectral}(\bar{r}, \bar{r}')|_{m \to +\infty} = \frac{1}{4d} \sum_{m=-\infty}^{+\infty} e^{-jk_{xm}(x-x')} \left\{ \frac{1}{|k_{xm}|} \times \left[ e^{|k_{xm}||z-z'|} \operatorname{erfc}\left(|z-z'|\varepsilon + \frac{|k_{xm}|}{2\varepsilon}\right) + e^{-|k_{xm}||z-z'|} \operatorname{erfc}\left(-|z-z'|\varepsilon + \frac{|k_{xm}|}{2\varepsilon}\right) \right] + \frac{k^2}{2} \left[ \frac{2e^{-|k_{xm}||z-z'|}}{|k_{xm}|^3} + \frac{2e^{-\frac{|k_{xm}|^2}{4\varepsilon^2} - |z-z'|^2\varepsilon^2}}{\sqrt{\pi} \varepsilon |k_{xm}|^2} + e^{-|k_{xm}||z-z'|} \left( \frac{-1 - \operatorname{erf}\left(\frac{|k_{xm}|}{2\varepsilon} - |z-z'|\varepsilon\right)}{|k_{xm}|^3} + \frac{|z-z'|\left(1 - \operatorname{erf}\left(\frac{|k_{xm}|}{2\varepsilon} - |z-z'|\varepsilon\right)\right)}{|k_{xm}|^2} \right) + e^{|k_{xm}||z-z'|} \left( \frac{1 - \operatorname{erf}\left(\frac{|k_{xm}|}{2\varepsilon} + |z-z'|\varepsilon\right)}{|k_{xm}|^3} + \frac{|z-z'|\left(-1 + \operatorname{erf}\left(\frac{|k_{xm}|}{2\varepsilon} - |z-z'|\varepsilon\right)\right)}{|k_{xm}|^2} \right) \right] \right\}$$

$$(1.77)$$

If we separate the term in m = 0,  $G_{spectral}(\bar{r}, \bar{r}')|_{m \to +\infty}$  is

$$G_{spectral}(\bar{r}, \bar{r}')|_{m \to +\infty} = \frac{1}{4d} \sum_{\substack{m = -\infty \\ m \neq 0}}^{+\infty} e^{-jk_{xm}(x-x')} \left\{ \frac{1}{|k_{xm}|} \right.$$

$$\times \left[ e^{|k_{xm}||z-z'|} \operatorname{erfc}\left(|z-z'|\varepsilon + \frac{|k_{xm}|}{2\varepsilon}\right) + e^{-|k_{xm}||z-z'|} \operatorname{erfc}\left(-|z-z'|\varepsilon + \frac{|k_{xm}|}{2\varepsilon}\right) \right]$$

$$+ \frac{k^2}{2} \left[ \frac{2e^{-|k_{xm}||z-z'|}}{|k_{xm}|^3} + \frac{2e^{-\frac{|k_{xm}|^2}{4\varepsilon^2} - |z-z'|^2\varepsilon^2}}{\sqrt{\pi} \varepsilon |k_{xm}|^2} \right.$$

$$+ e^{-|k_{xm}||z-z'|} \left( \frac{-1 - \operatorname{erf}\left(\frac{|k_{xm}|}{2\varepsilon} - |z-z'|\varepsilon\right)}{|k_{xm}|^3} + \frac{|z-z'|\left(1 - \operatorname{erf}\left(\frac{|k_{xm}|}{2\varepsilon} - |z-z'|\varepsilon\right)\right)}{|k_{xm}|^2} \right) \right.$$

$$+ e^{|k_{xm}||z-z'|} \left( \frac{1 - \operatorname{erf}\left(\frac{|k_{xm}|}{2\varepsilon} + |z-z'|\varepsilon\right)}{|k_{xm}|^3} + \frac{|z-z'|\left(-1 + \operatorname{erf}\left(\frac{|k_{xm}|}{2\varepsilon} - |z-z'|\varepsilon\right)\right)}{|k_{xm}|^2} \right) \right] \right\}$$

$$+ G_{e0}(\bar{r}, \bar{r}') \tag{1.78}$$

where  $G_{e0}(\bar{r}, \bar{r}')$  contains the value of this component when m = 0. On the other hand, the spatial Ewald's method component  $G_{spatial}(\bar{r}, \bar{r}')$  is [5,11]

$$G_{spatial}(\bar{r}, \bar{r}') = \frac{1}{4\pi} \sum_{m=-\infty}^{+\infty} e^{-jk_{x0}md} \sum_{q=0}^{+\infty} \left(\frac{k}{2\varepsilon}\right)^{2q} \frac{1}{q!} \operatorname{E}_{q+1}(R_m^2 \varepsilon^2)$$
 (1.79)

where the summation in q corresponds to the expansion of  $e^{\frac{k^2}{4s^2}}$  previously done in the proof of the spectral series and in the proof of the spectral Ewald's component. This expansion is originally carried out in the development of the spatial Ewald's component. For more detail see [5,11]. Knowing that, the second order expansion of  $G_{spatial}(\bar{r},\bar{r}')$  when  $k\to 0$  corresponds to the use of two terms in the q-summation

$$\lim_{k \to 0} G_{spatial}(\bar{r}, \bar{r}') = \lim_{k \to 0} \left\{ \frac{1}{4\pi} \sum_{m = -\infty}^{+\infty} e^{-jk_{x0}md} \sum_{q = 0}^{+\infty} \left(\frac{k}{2\varepsilon}\right)^{2q} \frac{1}{q!} \operatorname{E}_{q+1}(R_m^2 \varepsilon^2) \right\}$$

$$= \frac{1}{4\pi} \sum_{m = -\infty}^{+\infty} e^{-jk_{x0}md} \left[ \operatorname{E}_1(R_m^2 \varepsilon^2) + \left(\frac{k}{2\varepsilon}\right)^2 \operatorname{E}_2(R_m^2 \varepsilon^2) \right]$$
(1.80)

Once we have the second order expansion of the Ewald's method components, we can summarize how to sum the asymptotic retained part through Ewald's method.

$$\widetilde{G}_{e}(\bar{r}, \bar{r}') = \widetilde{G}_{e'}(\bar{r}, \bar{r}') - \frac{1}{2d} \left( \frac{1}{|k_{x0}|} + \frac{k^{2}}{2|k_{x0}|^{3}} + \frac{k^{2}|z - z'|}{2|k_{x0}|^{2}} \right) e^{-|k_{x0}||z - z'|} e^{-jk_{x0}(x - x')}$$
(1.81)

The series  $\widetilde{G}_{e'}(\bar{r}, \bar{r}')$  has been efficiently summed as

$$\begin{split} &\widetilde{G}_{e'}(\bar{r}, \bar{r}') = \left[ G_{spectral}(\bar{r}, \bar{r}') + G_{spatial}(\bar{r}, \bar{r}') \right] \Big|_{m \to +\infty} \\ &= \frac{1}{4d} \sum_{\substack{m = -\infty \\ m \neq 0}}^{+\infty} e^{-jk_{xm}(x-x')} \left\{ \frac{1}{|k_{xm}|} \right. \\ &\times \left[ e^{|k_{xm}||z-z'|} \operatorname{erfc} \left( |z-z'|\varepsilon + \frac{|k_{xm}|}{2\varepsilon} \right) + e^{-|k_{xm}||z-z'|} \operatorname{erfc} \left( -|z-z'|\varepsilon + \frac{|k_{xm}|}{2\varepsilon} \right) \right] \\ &+ \frac{k^2}{2} \left[ \frac{2e^{-|k_{xm}||z-z'|}}{|k_{xm}|^3} + \frac{2e^{-\frac{|k_{xm}|^2}{4\varepsilon^2} - |z-z'|^2\varepsilon^2}}{\sqrt{\pi} \varepsilon |k_{xm}|^2} \right. \\ &+ e^{-|k_{xm}||z-z'|} \left( \frac{-1 - \operatorname{erf} \left( \frac{|k_{xm}|}{2\varepsilon} - |z-z'|\varepsilon \right)}{|k_{xm}|^3} + \frac{|z-z'| \left( 1 - \operatorname{erf} \left( \frac{|k_{xm}|}{2\varepsilon} - |z-z'|\varepsilon \right) \right)}{|k_{xm}|^2} \right) \\ &+ e^{|k_{xm}||z-z'|} \left( \frac{1 - \operatorname{erf} \left( \frac{|k_{xm}|}{2\varepsilon} + |z-z'|\varepsilon \right)}{|k_{xm}|^3} + \frac{|z-z'| \left( -1 + \operatorname{erf} \left( \frac{|k_{xm}|}{2\varepsilon} - |z-z'|\varepsilon \right) \right)}{|k_{xm}|^2} \right) \right] \right\} \\ &+ G_{e0}(\bar{r}, \bar{r}') + \frac{1}{4\pi} \sum_{m = -\infty}^{+\infty} e^{-jk_{x0}md} \left[ \operatorname{E}_{1}(R_{m}^{2}\varepsilon^{2}) + \left( \frac{k}{2\varepsilon} \right)^{2} \operatorname{E}_{2}(R_{m}^{2}\varepsilon^{2}) \right] \end{split}$$

$$(1.82)$$

If we insert (1.82) in (1.81), the asymptotic part  $\widetilde{G}_e(\bar{r}, \bar{r}')$  remains

$$\widetilde{G}_{e}(\overline{r}, \overline{r}') = \frac{1}{4d} \sum_{\substack{m=-\infty\\m\neq 0}}^{+\infty} e^{-jk_{xm}(x-x')} \left\{ \frac{1}{|k_{xm}|} \times \left[ e^{|k_{xm}||z-z'|} \operatorname{erfc} \left( |z-z'|\varepsilon + \frac{|k_{xm}|}{2\varepsilon} \right) \right. \right. \\
+ e^{-|k_{xm}||z-z'|} \operatorname{erfc} \left( -|z-z'|\varepsilon + \frac{|k_{xm}|}{2\varepsilon} \right) \right] + \frac{k^{2}}{2} \left[ \frac{2e^{-|k_{xm}||z-z'|}}{|k_{xm}|^{3}} + \frac{2e^{-\frac{|k_{xm}|^{2}}{4\varepsilon^{2}} - |z-z'|^{2}\varepsilon^{2}}}{\sqrt{\pi} \varepsilon |k_{xm}|^{2}} \right. \\
+ e^{-|k_{xm}||z-z'|} \left( \frac{-1 - \operatorname{erf} \left( \frac{|k_{xm}|}{2\varepsilon} - |z-z'|\varepsilon \right)}{|k_{xm}|^{3}} + \frac{|z-z'| \left( 1 - \operatorname{erf} \left( \frac{|k_{xm}|}{2\varepsilon} - |z-z'|\varepsilon \right) \right)}{|k_{xm}|^{2}} \right) \right. \\
+ e^{|k_{xm}||z-z'|} \left( \frac{1 - \operatorname{erf} \left( \frac{|k_{xp}|}{2\varepsilon} + |z-z'|\varepsilon \right)}{|k_{xm}|^{3}} + \frac{|z-z'| \left( -1 + \operatorname{erf} \left( \frac{|k_{xm}|}{2\varepsilon} - |z-z'|\varepsilon \right) \right)}{|k_{xm}|^{2}} \right) \right] \right\} \\
+ G_{e0}(\overline{r}, \overline{r}') + \frac{1}{4\pi} \sum_{m=-\infty}^{+\infty} e^{-jk_{x0}md} \left[ \operatorname{E}_{1}(R_{m}^{2}\varepsilon^{2}) + \left( \frac{k}{2\varepsilon} \right)^{2} \operatorname{E}_{2}(R_{m}^{2}\varepsilon^{2}) \right] \\
- \frac{1}{2d} \left( \frac{1}{|k_{x0}|} + \frac{k^{2}}{2|k_{x0}|^{3}} + \frac{k^{2}|z-z'|}{2|k_{x0}|^{2}} \right) e^{-|k_{x0}||z-z'|} e^{-jk_{x0}(x-x')} \tag{1.83}$$

Regrouping terms,  $\widetilde{G}_e(\bar{r}, \bar{r}')$  remains

$$\begin{split} \widetilde{G}_{e}(\bar{r},\bar{r}') &= \frac{1}{4d} \sum_{\substack{m=-\infty\\m\neq 0}}^{+\infty} e^{-jk_{xm}(x-x')} \left\{ \frac{1}{|k_{xm}|} \times \left[ e^{|k_{xm}||z-z'|} \operatorname{erfc} \left( |z-z'|\varepsilon + \frac{|k_{xm}|}{2\varepsilon} \right) \right. \right. \\ &+ e^{-|k_{xm}||z-z'|} \operatorname{erfc} \left( -|z-z'|\varepsilon + \frac{|k_{xm}|}{2\varepsilon} \right) \right] + \frac{k^{2}}{2} \left[ \frac{2e^{-|k_{xm}||z-z'|}}{|k_{xm}|^{3}} + \frac{2e^{-\frac{|k_{xm}|^{2}}{4\varepsilon^{2}} - |z-z'|^{2}\varepsilon^{2}}}{\sqrt{\pi} \varepsilon |k_{xm}|^{2}} \right. \\ &+ e^{-|k_{xm}||z-z'|} \left( \frac{-1 - \operatorname{erf} \left( \frac{|k_{xm}|}{2\varepsilon} - |z-z'|\varepsilon \right)}{|k_{xm}|^{3}} + \frac{|z-z'| \left( 1 - \operatorname{erf} \left( \frac{|k_{xm}|}{2\varepsilon} - |z-z'|\varepsilon \right) \right)}{|k_{xm}|^{2}} \right) \right. \\ &+ e^{|k_{xm}||z-z'|} \left( \frac{1 - \operatorname{erf} \left( \frac{|k_{xp}|}{2\varepsilon} + |z-z'|\varepsilon \right)}{|k_{xm}|^{3}} + \frac{|z-z'| \left( -1 + \operatorname{erf} \left( \frac{|k_{xm}|}{2\varepsilon} - |z-z'|\varepsilon \right) \right)}{|k_{xm}|^{2}} \right) \right] \right\} \\ &+ \frac{1}{4\pi} \sum_{m=-\infty}^{+\infty} e^{-jk_{x0}md} \left[ \operatorname{E}_{1}(R_{m}^{2}\varepsilon^{2}) + \left( \frac{k}{2\varepsilon} \right)^{2} \operatorname{E}_{2}(R_{m}^{2}\varepsilon^{2}) \right] \\ &+ \underbrace{G_{e0}(\bar{r},\bar{r}') - \frac{1}{2d} \left( \frac{1}{|k_{x0}|} + \frac{k^{2}}{2|k_{x0}|^{3}} + \frac{k^{2}|z-z'|}{2|k_{x0}|^{2}} \right) e^{-|k_{x0}||z-z'|} e^{-jk_{x0}(x-x')} } \right. \end{split}$$

where the last term T contains the residual value when m = 0. Despite there is no problem with T when  $k_{x0} \neq 0$ , we have to use its limit when  $k_{x0} = 0$ .

$$T = \frac{1}{4d} e^{-jk_{x0}(x-x')} \left\{ \frac{1}{|k_{x0}|} \times \left[ e^{|k_{x0}||z-z'|} \operatorname{erfc} \left( |z-z'|\varepsilon + \frac{|k_{x0}|}{2\varepsilon} \right) \right] + e^{-|k_{x0}||z-z'|} \operatorname{erfc} \left( -|z-z'|\varepsilon + \frac{|k_{x0}|}{2\varepsilon} \right) \right] + \frac{k^2}{2} \left[ \frac{2e^{-|k_{x0}||z-z'|}}{|k_{x0}|^3} + \frac{2e^{-\frac{|k_{x0}|^2}{4\varepsilon^2} - |z-z'|^2\varepsilon^2}}{\sqrt{\pi} \varepsilon |k_{x0}|^2} \right] + e^{-|k_{x0}||z-z'|} \left( \frac{-1 - \operatorname{erf} \left( \frac{|k_{x0}|}{2\varepsilon} - |z-z'|\varepsilon \right)}{|k_{x0}|^3} + \frac{|z-z'| \left( 1 - \operatorname{erf} \left( \frac{|k_{x0}|}{2\varepsilon} - |z-z'|\varepsilon \right) \right)}{|k_{x0}|^2} \right) \right] + e^{|k_{x0}||z-z'|} \left( \frac{1 - \operatorname{erf} \left( \frac{|k_{x0}|}{2\varepsilon} + |z-z'|\varepsilon \right)}{|k_{x0}|^3} + \frac{|z-z'| \left( -1 + \operatorname{erf} \left( \frac{|k_{x0}|}{2\varepsilon} - |z-z'|\varepsilon \right) \right)}{|k_{x0}|^2} \right) \right] \right\} - \frac{1}{2d} \left( \frac{1}{|k_{x0}|} + \frac{k^2}{2|k_{x0}|^3} + \frac{k^2|z-z'|}{2|k_{x0}|^2} \right) e^{-|k_{x0}||z-z'|} e^{-jk_{x0}(x-x')}$$

$$(1.85)$$

Resolving this limit by the same procedure as the followed in the previous part, the term T that we have to use when  $k_{x0} = 0$  is

$$T = \frac{|z - z'|}{2d} - \frac{e^{-|z - z'|^2 \varepsilon^2}}{2\varepsilon d\sqrt{\pi}} - \frac{|z - z'|\operatorname{erf}(|z - z'|\varepsilon)}{2d} - \frac{|z - z'|^3 k^2}{12d} + \frac{k^2}{8d} \left[ -\frac{|z - z'|^3}{3} - \frac{e^{-|z - z'|^2 \varepsilon^2}}{2\varepsilon^3 \sqrt{\pi}} + \frac{|z - z'|^2 e^{-|z - z'|^2 \varepsilon^2}}{\varepsilon \sqrt{\pi}} - \frac{(-1 + 2|z - z'|^2 \varepsilon^2) e^{-|z - z'|^2 \varepsilon^2}}{6\varepsilon^3 \sqrt{\pi}} + \frac{|z - z'|^3}{6} (1 - \operatorname{erf}(|z - z'|\varepsilon)) + \frac{|z - z'|^3}{3} (-1 + \operatorname{erf}(|z - z'|\varepsilon)) + \frac{|z - z'|^3}{2} (1 + \operatorname{erf}(|z - z'|\varepsilon)) \right]$$

$$(1.86)$$

In order to summarize, in this subsection we have accelerated the 1-D periodic spectral Green's function by using Kummer's transformation and summing efficiently the asymptotic retained part through Ewald's method.

We have outlined the connection between the first and the second asymptotic term in the spectral series and the summation of these with Ewald's method. This approach has not been generalized to Q terms due to the difficulty that arises from the Ewald's integrals when we extract more than two terms. Nevertheless, the development done in

this approach implies a significant improvement over the slow convergence of the original series, as will be shown in Chapter 3.

## 1.1.2 Option A.2. Approach of $k_{xm}$ : Lerch Transcendent.

The strategy of this second alternative in the  $k_{xm}$  - approach is to develop the formulation without applying any transformation on it. It can be seen as the analogous technique of the polylogarithmic formulation for the case of  $\left(\frac{2\pi m}{d}\right)$  - approach. The final expression of this procedure will be expressed in a semi-closed form using the Lerch transcendent.

For this aim, we first remove the absolute value in (1.9) taking into account that for positive m

$$|k_{xm}| = \left| \frac{2\pi m}{d} + k_{x0} \right| = \left( \frac{2\pi m}{d} + k_{x0} \right)$$
 (1.87)

and for negative m

$$|k_{xm}| = \left| \frac{-2\pi m}{d} + k_{x0} \right| = \left( \frac{2\pi m}{d} - k_{x0} \right)$$
 (1.88)

Using this, we can write (1.9) as

$$\widetilde{G}_{e}(\overline{r}, \overline{r}') = \frac{e^{-jk_{x0}(x-x')}}{2d} \left[ \sum_{m=1}^{+\infty} \left( \sum_{q=0}^{Q} \frac{f_{q} k^{2q}}{\left(\frac{2\pi m}{d} + k_{x0}\right)^{2q+1}} \right) e^{-\left(\frac{2\pi m}{d} + k_{x0}\right)|z-z'|} e^{-j\frac{2\pi m}{d}(x-x')} \right] \\
+ \sum_{m=1}^{+\infty} \left( \sum_{q=0}^{Q} \frac{f_{q} k^{2q}}{\left(\frac{2\pi m}{d} - k_{x0}\right)^{2q+1}} \right) e^{-\left(\frac{2\pi m}{d} - k_{x0}\right)|z-z'|} e^{j\frac{2\pi m}{d}(x-x')} \right] \\
= \frac{e^{-jk_{x0}(x-x')}}{2d} \left[ e^{-k_{x0}|z-z'|} \sum_{m=1}^{+\infty} \left( \sum_{q=0}^{Q} \frac{f_{q} k^{2q}}{\left(\frac{2\pi m}{d} + k_{x0}\right)^{2q+1}} \right) e^{-\frac{2\pi m}{d}|z-z'|} e^{-j\frac{2\pi m}{d}(x-x')} \right] \\
+ e^{k_{x0}|z-z'|} \sum_{m=1}^{+\infty} \left( \sum_{q=0}^{Q} \frac{f_{q} k^{2q}}{\left(\frac{2\pi m}{d} - k_{x0}\right)^{2q+1}} \right) e^{-\frac{2\pi m}{d}|z-z'|} e^{j\frac{2\pi m}{d}(x-x')} \right] \\
\xrightarrow{S_{2}} \tag{1.89}$$

Using this notation,  $\widetilde{G}_e(\bar{r}, \bar{r}')$  can be expressed as the following summation

$$\widetilde{G}_e(\bar{r}, \bar{r}') = \frac{e^{-jk_{x0}(x-x')}}{2d} \left[ e^{-k_{x0}|z-z'|} S_1 + e^{k_{x0}|z-z'|} S_2 \right]$$
(1.90)

We have to sum the series  $S_1$  and  $S_2$  which have the same general form S

$$S = \sum_{m=1}^{+\infty} \left( \sum_{q=0}^{Q} \frac{f_q k^{2q}}{\left(\frac{2\pi m}{d} \pm k_{x0}\right)^{2q+1}} \right) e^{-\frac{2\pi m}{d} [|z-z'| \pm j(x-x')]}$$

$$= \sum_{q=0}^{Q} f_q k^{2q} \sum_{m=1}^{+\infty} \frac{1}{\left(\frac{2\pi m}{d} \pm k_{x0}\right)^{2q+1}} \left( \underbrace{e^{-\frac{2\pi}{d} [|z-z'| \pm j(x-x')]}}_{z_{\pm}} \right)^m$$

$$= \sum_{q=0}^{Q} f_q k^{2q} \sum_{m=1}^{+\infty} \frac{z_{\pm}^m}{\left(\frac{2\pi}{d}\right)^{2q+1} \left(m \pm \frac{k_{x0}d}{2\pi}\right)^{2q+1}}$$

$$= \sum_{q=0}^{Q} \frac{f_q k^{2q}}{\left(\frac{2\pi}{d}\right)^{2q+1}} \sum_{m=1}^{+\infty} \frac{z_{\pm}^m}{\left(m \pm \frac{k_{x0}d}{2\pi}\right)^{2q+1}}$$

$$\left(m + \underbrace{\left(\pm \frac{k_{x0}d}{2\pi}\right)}_{a}\right)^{2q+1}$$

$$(1.91)$$

Knowing that the Lerch transcendent is defined as

$$\Phi(z, s, a) = \sum_{k=0}^{+\infty} \frac{z^k}{(a+k)^s}$$
 (1.92)

Therefore, the summation that we are interested in can be written as

$$\sum_{k=1}^{+\infty} \frac{z^k}{(a+k)^s} = \sum_{k=0}^{+\infty} \frac{z^k}{(a+k)^s} - \frac{1}{a^s} = \Phi(z,s,a) - \frac{1}{a^s}$$
 (1.93)

We can use this notation to express the general summation S as

$$S = \sum_{q=0}^{Q} \frac{f_q k^{2q}}{\left(\frac{2\pi}{d}\right)^{2q+1}} \left[ \Phi\left(z_{\pm}, 2q+1, \pm \frac{k_{x0}d}{2\pi}\right) - \frac{1}{\left(\pm \frac{k_{x0}d}{2\pi}\right)^{2q+1}} \right]$$
(1.94)

and consequently,  $S_1$  and  $S_2$  can be written as follows

$$S_{1} = \sum_{q=0}^{Q} \frac{f_{q} k^{2q}}{\left(\frac{2\pi}{d}\right)^{2q+1}} \left[ \Phi\left(e^{-\frac{2\pi}{d}[|z-z'|+j(x-x')]}, 2q+1, \frac{k_{x0}d}{2\pi}\right) - \frac{1}{\left(\frac{k_{x0}d}{2\pi}\right)^{2q+1}} \right]$$
(1.95)

$$S_2 = \sum_{q=0}^{Q} \frac{f_q k^{2q}}{\left(\frac{2\pi}{d}\right)^{2q+1}} \left[ \Phi\left(e^{-\frac{2\pi}{d}[|z-z'|-j(x-x')]}, 2q+1, -\frac{k_{x0}d}{2\pi}\right) - \frac{1}{\left(-\frac{k_{x0}d}{2\pi}\right)^{2q+1}} \right]$$
(1.96)

So, we have accelerated the spectral Green's function by retaining Q terms in Kummer's transformation. These Q asymptotic retained terms can be summed using this method as a semi-closed form with Lerch transcendent formulation.

## 1.1.3 Option A.3. Approach of $k_{xm}$ : Summation by Parts.

In this subsection, we study an alternative to sum the remaining part using the summation by parts technique [9]. In this case, the series  $\tilde{G}_e(\bar{r}, \bar{r}')$  can be written as the sum of two parts, one analytical and the other numerical but finite.

For this technique, we start from (1.89)

$$\widetilde{G}_{e}(\overline{r}, \overline{r}') = \frac{e^{-jk_{x0}(x-x')}}{2d} \left[ e^{-k_{x0}|z-z'|} \sum_{m=1}^{+\infty} \left( \sum_{q=0}^{Q} \frac{f_{q} k^{2q}}{\left(\frac{2\pi m}{d} + k_{x0}\right)^{2q+1}} \right) e^{-\frac{2\pi m}{d}|z-z'|} e^{-j\frac{2\pi m}{d}(x-x')} \right] + e^{k_{x0}|z-z'|} \sum_{m=1}^{+\infty} \left( \sum_{q=0}^{Q} \frac{f_{q} k^{2q}}{\left(\frac{2\pi m}{d} - k_{x0}\right)^{2q+1}} \right) e^{-\frac{2\pi m}{d}|z-z'|} e^{j\frac{2\pi m}{d}(x-x')} \right]$$

$$S_{2}$$

$$(1.97)$$

As stated above,  $\widetilde{G}_e(\bar{r}, \bar{r}')$  can be expressed as the sum of two series with the same general form

$$\widetilde{G}_e(\bar{r}, \bar{r}') = \frac{e^{-jk_{x0}(x-x')}}{2d} \left[ e^{-k_{x0}|z-z'|} S_1 + e^{k_{x0}|z-z'|} S_2 \right]$$
(1.98)

Applying the theory of the summation by parts technique (see Appendix A.1) reported in [9], the general series S can be split into

$$S = \sum_{m=1}^{+\infty} \left( \sum_{q=0}^{Q} \frac{f_q k^{2q}}{\left(\frac{2\pi m}{d} \pm k_{x0}\right)^{2q+1}} \right) e^{-\frac{2\pi m}{d} [|z-z'| \pm j(x-x')]}$$

$$= \sum_{m=1}^{M-1} \left( \sum_{q=0}^{Q} \frac{f_q k^{2q}}{\left(\frac{2\pi m}{d} \pm k_{x0}\right)^{2q+1}} \right) e^{-\frac{2\pi m}{d} [|z-z'| \pm j(x-x')]}$$

$$+ \sum_{m=M}^{+\infty} \left( \sum_{q=0}^{Q} \frac{f_q k^{2q}}{\left(\frac{2\pi m}{d} \pm k_{x0}\right)^{2q+1}} \right) e^{-\frac{2\pi m}{d} [|z-z'| \pm j(x-x')]}$$

$$R_M$$
(1.99)

Now, we modify  $R_M$  in order to sum it analytically

$$R_{M} = \sum_{m=M}^{+\infty} \underbrace{\left(\sum_{q=0}^{Q} \frac{f_{q} k^{2q}}{\left(\frac{2\pi m}{d} \pm k_{x0}\right)^{2q+1}}\right) e^{-\frac{2\pi m}{d}|z-z'|}}_{\widetilde{G}_{m}^{(-1)}} \underbrace{e^{\mp j\frac{2\pi m}{d}(x-x')}}_{f_{m}^{(+1)}}$$
(1.100)

Using the first order approximation of  $R_M$ 

$$R_M = \widetilde{G}_M^{(-1)} f_{M-1}^{(+2)} \tag{1.101}$$

where

$$\widetilde{G}_{M}^{(-1)} = \widetilde{G}_{m}^{(-1)} \Big|_{m=M} = \left( \sum_{q=0}^{Q} \frac{f_{q} k^{2q}}{\left(\frac{2\pi m}{d} \pm k_{x0}\right)^{2q+1}} \right) e^{-\frac{2\pi m}{d}|z-z'|} \Big|_{m=M}$$

$$= \left( \sum_{q=0}^{Q} \frac{f_{q} k^{2q}}{\left(\frac{2\pi M}{d} \pm k_{x0}\right)^{2q+1}} \right) e^{-\frac{2\pi M}{d}|z-z'|}$$
(1.102)

and

$$f_{M-1}^{(+2)} = \sum_{k=m+1}^{+\infty} f_k^{(+1)} \Big|_{m=M-1} = \sum_{k=m+1}^{+\infty} e^{\mp j \frac{2\pi k}{d} (x-x')} \Big|_{m=M-1} = \frac{e^{\mp j \frac{2\pi (m+1)}{d} (x-x')}}{1 - e^{\mp j \frac{2\pi}{d} (x-x')}} \Big|_{m=M-1}$$

$$= \frac{e^{\mp j \frac{2\pi M}{d} (x-x')}}{1 - e^{\mp j \frac{2\pi}{d} (x-x')}}$$
(1.103)

 $R_M$  can be analytically summed as

$$R_M = \left(\sum_{q=0}^{Q} \frac{f_q \ k^{2q}}{\left(\frac{2\pi M}{d} \pm k_{x0}\right)^{2q+1}}\right) e^{-\frac{2\pi M}{d}|z-z'|} \frac{e^{\mp j\frac{2\pi M}{d}(x-x')}}{1 - e^{\mp j\frac{2\pi}{d}(x-x')}}$$
(1.104)

and therefore, S is given by the summation of the initial numerical part and the obtained analytical part

$$S = \sum_{m=1}^{M-1} \left( \sum_{q=0}^{Q} \frac{f_q \, k^{2q}}{\left(\frac{2\pi m}{d} \pm k_{x0}\right)^{2q+1}} \right) e^{-\frac{2\pi m}{d} [|z-z'| \pm j(x-x')]} + \left( \sum_{q=0}^{Q} \frac{f_q \, k^{2q}}{\left(\frac{2\pi M}{d} \pm k_{x0}\right)^{2q+1}} \right) e^{-\frac{2\pi M}{d} |z-z'|} \frac{e^{\mp j\frac{2\pi M}{d}(x-x')}}{1 - e^{\mp j\frac{2\pi}{d}(x-x')}}$$

$$(1.105)$$

where M has to be adjusted to sum each part in their optimum region. Using this general expression of S, the series  $S_1$  and  $S_2$  that we are interested in are

$$S_{1} = \sum_{m=1}^{M-1} \left( \sum_{q=0}^{Q} \frac{f_{q} k^{2q}}{\left(\frac{2\pi m}{d} + k_{x0}\right)^{2q+1}} \right) e^{-\frac{2\pi m}{d} [|z-z'| + j(x-x')]} + \left( \sum_{q=0}^{Q} \frac{f_{q} k^{2q}}{\left(\frac{2\pi M}{d} + k_{x0}\right)^{2q+1}} \right) e^{-\frac{2\pi M}{d} |z-z'|} \frac{e^{-j\frac{2\pi M}{d}(x-x')}}{1 - e^{-j\frac{2\pi}{d}(x-x')}}$$

$$(1.106)$$

$$S_{2} = \sum_{m=1}^{M-1} \left( \sum_{q=0}^{Q} \frac{f_{q} k^{2q}}{\left(\frac{2\pi m}{d} - k_{x0}\right)^{2q+1}} \right) e^{-\frac{2\pi m}{d} [|z-z'| - j(x-x')]} + \left( \sum_{q=0}^{Q} \frac{f_{q} k^{2q}}{\left(\frac{2\pi M}{d} - k_{x0}\right)^{2q+1}} \right) e^{-\frac{2\pi M}{d} |z-z'|} \frac{e^{j\frac{2\pi M}{d}}(x-x')}{1 - e^{j\frac{2\pi}{d}}(x-x')}$$

$$(1.107)$$

So, we have accelerated the spectral Green's function by retaining Q terms in Kummer's transformation. Thus, the Q asymptotic retained terms can be added using the summation by parts technique as a sum of an analytical part and a numerical but finite part.

A comparison between the different techniques reported in this section to sum the asymptotic series using this first approach of applying Kummer's transformation will be reported in Chapter 3.

## 1.1.4 Option B.1. Approach of $\left(\frac{2\pi m}{d}\right)$ : Sum by Ewald's Method.

The first alternative to sum the asymptotic retained terms obtained by the application of this second approach of Kummer's transformation is using the corresponding terms in Ewald's method. This can be considered a combination of both techniques. The strategy is similar to the followed in the subsection 1.1.1 but with the other approach to extract the asymptotic terms.

In this subsection we report the connection between the first asymptotic term in the spectral domain and the first asymptotic term in Ewald's method.

#### • Extraction of one term.

Here we suggest summing the static first term with Ewald's method. In this case, the series  $\widetilde{G}_e(\bar{r}, \bar{r}')$  that we have to efficiently sum is

$$\widetilde{G}_{e}(\bar{r}, \bar{r}') = \frac{1}{2d} \sum_{\substack{m = -\infty \\ m \neq 0}}^{+\infty} \left| \frac{d}{2\pi m} \right| e^{-\left|\frac{2\pi m}{d}\right| |z - z'|} e^{-jk_{xm}(x - x')}$$
(1.108)

Therefore, the static series  $\widetilde{G}_{e'}(\bar{r}, \bar{r}')$  is

$$\widetilde{G}_{e}(\bar{r}, \bar{r}') = e^{-jk_{x0}(x-x')} \underbrace{\left(\frac{1}{2d} \sum_{\substack{m=-\infty\\m\neq 0}}^{+\infty} \left| \frac{d}{2\pi m} \right| e^{-\left|\frac{2\pi m}{d}\right||z-z'|} e^{-j\frac{2\pi m}{d}(x-x')}\right)}_{\widetilde{G}_{e'}(\bar{r}, \bar{r}')}$$
(1.109)

The idea, like in the subsection 1.1.1, is to identify this series with an approximation of the spectral one and then use Ewald's transformation to sum the asymptotic term.

For this purpose, we have to remember that the spectral Green's function is

$$\widetilde{G}(\bar{r}, \bar{r}') = \frac{1}{2d} \sum_{m=-\infty}^{\infty} \frac{e^{-\gamma_m|z-z'|}}{\gamma_m} e^{-jk_{xm}(x-x')}$$

$$= \frac{1}{2d} \sum_{\substack{m=-\infty\\m\neq 0}}^{+\infty} \frac{e^{-\gamma_m|z-z'|}}{\gamma_m} e^{-jk_{xm}(x-x')} + \frac{1}{2d} \frac{e^{-\gamma_0|z-z'|}}{\gamma_0} e^{-jk_{x0}(x-x')}$$
(1.110)

where  $k_{xm} = k_{x0} + \frac{2\pi m}{d}$  and  $\gamma_m = \sqrt{k_{xm}^2 - k^2}$ . We want to obtain the approximation of the previous series when  $m \to \infty$  using this second approach. It is important to note that we are assuming that  $\gamma_m$  is approximated by  $\left|\frac{2\pi m}{d}\right|$ , that is

$$\gamma_m \big|_{m \to \infty} = \sqrt{k_{xm}^2 - k^2} \Big|_{m \to \infty} = \sqrt{\left(k_{x0} + \frac{2\pi m}{d}\right)^2 - k^2} \Big|_{m \to \infty}$$

$$= \sqrt{\left(k_{x0} + \frac{2\pi m}{d}\right)^2 - k^2} = \left|\frac{2\pi m}{d}\right|$$
(1.111)

For this reason, in m=0 where we only have  $k_{x0}$ , we will use the static limit of this term when  $k_{x0} \to 0$ . That is, we are assuming not only is  $\left(k_{x0} + \frac{2\pi m}{d}\right)$  more important than k (like the other option) but also  $\left|\frac{2\pi m}{d}\right|$  is more important than  $k_{x0}$ . This leads to believe that both k and  $k_{x0}$  tend to 0.

$$\widetilde{G}(\bar{r}, \bar{r}')\big|_{m \to \infty} = \frac{1}{2d} \sum_{\substack{m = -\infty \\ m \neq 0}}^{+\infty} \frac{1}{\gamma_m} e^{-\gamma_m |z - z'| - jk_{xm}(x - x')} \bigg|_{m \to \infty} \\
+ \lim_{k_{x_0} \to 0} \left( \frac{1}{2d} \frac{e^{-\gamma_0 |z - z'|}}{\gamma_0} e^{-jk_{x_0}(x - x')} \right) \\
= \frac{1}{2d} \sum_{\substack{m = -\infty \\ m \neq 0}}^{+\infty} \left| \frac{d}{2\pi m} \right| e^{-\left|\frac{2\pi m}{d}\right||z - z'|} e^{-j\frac{2\pi m}{d}(x - x')} \\
\widetilde{G}_{e'}(\bar{r}, \bar{r}') \\
+ \lim_{k_{x_0} \to 0} \left( \frac{1}{2d} \frac{1}{\gamma_0} e^{-\gamma_0 |z - z'| - jk_{x_0}(x - x')} \right) \tag{1.112}$$

As seen, we can identify the series  $\widetilde{G}_{e'}(\bar{r},\bar{r}')$  as a part of this approximation and therefore we can write  $\widetilde{G}_{e'}(\bar{r},\bar{r}')$  as a function of the approximation of the spectral Green's function when  $m \to \infty$ .

$$\widetilde{G}_{e'}(\bar{r}, \bar{r}') = \widetilde{G}(\bar{r}, \bar{r}') \Big|_{m \to \infty} - \lim_{k_{x_0} \to 0} \left( \frac{1}{2d} \frac{1}{\gamma_0} e^{-\gamma_0 |z - z'| - jk_{x_0}(x - x')} \right)$$
(1.113)

The idea is to sum  $\widetilde{G}_{e'}(\bar{r},\bar{r}')$  rapidly by using the approximation of the Ewald's method components when  $m \to \infty$ . Thus, the approximation of  $\widetilde{G}(\bar{r},\bar{r}')$  can be summed as  $[G_{spectral}(\bar{r},\bar{r}')+G_{spatial}(\bar{r},\bar{r}')]\big|_{m\to\infty}$ .

Remembering that the spectral Ewald's method component  $G_{spectral}(\bar{r}, \bar{r}')$  is [5,11]

$$G_{spectral}(\bar{r}, \bar{r}') = \frac{1}{4d} \sum_{m=-\infty}^{+\infty} \frac{e^{-jk_{xm}(x-x')}}{jk_{zm}} \times \left[ e^{jk_{zm}|z-z'|} \operatorname{erfc}\left(|z-z'|\varepsilon + \frac{jk_{zm}}{2\varepsilon}\right) + e^{-jk_{zm}|z-z'|} \operatorname{erfc}\left(-|z-z'|\varepsilon + \frac{jk_{zm}}{2\varepsilon}\right) \right]$$

$$(1.114)$$

where  $k_{xm} = k_{x0} + \frac{2\pi m}{d}$  and  $k_{zm} = \sqrt{k^2 - k_{xm}^2}$ . We sum separately the term m = 0

$$G_{spectral}(\bar{r}, \bar{r}') = \frac{1}{4d} \sum_{\substack{m=-\infty\\m\neq 0}}^{+\infty} \frac{e^{-jk_{xm}(x-x')}}{jk_{zm}} \times \left[ e^{jk_{zm}|z-z'|} \operatorname{erfc}\left(|z-z'|\varepsilon + \frac{jk_{zm}}{2\varepsilon}\right) + e^{-jk_{zm}|z-z'|} \operatorname{erfc}\left(-|z-z'|\varepsilon + \frac{jk_{zm}}{2\varepsilon}\right) \right] + \frac{1}{4d} \frac{e^{-jk_{x0}(x-x')}}{jk_{z0}} \times \left[ e^{jk_{z0}|z-z'|} \operatorname{erfc}\left(|z-z'|\varepsilon + \frac{jk_{z0}}{2\varepsilon}\right) + e^{-jk_{z0}|z-z'|} \operatorname{erfc}\left(-|z-z'|\varepsilon + \frac{jk_{z0}}{2\varepsilon}\right) \right]$$

$$(1.115)$$

The expansion of  $G_{spectral}(\bar{r}, \bar{r}')$  is given by

$$G_{spectral}(\bar{r}, \bar{r}')\big|_{m \to \infty} = \left\{ \frac{1}{4d} \sum_{\substack{m = -\infty \\ m \neq 0}}^{+\infty} \frac{e^{-jk_{xm}(x-x')}}{jk_{zm}} \right.$$

$$\times \left[ e^{jk_{zm}|z-z'|} \operatorname{erfc}\left(|z-z'|\varepsilon + \frac{jk_{zm}}{2\varepsilon}\right) + e^{-jk_{zm}|z-z'|} \operatorname{erfc}\left(-|z-z'|\varepsilon + \frac{jk_{zm}}{2\varepsilon}\right) \right]$$

$$+ \frac{1}{4d} \frac{e^{-jk_{x0}(x-x')}}{jk_{z0}} \times \left[ e^{jk_{z0}|z-z'|} \operatorname{erfc}\left(|z-z'|\varepsilon + \frac{jk_{z0}}{2\varepsilon}\right) + e^{-jk_{z0}|z-z'|} \operatorname{erfc}\left(-|z-z'|\varepsilon + \frac{jk_{z0}}{2\varepsilon}\right) \right] \right\} \Big|_{m \to \infty}$$

$$(1.116)$$

Using the following approximation of  $k_{zm}$  and  $k_{xm}$ 

$$k_{xm}\big|_{m\to\infty} = \left(k_{x0} + \frac{2\pi m}{d}\right)\bigg|_{m\to\infty} = \frac{2\pi m}{d}$$
 (1.117a)

$$k_{zm}\big|_{m\to\infty} = -\sqrt{k^2 - k_{xm}^2}\Big|_{m\to\infty} = -j\left|\frac{2\pi m}{d}\right|$$
 (1.117b)

the approximation of  $jk_{zm}$ , which is the term that we are interested in, can be obtained as

$$jk_{zm}\big|_{m\to\infty} = \left|\frac{2\pi m}{d}\right| \tag{1.118}$$

According to this, the expansion of  $G_{spectral}(\bar{r}, \bar{r}')$  can be expressed as

$$G_{spectral}(\bar{r}, \bar{r}')\big|_{m \to \infty} = \frac{1}{4d} \sum_{\substack{m = -\infty \\ m \neq 0}}^{+\infty} \frac{e^{-j\frac{2\pi m}{d}(x-x')}}{\left|\frac{2\pi m}{d}\right|} \times \left[e^{\left|\frac{2\pi m}{d}\right||z-z'|} \operatorname{erfc}\left(\left|z-z'\right|\varepsilon + \frac{\left|\frac{2\pi m}{d}\right|}{2\varepsilon}\right)\right] + e^{-\left|\frac{2\pi m}{d}\right||z-z'|} \operatorname{erfc}\left(-\left|z-z'\right|\varepsilon + \frac{\left|\frac{2\pi m}{d}\right|}{2\varepsilon}\right)\right] + \lim_{k_{x0} \to 0} \left(\frac{1}{4d} \frac{e^{-jk_{x0}(x-x')}}{jk_{z0}}\right) \times \left[e^{jk_{z0}|z-z'|} \operatorname{erfc}\left(\left|z-z'\right|\varepsilon + \frac{jk_{z0}}{2\varepsilon}\right) + e^{-jk_{z0}|z-z'|} \operatorname{erfc}\left(-\left|z-z'\right|\varepsilon + \frac{jk_{z0}}{2\varepsilon}\right)\right]\right)$$

$$(1.119)$$

As mentioned before, in m = 0 we have to calculate the limit of  $k_{x0}$  because we are using the approximation  $jk_{zm} = \left|\frac{2\pi m}{d}\right|$  neglecting not only k but also  $k_{x0}$ .

On the other hand, recalling that the spatial Ewald's method component  $G_{spatial}(\bar{r}, \bar{r}')$  is [5, 11]

$$G_{spatial}(\bar{r}, \bar{r}') = \frac{1}{4\pi} \sum_{m=-\infty}^{+\infty} e^{-jk_{x0}md} \sum_{q=0}^{+\infty} \left(\frac{k}{2\varepsilon}\right)^{2q} \frac{1}{q!} \operatorname{E}_{q+1}(R_m^2 \varepsilon^2)$$
(1.120)

the approximation when  $m \to \infty$  in the spectral domain corresponds to  $k \to 0$  in the spatial domain. Therefore, the limit of  $G_{spatial}(\bar{r}, \bar{r}')$  when  $k \to 0$  is given by

$$\lim_{\substack{k \to 0 \\ k_{x0} \to 0}} G_{spatial}(\bar{r}, \bar{r}') = \lim_{\substack{k \to 0 \\ k_{x0} \to 0}} \left\{ \frac{1}{4\pi} \sum_{m = -\infty}^{+\infty} e^{-jk_{x0}md} \sum_{q = 0}^{+\infty} \left( \frac{k}{2\varepsilon} \right)^{2q} \frac{1}{q!} \operatorname{E}_{q+1}(R_m^2 \varepsilon^2) \right\}$$

$$= \frac{1}{4\pi} \sum_{m = -\infty}^{+\infty} \operatorname{E}_1(R_m^2 \varepsilon^2) \tag{1.121}$$

The found approximations of Ewald's method components can be used to sum the series  $\widetilde{G}_e(\bar{r}, \bar{r}')$ 

$$\begin{split} \widetilde{G}_{e}(\bar{r}, \bar{r}') &= e^{-jk_{x0}(x-x')} \left\{ \widetilde{G}(\bar{r}, \bar{r}') \Big|_{m \to \infty} - \lim_{k_{x0} \to 0} \left( \frac{1}{2d} \frac{1}{\gamma_{0}} e^{-\gamma_{0}|z-z'| - jk_{x0}(x-x')} \right) \right\} \\ &= e^{-jk_{x0}(x-x')} \left\{ \left[ G_{spectral}(\bar{r}, \bar{r}') + G_{spatial}(\bar{r}, \bar{r}') \right] \Big|_{m \to \infty} \right. \\ &- \lim_{k_{x0} \to 0} \left( \frac{1}{2d} \frac{1}{\gamma_{0}} e^{-\gamma_{0}|z-z'| - jk_{x0}(x-x')} \right) \right\} \\ &= e^{-jk_{x0}(x-x')} \left\{ \frac{1}{4\pi} \sum_{m=-\infty}^{+\infty} \operatorname{E}_{1}(R_{m}^{2}\varepsilon^{2}) + \frac{1}{4d} \sum_{\substack{m=-\infty \\ m \neq 0}}^{+\infty} \frac{e^{-j\frac{2\pi m}{d}(x-x')}}{\left| \frac{2\pi m}{d} \right|} \right. \\ &\times \left[ e^{\left| \frac{2\pi m}{d} \right| |z-z'|} \operatorname{erfc} \left( |z-z'|\varepsilon + \frac{\left| \frac{2\pi m}{d} \right|}{2\varepsilon} \right) + e^{-\left| \frac{2\pi m}{d} \right| |z-z'|} \operatorname{erfc} \left( -|z-z'|\varepsilon + \frac{\left| \frac{2\pi m}{d} \right|}{2\varepsilon} \right) \right] \\ &+ \lim_{k_{x0} \to 0} \left( \frac{1}{4d} \frac{e^{-jk_{x0}(x-x')}}{jk_{z0}} \times \left[ e^{jk_{z0}|z-z'|} \operatorname{erfc} \left( |z-z'|\varepsilon + \frac{jk_{z0}}{2\varepsilon} \right) \right. \\ &+ e^{-jk_{z0}|z-z'|} \operatorname{erfc} \left( -|z-z'|\varepsilon + \frac{jk_{z0}}{2\varepsilon} \right) \right] - \frac{1}{2d} \frac{1}{\gamma_{0}} e^{-\gamma_{0}|z-z'| - jk_{x0}(x-x')} \right) \right\} \end{aligned} \tag{1.122}$$

where the last term T contains the residual value when m = 0. As discussed before, in this approach we have to calculate and use the limit of T when  $k_{x0} \to 0$  in all cases.

$$T = \lim_{k_{x0}\to 0} \left\{ \frac{1}{4d} \frac{e^{-jk_{x0}(x-x')}}{|k_{x0}|} \times \left[ e^{|k_{x0}||z-z'|} \operatorname{erfc} \left( |z-z'|\varepsilon + \frac{|k_{x0}|}{2\varepsilon} \right) + e^{-|k_{x0}||z-z'|} \right] \right\}$$

$$\operatorname{erfc} \left( -|z-z'|\varepsilon + \frac{|k_{x0}|}{2\varepsilon} \right) - \frac{1}{2d} \frac{1}{\gamma_0} e^{-\gamma_0|z-z'|-jk_{x0}(x-x')} \right\}$$

$$= \frac{1}{2d} \lim_{k_{x0}\to 0} \left\{ \frac{e^{-jk_{x0}(x-x')}}{|k_{x0}|} \left[ \frac{1}{2} \left( e^{|k_{x0}||z-z'|} \operatorname{erfc} \left( |z-z'|\varepsilon + \frac{|k_{x0}|}{2\varepsilon} \right) \right) + e^{-|k_{x0}||z-z'|} \operatorname{erfc} \left( -|z-z'|\varepsilon + \frac{|k_{x0}|}{2\varepsilon} \right) \right) - e^{-|k_{x0}||z-z'|} \right] \right\}$$

$$= \frac{|z-z'|}{2d} - \frac{e^{-|z-z'|^2\varepsilon^2}}{2\varepsilon d\sqrt{\pi}} - \frac{|z-z'|\operatorname{erf}(|z-z'|\varepsilon)}{2d}$$

$$(1.123)$$

Introducing (1.123) in (1.122),  $\widetilde{G}_e(\bar{r}, \bar{r}')$  remains

$$\widetilde{G}_{e}(\overline{r}, \overline{r}') = e^{-jk_{x0}(x-x')} \left\{ \frac{1}{4\pi} \sum_{m=-\infty}^{+\infty} \operatorname{E}_{1}(R_{m}^{2}\varepsilon^{2}) + \frac{1}{4d} \sum_{\substack{m=-\infty\\m\neq 0}}^{+\infty} \frac{e^{-j\frac{2\pi m}{d}(x-x')}}{\left|\frac{2\pi m}{d}\right|} \right. \\
\times \left[ e^{\left|\frac{2\pi m}{d}\right||z-z'|} \operatorname{erfc}\left(\left|z-z'\right|\varepsilon + \frac{\left|\frac{2\pi m}{d}\right|}{2\varepsilon}\right) + e^{-\left|\frac{2\pi m}{d}\right||z-z'|} \operatorname{erfc}\left(-\left|z-z'\right|\varepsilon + \frac{\left|\frac{2\pi m}{d}\right|}{2\varepsilon}\right) \right] \\
+ \frac{\left|z-z'\right|}{2d} - \frac{e^{-\left|z-z'\right|^{2}\varepsilon^{2}}}{2\varepsilon d\sqrt{\pi}} - \frac{\left|z-z'\right|\operatorname{erf}\left(\left|z-z'\right|\varepsilon\right)}{2d} \right\} \tag{1.124}$$

The extension of this formulation to one more term could be carried out by using the Taylor expansion not only for  $e^{\frac{k^2}{4s^2}}$  but also for  $e^{-jk_{x0}md}$ . These expansions have to be done in the spectral development (1.58) and in the developments of Ewald's method components (1.59) and (1.60).

$$G(\bar{r}, \bar{r}') = \frac{1}{2\pi} \sum_{m=-\infty}^{+\infty} \underbrace{e^{-jk_{x0}md}}_{\text{Taylor expansion}} \int_0^\infty \frac{e^{-R_m^2 s^2}}{s} \underbrace{e^{\frac{k^2}{4s^2}}}_{\text{Taylor expansion}} ds \qquad (1.125)$$

$$G_{spectral}(\bar{r}, \bar{r'}) = \frac{1}{2\pi} \sum_{m=-\infty}^{+\infty} \underbrace{e^{-jk_{x0}md}}_{\text{Taylor expansion}} \int_{0}^{\varepsilon} \frac{e^{-R_{m}^{2}s^{2}}}{s} \underbrace{e^{\frac{k^{2}}{4s^{2}}}}_{\text{Taylor expansion}} ds \quad (1.126)$$

$$G_{spatial}(\bar{r}, \bar{r'}) = \frac{1}{2\pi} \sum_{m=-\infty}^{+\infty} \underbrace{e^{-jk_{x0}md}}_{\text{Taylor expansion}} \int_{\varepsilon}^{\infty} \frac{e^{-R_m^2 s^2}}{s} \underbrace{e^{\frac{k^2}{4s^2}}}_{\text{Taylor expansion}} ds \quad (1.127)$$

The extraction of two terms and the generalization to Q terms is not carried out due to the difficulty that arises from the Ewald's integrals when we extract more than one term with this approach. This is because we have the product of two Taylor expansions and the integral resulted by this product become complicated.

But even so, in this subsection we have accelerated the spectral Green's function by using Kummer's transformation and summing efficiently the first asymptotic retained term through Ewald's method.

# 1.1.5 Option B.2. Approach of $(\frac{2\pi m}{d})$ : Polylogarithmic Functions.

This option consists of using polylogarithmic functions to write the asymptotic part when we use the  $\left(\frac{2\pi m}{d}\right)$  - approach. This alternative was studied in detail in [11].

The idea is that the Q retained terms are written in a semi-closed form as polylogarithmic funtions. The polylogarithm (also known as Jonquière's function) [16] is a special function  $\text{Li}_s(z)$  defined by the following series

$$\operatorname{Li}_{s}(z) = \sum_{k=1}^{\infty} \frac{z^{k}}{k^{s}} \tag{1.128}$$

where s is the order and z is the argument. Using the notation, when more and more terms are retained, more series with a higher order appear and more polylogarithms with a higher order have to be summed. The formulation start from

$$\widetilde{G}_{e}(\overline{r}, \overline{r}') = \frac{1}{2d} \sum_{\substack{m=-\infty\\m\neq 0}}^{+\infty} \left| \frac{d}{2\pi m} - \frac{k_{x0}d^{2}}{(2\pi m)^{2}} + \frac{(k^{2} - k_{x0}^{2})d^{3}}{2(2\pi m)^{3}} + \dots \right| e^{-\left|\frac{2\pi m}{d} + k_{x0}\right||z-z'|} e^{-jk_{xm}(x-x')}$$

$$= \frac{1}{2d} \sum_{\substack{m=-\infty\\m\neq 0}}^{+\infty} \left| \sum_{q=0}^{Q} \frac{d^{q+1}}{(\pi m)^{q+1}} \sum_{a=0}^{x} \frac{k_{x0}^{(q-2a)}(k_{x0}^{2} - k^{2})^{a}}{2^{2a+1}} {q-a \choose a} f_{q-a} \right| e^{-\left|\frac{2\pi m}{d} + k_{x0}\right||z-z'|} e^{-jk_{xm}(x-x')} \tag{1.129}$$

We can remove the absolute value as follows

$$\widetilde{G}_{e}(\bar{r},\bar{r}') = \frac{e^{-jk_{x0}(x-x')}}{2d} \left[ \sum_{m=1}^{+\infty} \left( \sum_{q=0}^{Q} \frac{d^{q+1}}{(\pi m)^{q+1}} \sum_{a=0}^{x} \frac{k_{x0}^{(q-2a)}(k_{x0}^{2} - k^{2})^{a}}{2^{2a+1}} \binom{q-a}{a} f_{q-a} \right) \right] \\
e^{-\left(\frac{2\pi m}{d} + k_{x0}\right)|z-z'|} e^{-j\frac{2\pi m}{d}(x-x')} - \sum_{m=1}^{+\infty} \left( \sum_{q=0}^{Q} \frac{(-1)^{q+1}d^{q+1}}{(\pi m)^{q+1}} \sum_{a=0}^{x} \frac{k_{x0}^{(q-2a)}(k_{x0}^{2} - k^{2})^{a}}{2^{2a+1}} \binom{q-a}{a} f_{q-a} \right) \\
e^{-\left(\frac{2\pi m}{d} - k_{x0}\right)|z-z'|} e^{j\frac{2\pi m}{d}(x-x')} \right] \tag{1.130}$$

Using the definition of polylogarithm given by (1.128),  $\widetilde{G}_e(\bar{r}, \bar{r}')$  can be written as

$$\widetilde{G}_{e}(\bar{r}, \bar{r}') = \frac{e^{-jk_{x0}(x-x')}}{2d} \left[ e^{-k_{x0}|z-z'|} \sum_{q=0}^{Q} \frac{d^{q+1}}{\pi^{q+1}} \sum_{a=0}^{x} \frac{k_{x0}^{(q-2a)}(k_{x0}^{2} - k^{2})^{a}}{2^{2a+1}} {q-a \choose a} f_{q-a} \right]$$

$$\operatorname{Li}_{q+1}(z_{1}) - e^{k_{x0}|z-z'|} \sum_{q=0}^{Q} \frac{(-1)^{q+1}d^{q+1}}{\pi^{q+1}} \sum_{a=0}^{x} \frac{k_{x0}^{(q-2a)}(k_{x0}^{2} - k^{2})^{a}}{2^{2a+1}} {q-a \choose a} f_{q-a} \operatorname{Li}_{q+1}(z_{2})$$

$$(1.131)$$

where

$$z_1 = e^{-\frac{2\pi}{d}[|z-z'|+j(x-x')]}$$
(1.132a)

$$z_2 = e^{-\frac{2\pi}{d}[|z-z'| - j(x-x')]}$$
(1.132b)

So, we have accelerated the spectral Green's function by retaining Q terms in Kummer's transformation. These Q asymptotic retained terms can be summed using this method as a semi-closed form with polylogarithmic formulation. For more detail about the general formulation see [11]. It is important to note that this development has been outlined in a Q generic form for both approaches using the Lerch transcendent formulation for the first one and the polylogarithmic functions as analogue for the second approach.

In addition to this expansion, we can consider an alternative approximation described in [17,18]. This alternative is reported for second order terms but is not generalized.

The idea starts from the expansion of  $\gamma_m$ . We have that  $\gamma_m$  is

$$\gamma_{m} = \sqrt{k_{xm}^{2} - k^{2}} = \sqrt{\left(k_{x0} + \frac{2\pi m}{d}\right)^{2} - k^{2}} = \sqrt{k_{x0}^{2} + \frac{2\pi m k_{x0}}{d} + \left(\frac{2\pi m}{d}\right)^{2} - k^{2}}$$

$$= \left(\frac{2\pi m}{d}\right) \sqrt{1 + \underbrace{\frac{k_{x0}d}{\pi m} + \frac{k_{x0}^{2} - k^{2}}{\left(\frac{2\pi m}{d}\right)^{2}}}_{u}}$$
(1.133)

The expansion of  $\gamma_m$  when  $u \to 0$  is

$$\gamma_m \approx \left(\frac{2\pi m}{d}\right) \left(1 + \frac{k_{x0}d}{2\pi m} - \frac{k^2}{2\left(\frac{2\pi m}{d}\right)^2} + \frac{k_{x0}^2}{2\left(\frac{2\pi m}{d}\right)^2} + \dots\right) 
= \left|\frac{2\pi m}{d} + k_{x0} - \frac{k^2d}{4\pi m} + \frac{k_{x0}^2d}{4\pi m} + \dots\right|$$
(1.134)

and thus the expansion of the exponential in the asymptotic term is given by

$$e^{-\gamma_m|z-z'|} \approx e^{-\left|\frac{2\pi m}{d} + k_{x0} - \frac{k^2 d}{4\pi m} + \frac{k_{x0}^2 d}{4\pi m}\right||z-z'|}$$
 (1.135)

We used the first two terms in our approximation [11] due to the third term,  $e^{-x/m}$ , when  $m \to +\infty$  does not improve the convergence. In [17,18] the first two terms of exponential are also use and the third one results in additional terms by Taylor expansion of the exponential. According to this, the final expansion of the exponential in the asymptotic

terms is given by

$$e^{-\gamma_m|z-z'|} \approx e^{-\left|\frac{2\pi m}{d} + k_{x0}\right||z-z'|}$$
 (1.136)

and the exponential, resulted by the third term in the expansion of  $\gamma_m$ , is used as follows

$$e^{\frac{k^2d|z-z'|}{4\pi|m|}} = 1 + \frac{k^2d|z-z'|}{4\pi|m|} + \frac{1}{2!} \left(\frac{k^2d|z-z'|}{4\pi|m|}\right)^2 + \frac{1}{3!} \left(\frac{k^2d|z-z'|}{4\pi|m|}\right)^3 + \dots$$

$$= 1 + \sum_{n=0}^{+\infty} \frac{1}{n!} \left(\frac{k^2d|z-z'|}{4\pi|m|}\right)^n$$
(1.137)

Thus, the asymptotic term can be generally written as

$$\frac{1}{\gamma_{m}} e^{-\gamma_{m}|z-z'|} \approx \frac{1}{\gamma_{m}} \left( 1 + \sum_{n=0}^{+\infty} \frac{1}{n!} \left( \frac{k^{2}d|z-z'|}{4\pi|m|} \right)^{n} \right) e^{-\left|\frac{2\pi m}{d} + k_{x0}\right||z-z'|}$$

$$= \left( \frac{1}{\gamma_{m}} + \underbrace{\frac{1}{\gamma_{m}} \sum_{n=0}^{+\infty} \frac{1}{n!} \left( \frac{k^{2}d|z-z'|}{4\pi|m|} \right)^{n}}_{\text{the new terms}} \right) e^{-\left|\frac{2\pi m}{d} + k_{x0}\right||z-z'|} \tag{1.138}$$

It can be noted that if we consider the first term of this new expansion, which is 1, the expansion of  $\frac{1}{\gamma_m}$  is the same we have taken into account in [11].

The improvement that these terms incorporate is the next terms of the exponential expansion. In addition, the following terms that are obtained in the expansion of  $\gamma_m$  will result in more exponential expansions like the reported one.

This alternative improves the convergence of Green's function when the observation point is far from the source because near the source this new terms are negligible due to the fact that contains |z - z'| and near the source  $|z - z'| \to 0$ .

The formulation with this consideration can become complicated due to the number of terms to take into account. In addition, it should be pointed out that far from the source the spectral Green's function without any transformation is rapidly convergent and for this reason, the improvement in the case that we are interested in (near the source) is negligible.

Because of that, we are going to detail the process following in [17,18] and show the change in our notation produced by this additional expansion. However, we are going to continue our formulation without taking into account these terms.

According to this development, the second order approximation of Kummer's transformation can be obtained as

$$\frac{1}{\gamma_m} e^{-\gamma_m |z-z'|} \approx \left| \frac{d}{2\pi m} - \frac{k_{x0}d^2}{(2\pi m)^2} \right| \left( 1 + \frac{(k^2 - k_{x0}^2)d|z-z'|}{4\pi |m|} \right) e^{-\left|\frac{2\pi m}{d} + k_{x0}\right||z-z'|} \tag{1.139}$$

where for positive m is

$$\left| \frac{d}{2\pi m} - \frac{k_{x0}d^2}{(2\pi m)^2} \right| = \frac{d}{2\pi m} - \frac{k_{x0}d^2}{(2\pi m)^2} = \frac{d}{2\pi m} - \frac{\operatorname{sgn}(m)k_{x0}d^2}{(2\pi m)^2}$$
(1.140)

and for negative m is

$$\left| -\frac{d}{2\pi m} - \frac{k_{x0}d^2}{(2\pi m)^2} \right| = \frac{d}{2\pi m} + \frac{k_{x0}d^2}{(2\pi m)^2} = \frac{d}{2\pi |m|} - \frac{\operatorname{sgn}(m)k_{x0}d^2}{(2\pi m)^2}$$
(1.141)

and in general for positive and negative m is

$$\left| \frac{d}{2\pi m} - \frac{k_{x0}d^2}{(2\pi m)^2} \right| = \frac{d}{2\pi |m|} - \frac{\operatorname{sgn}(m)k_{x0}d^2}{(2\pi m)^2}$$
 (1.142)

Using this,  $\frac{1}{\gamma_m}e^{-\gamma_m|z-z'|}$  can be expressed as its second order expansion but now we use the previous obtained terms in the expansion of third exponential.

$$\frac{1}{\gamma_{m}}e^{-\gamma_{m}|z-z'|} \approx \left(\frac{d}{2\pi|m|} - \frac{\operatorname{sgn}(m) k_{x0} d^{2}}{(2\pi m)^{2}}\right) \left(1 + \frac{(k^{2} - k_{x0}^{2}) d|z-z'|}{4\pi|m|}\right) e^{-\left|\frac{2\pi m}{d} + k_{x0}\right||z-z'|}$$

$$= \left(\frac{d}{2\pi|m|} - \frac{\operatorname{sgn}(m) k_{x0} d^{2}}{(2\pi m)^{2}} + \frac{(k^{2} - k_{x0}^{2}) d^{2}|z-z'|}{2(2\pi|m|)^{2}} + \frac{\operatorname{sgn}(m) (k^{2} - k_{x0}^{2}) k_{x0} d^{3}|z-z'|}{2(2\pi m)^{3}}\right)$$

$$e^{-\left|\frac{2\pi m}{d} + k_{x0}\right||z-z'|} \tag{1.143}$$

where we have in [11] that the second order expansion of the Kummer's transformation is

$$\widetilde{G}_{e} = \frac{e^{-jk_{x0}(x-x')}}{2d} \left\{ e^{k_{z0}|z-z'|} \left[ \frac{d}{2\pi} \operatorname{Li}_{1}(z_{1}) + \frac{k_{x0} d^{2}}{(2\pi)^{2}} \operatorname{Li}_{2}(z_{1}) \right] + e^{-k_{z0}|z-z'|} \left[ \frac{d}{2\pi} \operatorname{Li}_{1}(z_{2}) - \frac{k_{x0} d^{2}}{(2\pi)^{2}} \operatorname{Li}_{2}(z_{2}) \right] \right\}$$
(1.144)

where  $z_1 = e^{\frac{2\pi}{d}[|z-z'|-j(x-x')]}$  and  $z_2 = e^{\frac{2\pi}{d}[|z-z'|+j(x-x')]}$ . Now, with this alternative approximation, the second order expansion of the Kummer's transformation is

$$\widetilde{G}_{e} = \frac{e^{-jk_{x0}(x-x')}}{2d} \left\{ e^{k_{z0}|z-z'|} \left[ \frac{d}{2\pi} \operatorname{Li}_{1}(z_{1}) + \left( \frac{(k^{2}-k_{x0}^{2}) d^{2}|z-z'|}{2(2\pi)^{2}} + \frac{k_{x0} d^{2}}{(2\pi)^{2}} \right) \operatorname{Li}_{2}(z_{1}) \right] + e^{-k_{z0}|z-z'|} \left[ \frac{d}{2\pi} \operatorname{Li}_{1}(z_{2}) + \left( \frac{(k^{2}-k_{x0}^{2}) d^{2}|z-z'|}{2(2\pi)^{2}} - \frac{k_{x0} d^{2}}{(2\pi)^{2}} \right) \operatorname{Li}_{2}(z_{2}) \right] \right\}$$
(1.145)

As has been noticed, this procedure can be generalized for all terms presented in the exponential expansion, nonetheless all these terms would be proportional to the distance between the observation point and the source point |z - z'|. In our case, we are interested in accelerating the convergence of Green's functions when the observation point is close to the source and for this case, these additional terms would be negligible.

# 1.1.6 Option B.3. Approach of $(\frac{2\pi m}{d})$ : Summation by Parts.

In this subsection, we study an alternative to sum the remaining part using the summation by parts technique [9]. In this case, the series  $\tilde{G}_e(\bar{r}, \bar{r}')$  can be written as the sum of two parts, one analytical and the other numerical but finite.

For this purpose, we start from (1.16)

$$\widetilde{G}_{e}(\overline{r}, \overline{r}') = \frac{1}{2d} \sum_{\substack{m=-\infty\\m\neq 0}}^{+\infty} \left| \frac{d}{2\pi m} - \frac{k_{x0}d^{2}}{(2\pi m)^{2}} + \frac{(k^{2} - k_{x0}^{2})d^{3}}{2(2\pi m)^{3}} + \dots \right| 
e^{-\left|\frac{2\pi m}{d} + k_{x0}\right||z-z'|} e^{-jk_{xm}(x-x')} 
= \frac{1}{2d} \sum_{\substack{m=-\infty\\m\neq 0}}^{+\infty} \left| \sum_{q=0}^{Q} \sum_{a=0}^{q} {q \choose a} \frac{k_{x0}^{(q-a)}(k_{x0}^{2} - k^{2})^{a}}{2^{2a+1}} \left( \frac{d}{\pi m} \right)^{q+a+1} f_{q} \right| 
e^{-\left|\frac{2\pi m}{d} + k_{x0}\right||z-z'|} e^{-jk_{xm}(x-x')}$$
(1.146)

According to this, the asymptotic series that has to be accelerated is

$$\widetilde{G}_{e}(\overline{r}, \overline{r}') = \frac{e^{-jk_{x0}(x-x')}}{2d} \left[ e^{-k_{x0}|z-z'|} \\
\sum_{m=1}^{+\infty} \sum_{q=0}^{Q} \sum_{a=0}^{q} {q \choose a} \frac{k_{x0}^{(q-a)} (k_{x0}^{2} - k^{2})^{a}}{2^{2a+1}} \left( \frac{d}{\pi m} \right)^{q+a+1} f_{q} e^{-\frac{2\pi m}{d}[|z-z'|+j(x-x')]} - e^{k_{x0}|z-z'|} \\
\sum_{m=1}^{+\infty} \sum_{q=0}^{Q} (-1)^{q} \sum_{a=0}^{q} (-1)^{a+1} {q \choose a} \frac{k_{x0}^{(q-a)} (k_{x0}^{2} - k^{2})^{a}}{2^{2a+1}} \left( \frac{d}{\pi m} \right)^{q+a+1} f_{q} e^{-\frac{2\pi m}{d}[|z-z'|-j(x-x')]} \right] \\
\widetilde{S}_{2} \qquad (1.147)$$

As stated above,  $\widetilde{G}_e(\bar{r}, \bar{r}')$  can be expressed as the sum of two series with the following general form

$$\widetilde{G}_e(\bar{r}, \bar{r}') = \frac{e^{-jk_{x0}(x-x')}}{2d} \left[ e^{-k_{x0}|z-z'|} S_1 - e^{k_{x0}|z-z'|} S_2 \right]$$
(1.148)

We name the factors, which are multiplying,  $F_{+}$  and  $F_{-}$ , respectively.

$$F_{+} = {q \choose a} \frac{k_{x0}^{(q-a)} (k_{x0}^{2} - k^{2})^{a}}{2^{2a+1}} \left(\frac{d}{\pi}\right)^{q+a+1} f_{q}$$
 (1.149)

$$F_{-} = (-1)^{q} {q \choose a} (-1)^{a+1} \frac{k_{x0}^{(q-a)} (k_{x0}^{2} - k^{2})^{a}}{2^{2a+1}} \left(\frac{d}{\pi}\right)^{q+a+1} f_{q}$$
 (1.150)

Applying the theory of the summation by parts technique (see Appendix A.1) reported in [9], the general series S can be split into

$$S = \sum_{m=1}^{+\infty} \sum_{q=0}^{Q} \sum_{a=0}^{q} F_{\pm} \frac{e^{-\frac{2\pi m}{d}|z-z'|}}{m^{q+a+1}} e^{\mp j\frac{2\pi m}{d}}(x-x') = \underbrace{\sum_{m=1}^{M-1} \sum_{q=0}^{Q} \sum_{a=0}^{q} F_{\pm} \frac{e^{-\frac{2\pi m}{d}|z-z'|}}{m^{q+a+1}} e^{\mp j\frac{2\pi m}{d}}(x-x')}_{S_{M-1}} + \underbrace{\sum_{m=M}^{+\infty} \sum_{q=0}^{Q} \sum_{a=0}^{q} F_{\pm} \frac{e^{-\frac{2\pi m}{d}|z-z'|}}{m^{q+a+1}} e^{\mp j\frac{2\pi m}{d}}(x-x')}_{R_{M}}$$

$$(1.151)$$

Now, we modify  $R_M$  in order to sum it analytically

$$R_{M} = \sum_{m=M}^{+\infty} \underbrace{\sum_{q=0}^{Q} \sum_{a=0}^{q} F_{\pm} \frac{e^{-\frac{2\pi m}{d}|z-z'|}}{m^{q+a+1}}}_{\widetilde{G}_{m}^{(-1)}} \underbrace{e^{\mp j\frac{2\pi m}{d}(x-x')}}_{f_{m}^{(+1)}}$$
(1.152)

Using the first order approximation of  $R_M = \widetilde{G}_M^{(-1)} f_{M-1}^{(+2)}$  where

$$\widetilde{G}_{M}^{(-1)} = \widetilde{G}_{m}^{(-1)} \Big|_{m=M} = \sum_{q=0}^{Q} \sum_{a=0}^{q} F_{\pm} \frac{e^{-\frac{2\pi m}{d}|z-z'|}}{m^{q+a+1}} \Big|_{m=M} = \sum_{q=0}^{Q} \sum_{a=0}^{q} F_{\pm} \frac{e^{-\frac{2\pi M}{d}|z-z'|}}{M^{q+a+1}} \tag{1.153}$$

and

$$f_{M-1}^{(+2)} = \sum_{k=m+1}^{+\infty} f_k^{(+1)} \Big|_{m=M-1} = \sum_{k=m+1}^{+\infty} e^{\mp j \frac{2\pi k}{d} (x-x')} \Big|_{m=M-1} = \frac{e^{\mp j \frac{2\pi (m+1)}{d} (x-x')}}{1 - e^{\mp j \frac{2\pi}{d} (x-x')}} \Big|_{m=M-1}$$

$$= \frac{e^{\mp j \frac{2\pi M}{d} (x-x')}}{1 - e^{\mp j \frac{2\pi}{d} (x-x')}}$$

$$(1.154)$$

 $R_M$  can be summed as

$$R_M = \sum_{q=0}^{Q} \sum_{a=0}^{q} F_{\pm} \frac{e^{-\frac{2\pi M}{d}|z-z'|}}{M^{q+a+1}} \frac{e^{\mp j\frac{2\pi M}{d}(x-x')}}{1 - e^{\mp j\frac{2\pi}{d}(x-x')}}$$
(1.155)

and therefore, S is given by the summation of the initial numerical part and the obtained analytical part.

$$S = \sum_{m=1}^{M-1} \sum_{q=0}^{Q} \sum_{a=0}^{q} F_{\pm} \frac{e^{-\frac{2\pi m}{d}|z-z'|}}{m^{q+a+1}} e^{\mp j\frac{2\pi m}{d}(x-x')} + \sum_{q=0}^{Q} \sum_{a=0}^{q} F_{\pm} \frac{e^{-\frac{2\pi M}{d}|z-z'|}}{M^{q+a+1}} \frac{e^{\mp j\frac{2\pi M}{d}(x-x')}}{1 - e^{\mp j\frac{2\pi}{d}(x-x')}}$$

$$(1.156)$$

Using this general expression of S, the series that we are interesting in  $S_1$  and  $S_2$  are

$$S_{1} = \sum_{m=1}^{M-1} \sum_{q=0}^{Q} \sum_{a=0}^{q} F_{+} \frac{e^{-\frac{2\pi m}{d}|z-z'|}}{m^{q+a+1}} e^{-j\frac{2\pi m}{d}(x-x')} + \sum_{q=0}^{Q} \sum_{a=0}^{q} F_{+} \frac{e^{-\frac{2\pi M}{d}|z-z'|}}{M^{q+a+1}} \frac{e^{-j\frac{2\pi M}{d}(x-x')}}{1 - e^{-j\frac{2\pi}{d}(x-x')}}$$

$$(1.157)$$

$$S_{2} = \sum_{m=1}^{M-1} \sum_{q=0}^{Q} \sum_{a=0}^{q} F_{-} \frac{e^{-\frac{2\pi m}{d}|z-z'|}}{m^{q+a+1}} e^{+j\frac{2\pi m}{d}(x-x')} + \sum_{q=0}^{Q} \sum_{a=0}^{q} F_{-} \frac{e^{-\frac{2\pi M}{d}|z-z'|}}{M^{q+a+1}} \frac{e^{j\frac{2\pi M}{d}(x-x')}}{1 - e^{j\frac{2\pi}{d}(x-x')}}$$

$$(1.158)$$

So, we have accelerated the spectral Green's function by retaining Q terms in Kummer's transformation. These Q asymptotic retained terms can be summed using the summation by parts technique as a sum of an analytical part and a numerical but finite part. It should be pointed out that this development has been obtained in generic form using either approaches.

A comparison between the different techniques reported in this section to sum the asymptotic series in this second form of applying Kummer's transformation will be reported in Chapter 3.

Additionally, in Chapter 3 we compare the improvement that implies the use of each approach in the application of the spectral Kummer's transformation and we analyse the advantages of using one or the other strategy. In advance, we could suppose that, depending on the case that we are interested in, it would be better using one or the other approach.

As a general conclusion of this section, we have proposed for each approach three methods of summing the remaining part.

#### 1. The first one is using Ewald's method.

This alternative allows us to use the acceleration resulted by applying Kummer's transformation and sum efficiently the retained terms through Ewald's method. It provides that the Green's function can be written as the summation of two rapidly convergent components.

The relatively minor disadvantage of the original Ewald's method could be that its components require the evaluation of special functions like complementary error function with complex argument and the exponential integral.

Thanks to the proposed Kummer-Ewald technique, we can take advantage of the rapidly convergence of Ewald's components without the need to calculate all of these special functions. This is because in this case the error functions have a real argument and we only have to calculate one or two exponential integrals, not all of them. These two advantages could result in a significant improvement of the required computational time respect to the original Ewald's method. Obviously, these advantages arise from the combination of both Kummer's transformation and Ewald's method.

### 2. The second one is using the Lerch transcendent and the polylogarithm.

These functions allow us to express the remaining part as a semi-closed form. As can be noted, the Lerch transcendent and the polylogarithm are defined as an infinite summation. In addition, these two functions are analogous, one for the first approach and the other one for the second approach in the extraction of terms in Kummer's transformation. The difference between them lies in the factor  $k_{x0}$  that appears in the denominator of the infinite sum.

When this factor is null, the definition of these functions become the same. We should take into account that the difference between both approaches is that in the first one we consider  $k_{x0}$  in the approximation of  $\gamma_m$  whereas in the second one we disregard  $k_{x0}$ .

On this basis, the two approaches become the same when  $k_{x0} = 0$ . As we have mentioned before, when the factor that differentiates the Lerch transcendent and the poylogarithm is null, the functions are the same. As might be expected, this occurs when  $k_{x0} = 0$ .

Thus, the approaches become the same when  $k_{x0} = 0$  as well as the Lerch transcendent and the polylogarithm become the same. This is because they are the same way to express in a semi-closed form the retained part of each approach.

## 3. The last one is using the summation by parts technique.

This transformation consists of accelerating the series on the basis of their oscillation behaviours. It allows us to express the remaining series as a sum of an analytical part plus a numerical but finite part. It is important to note that this technique has been outlined for the extraction of Q terms in both approaches.

The above conclusions will be proved through programming these techniques. Numerical results will be shown in Chapter 3.

## 1.2 Green's Functions of Parallel-Plate Waveguides

In parallel-plate waveguide, the spatial Green's functions can be formulated using the classical theory of images with respect to two perfect electric conductors. This theory implies that the actual system can be replaced by the equivalent system formed by the combination of the real and the introduced virtual sources (images) [1].

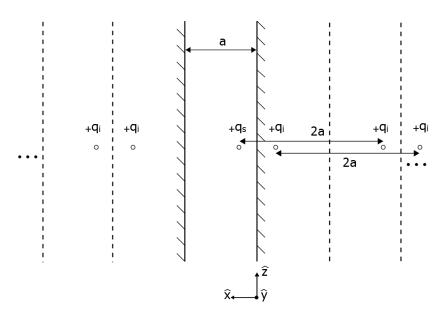
In this section, we first obtain the different components of the outstanding Green's functions involved in this problem from the general 2-D Green's function with 1-D periodicity. Once these components are formulated, we apply Kummer's transformation technique (Subsection 1.2.1) in order to accelerate their convergences.

To obtain the outstanding components of Green's functions it is advisable representing the possible scenarios in this problem. The Fig. 1.2(a) represents the combination of the actual source and its images when a magnetic charge is placed near the electric conductors. Being a magnetic charge, the images have the same sign as the actual source. This distribution is employed to evaluate the Green's function of the magnetic scalar potential  $G_W$ .

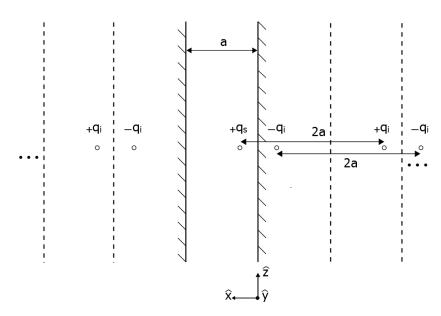
On the other hand, Fig. 1.2(b) represents the combination of the actual source and its images when an electric charge is placed near the electric conductors. Being an electric charge, the images alternate the positive and negative signs. This distribution is employed to evaluate the Green's function of the electric scalar potential  $G_V$ .

The Fig. 1.3 represents the combination of the actual source and its images when a magnetic current dipole  $\vec{m}_s$  is placed near the electric conductors in the x-direction (Fig. 1.3(a)), in the y-direction (Fig. 1.3(b)) and in the z-direction (Fig. 1.3(c)). Being a magnetic current dipole, the images change the sign or orientation when the actual source is in the x-direction. On the contrary, the images have the same sign as the actual source when the magnetic current dipole is in the y-direction and in the z-direction. These distributions are employed to calculate the dyadic components of the Green's function of the electric vector potential  $G_F^{xx}$ ,  $G_F^{yy}$  and  $G_F^{zz}$ , respectively.

Finally, the Fig. 1.4 represents the combination of the actual source and its images when an electric current dipole  $\vec{j}_s$  is placed near the electric conductors in the x-direction (Fig. 1.4(a)), in the y-direction (Fig. 1.4(b)) and in the z-direction (Fig. 1.4(c)). Being an electric current dipole, the images change the sign or orientation when the actual source is in the y-direction and in the z-direction. On the contrary, the images have the same sign as the actual source when the electric current dipole is in the x-direction. These distributions are employed to calculate the dyadic components of the Green's function of the magnetic vector potential  $G_A^{xx}$ ,  $G_A^{yy}$  and  $G_A^{zz}$ , respectively.

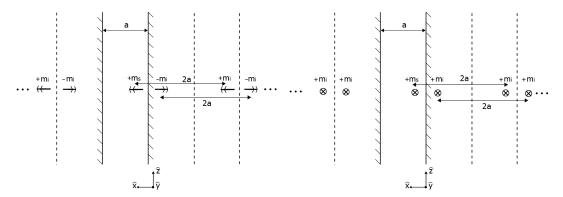


(a) Distribution of the actual magnetic charge  $q_s$  and its images  $q_i$  for a parellel-plate waveguide.

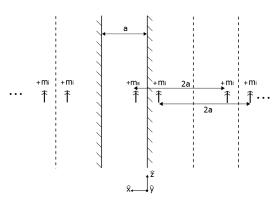


(b) Distribution of the actual electric charge  $q_s$  and its images  $q_i$  for a parellel-plate waveguide.

Figure 1.2: Distribution of the actual and virtual sources. The width of the parallel-plate waveguide in the x-direction is a and the images are distributed in pairs separated by a distance of 2a. It is satisfied that  $q_s = q_i$ .

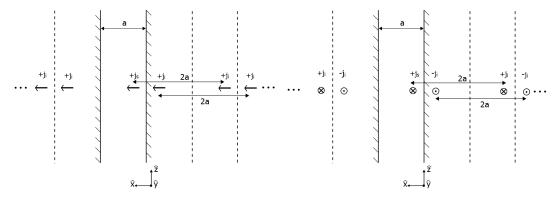


(a) Actual and virtual sources produced by a magnetic current dipole oriented in x-direction. Note that the following produced by a magnetic current dipole oriented in y-direction.

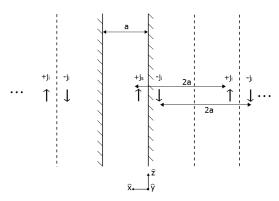


(c) Actual and virtual sources produced by a magnetic current dipole oriented in z-direction.

Figure 1.3: Distribution of the actual magnetic current dipole  $\vec{m}_s$  and its images  $\vec{m}_i$  for a parellel-plate waveguide. It is satisfied that  $m_s = m_i$ . The width of the waveguide in the x-direction is a and the images are distributed in pairs separated by a distance of 2a.



(a) Actual and virtual sources produced by an (b) Actual and virtual sources produced by an electelectric current dipole oriented in x-direction. tric current dipole oriented in y-direction.



(c) Actual and virtual sources produced by an electric current dipole oriented in z-direction.

Figure 1.4: Distribution of the actual electric current dipole  $\vec{j}_s$  and its images  $\vec{j}_i$  for a parellel-plate waveguide. It is satisfied that  $j_s = j_i$ . The width of the waveguide in the x-direction is a and the images are distributed in pairs separated by a distance of 2a.

If we define the series  $\widetilde{G}_{+}(\bar{r},\bar{r}')$  and  $\widetilde{G}_{-}(\bar{r},\bar{r}')$  as the basis of the Green's functions involved in parallel-plate waveguide problems, the most relevant components are expressed by the following spectral and spatial series

• Green's function of the magnetic scalar potential

$$G_W = \frac{1}{\mu_0} G_+(\bar{r}, \bar{r}') = \frac{1}{\mu_0} \tilde{G}_+(\bar{r}, \bar{r}')$$
 (1.159)

• Green's function of the electric scalar potential

$$G_V = \frac{1}{\epsilon_0} G_-(\bar{r}, \bar{r}') = \frac{1}{\epsilon_0} \widetilde{G}_-(\bar{r}, \bar{r}')$$
 (1.160)

- Dyadic components of Green's function of the electric vector potential
  - x-Dyadic component of Green's function of the electric vector potential

$$G_F^{xx} = \epsilon_0 G_-(\bar{r}, \bar{r}') = \epsilon_0 \widetilde{G}_-(\bar{r}, \bar{r}') \tag{1.161}$$

- y-Dyadic component of Green's function of the electric vector potential

$$G_F^{yy} = \epsilon_0 G_+(\bar{r}, \bar{r}') = \epsilon_0 \widetilde{G}_+(\bar{r}, \bar{r}') \tag{1.162}$$

- z-Dyadic component of Green's function of the electric vector potential

$$G_F^{zz} = \epsilon_0 G_+(\bar{r}, \bar{r}') = \epsilon_0 \widetilde{G}_+(\bar{r}, \bar{r}') \tag{1.163}$$

- Dyadic components of Green's function of the magnetic vector potential
  - x-Dyadic component of Green's function of the magnetic vector potential

$$G_A^{xx} = \mu_0 G_+(\bar{r}, \bar{r}') = \mu_0 \tilde{G}_+(\bar{r}, \bar{r}')$$
 (1.164)

- y-Dyadic component of Green's function of the magnetic vector potential

$$G_A^{yy} = \mu_0 G_-(\bar{r}, \bar{r}') = \mu_0 \widetilde{G}_-(\bar{r}, \bar{r}')$$
 (1.165)

- z-Dyadic component of Green's function of the magnetic vector potential

$$G_A^{zz} = \mu_0 G_-(\bar{r}, \bar{r}') = \mu_0 \widetilde{G}_-(\bar{r}, \bar{r}')$$
 (1.166)

where the series  $\widetilde{G}_{+}(\bar{r}, \bar{r}')$  and  $\widetilde{G}_{-}(\bar{r}, \bar{r}')$  are going to be formulated using the general spatial and spectral 2-D Green's functions with 1-D periodicity. The spatial general Green's function  $G(\bar{r}, \bar{r}')$  is given by

$$G(\bar{r}, \bar{r}') = \frac{1}{4j} \sum_{m=-\infty}^{+\infty} H_0^{(2)}(kR_m) e^{-jk_{x0}md}$$
(1.167)

where 
$$R_m = \sqrt{(x - x' - md)^2 + (z - z')^2}$$
.

On the other hand, the spectral general Green's function  $\widetilde{G}(\bar{r}, \bar{r}')$  is given by

$$\widetilde{G}(\bar{r}, \bar{r}') = \frac{1}{2d} \sum_{m=-\infty}^{+\infty} \frac{e^{-\gamma_m |z-z'|}}{\gamma_m} e^{-jk_{xm}(x-x')}$$
(1.168)

where 
$$k_{xm} = k_{x0} + \frac{2\pi m}{d} = k \sin(\theta) + \frac{2\pi m}{d}$$
 and  $\gamma_m = \sqrt{k_{xm}^2 - k^2}$ .

The series  $\widetilde{G}_{+}(\overline{r},\overline{r}')$  and  $\widetilde{G}_{-}(\overline{r},\overline{r}')$  are composed by the combination of two general 1-D periodic Green's functions with different sources. In the first one the source is (x',z') and in the second one is (-x',z'). In both cases, the period is d=2a and  $\theta=0^{\circ}$  due to the direction of the incident wave on the array. We use the following notation for these two sources

$$R_{m+} = \sqrt{(x - x' - 2am)^2 + (z - z')^2}$$
(1.169)

$$R_{m-} = \sqrt{(x+x'-2am)^2 + (z-z')^2}$$
(1.170)

In the case of the function composed by the addition of the images, the spatial Green's function  $G_{+}(\bar{r}, \bar{r}')$  can be expressed as the sum of two general periodic Green's functions as

$$G_{+}(\bar{r},\bar{r}') = \frac{1}{4j} \sum_{m=-\infty}^{+\infty} H_{0}^{(2)}(kR_{m+}) e^{-jk_{xx} 2 dm} + \frac{1}{4j} \sum_{m=-\infty}^{\infty} H_{0}^{(2)}(kR_{m-}) e^{-jk_{xx} 2 dm}$$

$$= \sum_{m=-\infty}^{+\infty} \left[ \frac{1}{4j} H_{0}^{(2)}(k\sqrt{(x-x'-2am)^{2}+(z-z')^{2}}) + \frac{1}{4j} H_{0}^{(2)}(k\sqrt{(x+x'-2am)^{2}+(z-z')^{2}}) \right]$$

$$(1.171)$$

Using Poisson's formula, its alternative spectral  $\widetilde{G}_{+}(\bar{r}, \bar{r}')$  series is obtained

$$\widetilde{G}_{+}(\bar{r},\bar{r}') = \frac{1}{4a} \sum_{m=-\infty}^{+\infty} \left[ \frac{e^{-\gamma_{m}|z-z'|}}{\gamma_{m}} e^{-jk_{x}(x-x')} + \frac{e^{-\gamma_{m}|z-z'|}}{\gamma_{m}} e^{-jk_{x}(x+x')} \right]$$

$$= \frac{1}{4a} \sum_{m=-\infty}^{+\infty} \frac{e^{-\gamma_{m}|z-z'|}}{\gamma_{m}} \left[ e^{-jk_{x}(x-x')} + e^{-jk_{x}(x+x')} \right]$$
(1.172)

where  $k_x = k_{x0} + \frac{2\pi m}{d} = \frac{\pi m}{a}$  and therefore  $\gamma_m = \sqrt{k_x^2 - k^2} = \sqrt{\left(\frac{\pi m}{a}\right)^2 - k^2}$ . This series can be rewritten by grouping terms as

$$\widetilde{G}_{+}(\bar{r}, \bar{r}') = \frac{1}{4a} \sum_{m=-\infty}^{+\infty} \frac{e^{-\gamma_{m}|z-z'|}}{\gamma_{m}} \left[ e^{-jk_{x}x} e^{jk_{x}x'} + e^{-jk_{x}x} e^{-jk_{x}x'} \right] 
= \frac{1}{4a} \sum_{m=-\infty}^{+\infty} \frac{e^{-\gamma_{m}|z-z'|}}{\gamma_{m}} e^{-jk_{x}x} \frac{2\left[ e^{jk_{x}x'} + e^{-jk_{x}x'} \right]}{2} 
= \frac{1}{4a} \sum_{m=-\infty}^{+\infty} 2\frac{e^{-\gamma_{m}|z-z'|}}{\gamma_{m}} e^{-jk_{x}x} \cos(k_{x}x')$$
(1.173)

Due to the fact that this is an even function with respect to  $k_x$ , the exponential  $e^{-jk_xx}$  evaluated in m between  $(-\infty, +\infty)$  can be written as  $2\epsilon_m \cos(k_x x)$  evaluated in m between  $(0, +\infty)$ . For more details see Appendix A.2.

According to this,  $\widetilde{G}_{+}(\bar{r},\bar{r}')$  is given by

$$\widetilde{G}_{+}(\bar{r},\bar{r}') = \frac{\epsilon_m}{4a} \sum_{m=0}^{+\infty} 2 \cdot 2 \frac{e^{-\gamma_m|z-z'|}}{\gamma_m} \cos(k_x x) \cos(k_x x')$$

$$= \frac{\epsilon_m}{a} \sum_{m=0}^{+\infty} \frac{e^{-\gamma_m|z-z'|}}{\gamma_m} \cos(k_x x) \cos(k_x x')$$
(1.174)

where  $\epsilon_m = 1/2$  if m = 0 or  $\epsilon_m = 1$  if  $m \neq 0$  (see Appendix A.2).

On the other hand, in the case of the functions composed by the subtraction of the images, we have the sum of two periodic Green's functions with different sources and additionally, one of them is inverted. Thus, the spatial series  $G_{-}(\bar{r}, \bar{r}')$  in this case is

$$G_{-}(\bar{r}, \bar{r}') = \frac{1}{4j} \sum_{m=-\infty}^{+\infty} H_{0}^{(2)}(kR_{m+}) e^{-jk_{x0}2am} - \frac{1}{4j} \sum_{m=-\infty}^{\infty} H_{0}^{(2)}(kR_{m-}) e^{-jk_{x0}2am}$$

$$= \sum_{m=-\infty}^{+\infty} \left[ \frac{1}{4j} H_{0}^{(2)}(k\sqrt{(x-x'-2am)^{2}+(z-z')^{2}}) - \frac{1}{4j} H_{0}^{(2)}(k\sqrt{(x+x'-2am)^{2}+(z-z')^{2}}) \right]$$

$$(1.175)$$

The alternative spectral series  $\widetilde{G}_{-}(\bar{r},\bar{r}')$  given by the application of Poisson's formula is

$$\widetilde{G}_{-}(\bar{r}, \bar{r}') = \frac{1}{4a} \sum_{m=-\infty}^{+\infty} \left[ \frac{e^{-\gamma_m|z-z'|}}{\gamma_m} e^{-jk_x(x-x')} - \frac{e^{-\gamma_m|z-z'|}}{\gamma_m} e^{-jk_x(x+x')} \right] 
= \frac{1}{4a} \sum_{m=-\infty}^{+\infty} \frac{e^{-\gamma_m|z-z'|}}{\gamma_m} \left[ e^{-jk_x(x-x')} - e^{-jk_x(x+x')} \right]$$
(1.176)

This series can be rewritten by grouping terms as

$$\widetilde{G}_{-}(\overline{r}, \overline{r}') = \frac{1}{4a} \sum_{m=-\infty}^{+\infty} \frac{e^{-\gamma_m|z-z'|}}{\gamma_m} \left[ e^{-jk_x x} e^{jk_x x'} - e^{-jk_x x} e^{-jk_x x'} \right] 
= \frac{1}{4a} \sum_{m=-\infty}^{+\infty} \frac{e^{-\gamma_m|z-z'|}}{\gamma_m} e^{-jk_x x} \frac{2j \left[ e^{jk_x x'} - e^{-jk_x x'} \right]}{2j} 
= \frac{1}{4a} \sum_{m=-\infty}^{+\infty} 2j \frac{e^{-\gamma_m|z-z'|}}{\gamma_m} e^{-jk_x x} \sin(k_x x')$$
(1.177)

Due to the fact that this is an odd function with respect to  $k_x$ , the exponential  $e^{-jk_xx}$  evaluated in m between  $(-\infty, +\infty)$  can be written as  $-2j\sin(k_xx)$  evaluated in m between  $(0, +\infty)$ . For more details see Appendix A.2. According to this,  $\widetilde{G}_+(\bar{r}, \bar{r}')$  is given by

$$\widetilde{G}_{-}(\bar{r}, \bar{r}') = \frac{1}{4a} \sum_{m=1}^{+\infty} 2j \cdot (-2j) \frac{e^{-\gamma_m|z-z'|}}{\gamma_m} \sin(k_x x) \sin(k_x x')$$

$$= \frac{1}{a} \sum_{m=1}^{+\infty} \frac{e^{-\gamma_m|z-z'|}}{\gamma_m} \sin(k_x x) \sin(k_x x')$$
(1.178)

where  $\gamma_m = \sqrt{k_x^2 - k^2} = \sqrt{\left(\frac{\pi m}{a}\right)^2 - k^2}$ . As the series  $\widetilde{G}_+(\bar{r}, \bar{r}')$  and  $\widetilde{G}_-(\bar{r}, \bar{r}')$  are slowly convergent, it is important to apply some acceleration technique to improve their convergences. For this reason, they are our starting point in the following developments.

#### 1.2.1 Application of Kummer's Transformation

Once we have obtained the functions involved in parallel-plate waveguide problems, the transformations applied in general Green's functions will be also applied in this case. As in the general case of 2-D Green's functions with 1-D periodicity, when evaluating Green's functions of the magnetic and electric scalar and vector potentials, it is also necessary to accelerate these functions [21]. The same techniques can be used in these problems and, for instance, Ewald's method was proposed in [22]. In [20], Green's functions for parallel-plate waveguide have been accelerated using Kummer's transformation.

The difference in this case with respect to the general Green's function is that  $k_{x0} = 0$  due to  $\theta = 0^{\circ}$ . As we have mentioned before, if  $k_{x0} = 0$ , the two different approaches considered in Kummer's transformation become the same and therefore we can take the advantages of each approach. All the proposed methods in the previous section can be also particularized for  $k_{x0} = 0$  to sum the remaining part.

In particular, in this section we continue applying the spectral Kummer's transformation through the extraction of one, two, three and Q terms to the spectral parallel-plate Green's functions. Specifically, we focus on summing the asymptotic terms through polylogarithmic functions. Numerical results will be shown in Chapter 3.

#### • Extraction of one term.

The procedure to be followed is the same as in the previous section. First, we start with the series  $\widetilde{G}_{+}(\bar{r},\bar{r}')$ .

$$\widetilde{G}_{+}(\bar{r}, \bar{r}') = \frac{1}{a} \sum_{m=0}^{+\infty} \frac{e^{-\gamma_{m}|z-z'|}}{\gamma_{m}} \cos(k_{x}x) \cos(k_{x}x')$$

$$= \widetilde{G}_{+0}(\bar{r}, \bar{r}') + \frac{1}{a} \sum_{m=1}^{+\infty} \cos(k_{x}x) \cos(k_{x}x') \frac{e^{-\gamma_{m}|z-z'|}}{\gamma_{m}}$$

$$= \widetilde{G}_{+0}(\bar{r}, \bar{r}') + \frac{1}{a} \sum_{m=1}^{+\infty} \cos(k_{x}x) \cos(k_{x}x') \left(\frac{e^{-\gamma_{m}|z-z'|}}{\gamma_{m}} - \frac{e^{-\frac{\pi m}{a}|z-z'|}}{\frac{\pi m}{a}}\right)$$

$$+ \underbrace{\frac{1}{a} \sum_{m=1}^{+\infty} \cos(k_{x}x) \cos(k_{x}x') \frac{e^{-\frac{\pi m}{a}|z-z'|}}{\frac{\pi m}{a}}}_{\widetilde{G}_{e+}} \tag{1.179}$$

 $\widetilde{G}_{+0}(\bar{r},\bar{r}')$  is the series in m=0 where we do not apply the extraction. Thus, the series  $\widetilde{G}_{e+}$  has to be efficiently summed

$$\widetilde{G}_{e+} = \frac{1}{a} \sum_{m=1}^{+\infty} \cos(k_x x) \cos(k_x x') \frac{e^{-\frac{\pi m}{a}|z-z'|}}{\frac{\pi m}{a}}$$
 (1.180)

Applying the following trigonometric identity

$$\cos(A)\cos(B) = \frac{\cos(A-B) + \cos(A+B)}{2}$$
 (1.181)

 $\widetilde{G}_{e+}$  can be expressed as follows

$$\widetilde{G}_{e+} = \frac{1}{2\pi} \sum_{m=1}^{+\infty} \left[ \cos(k_x(x - x')) + \cos(k_x(x + x')) \right] \frac{e^{-\frac{\pi m}{a}|z - z'|}}{m}$$

$$= \frac{1}{2\pi} \sum_{m=1}^{+\infty} \cos(k_x(x - x')) \frac{e^{-\frac{\pi m}{a}|z - z'|}}{m} + \frac{1}{2\pi} \sum_{m=1}^{+\infty} \cos(k_x(x + x')) \frac{e^{-\frac{\pi m}{a}|z - z'|}}{m}$$
(1.182)

Since  $k_x$  is defined as  $k_x = \frac{\pi m}{a}$ ,  $\widetilde{G}_{e+}$  is

$$\widetilde{G}_{e+} = \frac{1}{2\pi} \sum_{m=1}^{+\infty} \cos\left(\frac{\pi m}{a}(x - x')\right) \frac{e^{-\frac{\pi m}{a}|z - z'|}}{m} + \frac{1}{2\pi} \sum_{m=1}^{+\infty} \cos\left(\frac{\pi m}{a}(x + x')\right) \frac{e^{-\frac{\pi m}{a}|z - z'|}}{m}$$
(1.183)

In the knowledge that the summations in (1.183) can be analytically expressed (see Appendix A.3) as follows

$$\sum_{m=1}^{+\infty} \frac{\cos(nx)}{n} e^{-nz} = -\mathbb{R}e \left\{ \ln \left[ 1 - e^{(-z+jx)} \right] \right\}$$
 (1.184)

 $\widetilde{G}_{e+}$  can be written as

$$\widetilde{G}_{e+} = \frac{1}{2\pi} \left[ -\mathbb{R}e \left\{ \ln \left[ 1 - e^{-\frac{\pi}{a}[|z - z'| - j(x - x')]} \right] \right\} - \mathbb{R}e \left\{ \ln \left[ 1 - e^{-\frac{\pi}{a}[|z - z'| - j(x + x')]} \right] \right\} \right] \\
= \frac{-1}{2\pi} \left[ \mathbb{R}e \left\{ \ln \left[ \left( 1 - e^{-\frac{\pi}{a}[|z - z'| - j(x - x')]} \right) \left( 1 - e^{-\frac{\pi}{a}[|z - z'| - j(x + x')]} \right) \right] \right\} \right] \tag{1.185}$$

Now, we continue with series  $\widetilde{G}_{-}(\bar{r},\bar{r}')$ .

$$\widetilde{G}_{-}(\bar{r}, \bar{r}') = \frac{1}{a} \sum_{m=1}^{+\infty} \frac{e^{-\gamma_m|z-z'|}}{\gamma_m} \sin(k_x x) \sin(k_x x')$$
 (1.186)

Applying Kummer's transformation

$$\widetilde{G}_{-}(\overline{r}, \overline{r}') = \frac{1}{a} \sum_{m=1}^{+\infty} \frac{e^{-\gamma_m|z-z'|}}{\gamma_m} \sin(k_x x) \sin(k_x x') 
= \frac{1}{a} \sum_{m=1}^{+\infty} \sin(k_x x) \sin(k_x x') \left( \frac{e^{-\gamma_m|z-z'|}}{\gamma_m} - \frac{e^{-\frac{\pi m}{a}|z-z'|}}{\frac{\pi m}{a}} \right) 
+ \underbrace{\frac{1}{a} \sum_{m=1}^{+\infty} \sin(k_x x) \sin(k_x x') \frac{e^{-\frac{\pi m}{a}|z-z'|}}{\frac{\pi m}{a}}}_{\widetilde{G}_{e-}} \tag{1.187}$$

Where we have to sum  $\widetilde{G}_{e-}$  efficiently

$$\widetilde{G}_{e-} = \frac{1}{a} \sum_{m=1}^{+\infty} \sin(k_x x) \sin(k_x x) \frac{e^{-\frac{\pi m}{a}|z-z'|}}{\frac{\pi m}{a}}$$
(1.188)

Using the following trigonometric identity

$$\sin(A)\sin(B) = \frac{\cos(A-B) - \cos(A+B)}{2}$$
 (1.189)

 $\widetilde{G}_{e-}$  can be expressed as follows

$$\widetilde{G}_{e-} = \frac{1}{2\pi} \sum_{m=1}^{+\infty} \left[ \cos(k_x(x - x')) - \cos(k_x(x + x')) \right] \frac{e^{-\frac{\pi m}{a}|z - z'|}}{m}$$

$$= \frac{1}{2\pi} \sum_{m=1}^{+\infty} \cos(k_x(x - x')) \frac{e^{-\frac{\pi m}{a}|z - z'|}}{m} - \frac{1}{2\pi} \sum_{m=1}^{+\infty} \cos(k_x(x + x')) \frac{e^{-\frac{\pi m}{a}|z - z'|}}{m}$$
(1.190)

where  $k_x = \frac{\pi m}{a}$  and therefore

$$\widetilde{G}_{e-} = \frac{1}{2\pi} \sum_{m=1}^{+\infty} \cos\left(\frac{\pi m}{a}(x - x')\right) \frac{e^{-\frac{\pi m}{a}|z - z'|}}{m} - \frac{1}{2\pi} \sum_{m=1}^{+\infty} \cos\left(\frac{\pi m}{a}(x + x')\right) \frac{e^{-\frac{\pi m}{a}|z - z'|}}{m}$$
(1.191)

Using the relation proved in Appendix A.3 and given in (1.184),  $\widetilde{G}_{e-}$  can be written as

$$\widetilde{G}_{e-} = \frac{1}{2\pi} \left[ -\mathbb{R}e \left\{ \ln \left[ 1 - e^{-\frac{\pi}{a}[|z-z'|-j(x-x')]} \right] \right\} + \mathbb{R}e \left\{ \ln \left[ 1 - e^{-\frac{\pi}{a}[|z-z'|-j(x+x')]} \right] \right\} \right] \\
= \frac{1}{2\pi} \left[ \mathbb{R}e \left\{ \ln \left( \frac{1 - e^{-\frac{\pi}{a}[|z-z'|-j(x-x')]}}{1 - e^{-\frac{\pi}{a}[|z-z'|-j(x-x')]}} \right) \right\} \right] \tag{1.192}$$

Through Kummer's transformation we have been able to accelerate the convergence of the spectral series involved in parallel-plate problems by the extraction of one term and the analytical sum of this one.

#### • Extraction of two terms.

In this part we are interested in the extraction of one more term in order to accelerate even more the convergence of these functions. The disadvantage is that the following retained term is not analytical. Nevertheless, it is rapidly convergent and its convergence is independent of the frequency (semi-static).

We are looking for the asymptotic terms of the part which is involved in the convergence of the series

$$\frac{e^{-\gamma_m|z-z'|}}{\gamma_m} \tag{1.193}$$

Using Kummer's transformation proof in [11] the asymptotic expansion when we extract two terms is

$$\widetilde{G}_m = \left| \frac{d}{2\pi m} - \frac{k_{x0}d^2}{(2\pi m)^2} \right| e^{-\left| \frac{2\pi m}{d} + k_{x0} \right| |z - z'|}$$
(1.194)

Particularizing for the case of parallel-plate waveguides, d=2a and  $\theta=0^{\circ} \to k_{x0}=k\sin(\theta)=0$ ,  $\widetilde{G}_m$  is

$$\widetilde{G}_m = \frac{e^{-\frac{\pi m}{a}|z-z'|}}{\frac{\pi m}{a}} \tag{1.195}$$

As can be seen, it is the same as the term retained in (1.179) and therefore we do not improve the convergence. According to the analysis done in [11] about the particular case of  $\theta = 0^{\circ}$ , the retained terms that contain the factor  $k_{x0}$  are cancelled and therefore there is no improvement when we extract these terms.

Thus, in this case there is no improvement with the extraction of the second term in the general Kummer's transformation due to the cancellation of the new term because of  $\theta = 0$ .

Even so, we can apply here the extraction of the terms explained in [17, 18] and reviewed in the subsection 1.1.5. Following this procedure, the asymptotic expansion when we extract two terms in general case is

$$\widetilde{G}_m = \left| \frac{d}{2\pi m} + \frac{k^2 d^2 |z - z'|}{2(2\pi m)^2} - \frac{k_{x0} d^2}{(2\pi m)^2} \right| e^{-\left|\frac{2\pi m}{d} + k_{x0}\right||z - z'|}$$
(1.196)

In the case of parallel-plate waveguide, d = 2a and  $k_{x0} = k \sin(\theta) = 0$  because  $\theta = 0$  so  $\widetilde{G}_m$  is given by this second order approximation

$$\widetilde{G}_m = \left| \frac{a}{\pi m} + \frac{k^2 a^2 |z - z'|}{2(\pi m)^2} \right| e^{-\frac{\pi |m|}{a} |z - z'|}$$
(1.197)

Based on this, the spectral Kummer's transformation in Green's functions of parallelplates waveguide can be applied.

First, we start with the series  $\widetilde{G}_{+}(\bar{r}, \bar{r}')$ .

$$\widetilde{G}_{+}(\bar{r}, \bar{r}') = \frac{1}{a} \sum_{m=0}^{+\infty} \frac{e^{-\gamma_{m}|z-z'|}}{\gamma_{m}} \cos(k_{x}x) \cos(k_{x}x')$$

$$= \widetilde{G}_{+0}(\bar{r}, \bar{r}') + \frac{1}{a} \sum_{m=1}^{+\infty} \cos(k_{x}x) \cos(k_{x}x') \frac{e^{-\gamma_{m}|z-z'|}}{\gamma_{m}}$$

$$= \widetilde{G}_{+0}(\bar{r}, \bar{r}') + \frac{1}{a} \sum_{m=1}^{+\infty} \cos(k_{x}x) \cos(k_{x}x') \left[ \frac{e^{-\gamma_{m}|z-z'|}}{\gamma_{m}} - \left( \frac{a}{\pi m} + \frac{k^{2} a^{2} |z-z'|}{2(\pi m)^{2}} \right) \right]$$

$$e^{-\frac{\pi m}{a}|z-z'|} + \underbrace{\frac{1}{a} \sum_{m=1}^{+\infty} \cos(k_{x}x) \cos(k_{x}x') \left( \frac{a}{\pi m} + \frac{k^{2} a^{2} |z-z'|}{2(\pi m)^{2}} \right) e^{-\frac{\pi m}{a}|z-z'|}}_{\widetilde{G}_{e+}} \tag{1.198}$$

The series  $\widetilde{G}_{e+}$  has to be efficiently summed

$$\widetilde{G}_{e+} = \frac{1}{a} \sum_{m=1}^{+\infty} \cos(k_x x) \cos(k_x x') \left( \frac{a}{\pi m} + \frac{k^2 a^2 |z - z'|}{2(\pi m)^2} \right) e^{-\frac{\pi m}{a} |z - z'|}$$

$$= \frac{1}{a} \sum_{m=1}^{+\infty} \cos(k_x x) \cos(k_x x') \left( \frac{a}{\pi m} \right) e^{-\frac{\pi m}{a} |z - z'|}$$

$$+ \frac{1}{a} \sum_{m=1}^{+\infty} \cos(k_x x) \cos(k_x x') \left( \frac{k^2 a^2 |z - z'|}{2(\pi m)^2} \right) e^{-\frac{\pi m}{a} |z - z'|}$$
(1.199)

The first series  $\widetilde{G}_{e1+}$  is summed in the previous part (One term: 1.185)

$$\widetilde{G}_{e1+} = \frac{-1}{2\pi} \left[ \mathbb{R}e \left\{ \ln \left[ \left( 1 - e^{-\frac{\pi}{a} [|z - z'| - j(x - x')]} \right) \left( 1 - e^{-\frac{\pi}{a} [|z - z'| - j(x + x')]} \right) \right] \right\} \right]$$
(1.200)

The second series  $\widetilde{G}_{e2+}$  is the subject of study in this part. Using the trigonometric identity written in (1.181),  $\widetilde{G}_{e2+}$  can be summed as follows

$$\widetilde{G}_{e2+} = \frac{1}{a} \sum_{m=1}^{+\infty} \left( \frac{k^2 a^2 |z - z'|}{2(\pi m)^2} \right) \frac{1}{2} \left[ \cos(k_x(x - x')) + \cos(k_x(x + x')) \right] e^{-\frac{\pi m}{a}|z - z'|}$$

$$= \frac{k^2 a |z - z'|}{(2\pi)^2} \sum_{m=1}^{+\infty} \frac{e^{-\frac{\pi m}{a}|z - z'|}}{m^2} \left[ \cos(k_x(x - x')) + \cos(k_x(x + x')) \right]$$

$$= \frac{k^2 a |z - z'|}{(2\pi)^2} \sum_{m=1}^{+\infty} \cos(k_x(x - x')) \frac{e^{-\frac{\pi m}{a}|z - z'|}}{m^2}$$

$$+ \frac{k^2 a |z - z'|}{(2\pi)^2} \sum_{m=1}^{+\infty} \cos(k_x(x + x')) \frac{e^{-\frac{\pi m}{a}|z - z'|}}{m^2}$$

$$(1.201)$$

where  $k_x = \frac{\pi m}{a}$  and therefore

$$\widetilde{G}_{e2+} = \frac{k^2 a |z - z'|}{(2\pi)^2} \sum_{m=1}^{+\infty} \cos\left(\frac{\pi m}{a}(x - x')\right) \frac{e^{-\frac{\pi m}{a}|z - z'|}}{m^2} + \frac{k^2 a |z - z'|}{(2\pi)^2} \sum_{m=1}^{+\infty} \cos\left(\frac{\pi m}{a}(x + x')\right) \frac{e^{-\frac{\pi m}{a}|z - z'|}}{m^2}$$
(1.202)

In the knowledge that the summations in (1.202) can be expressed in a semi-closed form (see Appendix A.3) as follows

$$\sum_{m=1}^{+\infty} \frac{e^{-nz}}{n^2} \cos(nx) = \mathbb{R}e\left\{ \text{Li}_2\left[e^{(-z+jx)}\right] \right\}$$
 (1.203)

where  $\text{Li}_2(z)$  is the second order polylogarithm of the argument z,  $\widetilde{G}_{e2+}$  can be written as

$$\widetilde{G}_{e2+} = \frac{k^2 a |z - z'|}{(2\pi)^2} \left[ \mathbb{R}e \left\{ \operatorname{Li}_2 \left[ e^{-\frac{\pi}{a}[|z - z'| - j(x - x')]} \right] \right\} + \mathbb{R}e \left\{ \operatorname{Li}_2 \left[ e^{-\frac{\pi}{a}[|z - z'| - j(x + x')]} \right] \right\} \right]$$
(1.204)

Next, we continue applying the same procedure with the series  $\widetilde{G}_{-}(\bar{r},\bar{r}')$ .

$$\widetilde{G}_{-}(\overline{r}, \overline{r}') = \frac{1}{a} \sum_{m=1}^{+\infty} \sin(k_{x}x) \sin(k_{x}x') \frac{e^{-\gamma_{m}|z-z'|}}{\gamma_{m}} 
= \frac{1}{a} \sum_{m=1}^{+\infty} \sin(k_{x}x) \sin(k_{x}x') \left( \frac{e^{-\gamma_{m}|z-z'|}}{\gamma_{m}} - \left( \frac{a}{\pi m} + \frac{k^{2} a^{2} |z-z'|}{2(\pi m)^{2}} \right) e^{-\frac{\pi m}{a}|z-z'|} \right) 
+ \underbrace{\frac{1}{a} \sum_{m=1}^{+\infty} \sin(k_{x}x) \sin(k_{x}x') \left( \frac{a}{\pi m} + \frac{k^{2} a^{2} |z-z'|}{2(\pi m)^{2}} \right) e^{-\frac{\pi m}{a}|z-z'|}}_{\widetilde{G}_{e-}} \tag{1.205}$$

The asymptotic part that has to be summed is

$$\widetilde{G}_{e-} = \frac{1}{a} \sum_{m=1}^{+\infty} \sin(k_x x) \sin(k_x x') \left( \frac{a}{\pi m} + \frac{k^2 a^2 |z - z'|}{2(\pi m)^2} \right) e^{-\frac{\pi m}{a} |z - z'|}$$

$$= \frac{1}{a} \sum_{m=1}^{+\infty} \sin(k_x x) \sin(k_x x') \left( \frac{a}{\pi m} \right) e^{-\frac{\pi m}{a} |z - z'|}$$

$$+ \frac{1}{a} \sum_{m=1}^{+\infty} \sin(k_x x) \sin(k_x x') \left( \frac{k^2 a^2 |z - z'|}{2(\pi m)^2} \right) e^{-\frac{\pi m}{a} |z - z'|}$$
(1.206)

The first series  $\widetilde{G}_{e1-}$  is summed in the previous part (One term: 1.192)

$$\widetilde{G}_{e1-} = \frac{1}{2\pi} \left[ \mathbb{R}e \left\{ \ln \left( \frac{1 - e^{-\frac{\pi}{a}[|z - z'| - j(x + x')]}}{1 - e^{-\frac{\pi}{a}[|z - z'| - j(x - x')]}} \right) \right\} \right]$$
(1.207)

The second series  $\widetilde{G}_{e2-}$  is the subject of study in this part. Using the trigonometric identity defined in (1.189),  $\widetilde{G}_{e2-}$  can be expressed as follows

$$\widetilde{G}_{e2-} = \frac{1}{a} \sum_{m=1}^{+\infty} \left( \frac{k^2 a^2 |z - z'|}{2(\pi m)^2} \right) \frac{1}{2} \left[ \cos(k_x(x - x')) - \cos(k_x(x + x')) \right] e^{-\frac{\pi m}{a}|z - z'|} \\
= \frac{k^2 a |z - z'|}{(2\pi)^2} \sum_{m=1}^{+\infty} \frac{e^{-\frac{\pi m}{a}|z - z'|}}{m^2} \left[ \cos(k_x(x - x')) - \cos(k_x(x + x')) \right] \\
= \frac{k^2 a |z - z'|}{(2\pi)^2} \sum_{m=1}^{+\infty} \cos(k_x(x - x')) \frac{e^{-\frac{\pi m}{a}|z - z'|}}{m^2} \\
- \frac{k^2 a |z - z'|}{(2\pi)^2} \sum_{m=1}^{+\infty} \cos(k_x(x + x')) \frac{e^{-\frac{\pi m}{a}|z - z'|}}{m^2} \tag{1.208}$$

where  $k_x = \frac{\pi m}{a}$  and therefore

$$\widetilde{G}_{e2-} = \frac{k^2 a |z - z'|}{(2\pi)^2} \sum_{m=1}^{+\infty} \cos\left(\frac{\pi m}{a}(x - x')\right) \frac{e^{-\frac{\pi m}{a}|z - z'|}}{m^2} - \frac{k^2 a |z - z'|}{(2\pi)^2} \sum_{m=1}^{+\infty} \cos\left(\frac{\pi m}{a}(x + x')\right) \frac{e^{-\frac{\pi m}{a}|z - z'|}}{m^2}$$
(1.209)

Assuming that the summations in (1.209) can be expressed in a semi-closed form (see Appendix A.3) by using (1.203),  $\tilde{G}_{e2-}$  can be written as

$$\widetilde{G}_{e2-} = \frac{k^2 a |z - z'|}{(2\pi)^2} \left[ \mathbb{R}e \left\{ \operatorname{Li}_2 \left[ e^{-\frac{\pi}{a}[|z - z'| - j(x - x')]} \right] \right\} - \mathbb{R}e \left\{ \operatorname{Li}_2 \left[ e^{-\frac{\pi}{a}[|z - z'| - j(x + x')]} \right] \right\} \right]$$
(1.210)

This can be an alternative to improve the convergence of Green's functions involved in parallel-plate waveguide problems using only the second order approximation in Kummer's transformation. Nevertheless, these new terms will be not very significant when the observation point is near the source. The acceleration of the Green's functions in this particular case is the most interesting problem for us due to the fact that they are slowly convergent. For this reason, the new terms that appear not only here but also in this alternative extraction are negligible, as discussed in 1.1.5.

#### • Extraction of three terms.

To improve the convergence with respect to one retained term, we have to follow the development done in [11] when we extract three terms. The asymptotic term in general spectral Green's function is given by - the option A:  $k_{xm}$  - approach

$$\widetilde{G}_m = \left(\frac{1}{|k_{xm}|} + \frac{k^2}{2|k_{xm}|^3}\right) e^{-|k_{xm}||z-z'|}$$
(1.211)

– the option B:  $\left(\frac{2\pi m}{d}\right)$  - approach

$$\widetilde{G}_m = \left| \frac{d}{2\pi m} - \frac{k_{x0}d^2}{(2\pi m)^2} + \frac{(k^2 - k_{x0}^2)d^3}{2(2\pi m)^3} \right| e^{-\left|\frac{2\pi m}{d} + k_{x0}\right||z - z'|}$$
(1.212)

Particularizing for the case of parallel-plate waveguide, d=2a and  $\theta=0^{\circ} \to k_{x0}=k\sin(\theta)=0$ , the two previous alternatives become the same and  $\widetilde{G}_m$  is

$$\widetilde{G}_m = \left| \frac{a}{\pi m} + \frac{k^2 a^3}{2(\pi m)^3} \right| e^{-\frac{\pi |m|}{a}|z-z'|}$$
 (1.213)

Therefore, we can apply Kummer's transformation to the spectral parallel-plate Green's functions. First, we start with the series  $\widetilde{G}_{+}(\bar{r},\bar{r}')$ .

$$\widetilde{G}_{+}(\bar{r}, \bar{r}') = \frac{1}{a} \sum_{m=0}^{+\infty} \frac{e^{-\gamma_{m}|z-z'|}}{\gamma_{m}} \cos(k_{x}x) \cos(k_{x}x')$$

$$= \widetilde{G}_{+0}(\bar{r}, \bar{r}') + \frac{1}{a} \sum_{m=1}^{+\infty} \cos(k_{x}x) \cos(k_{x}x') \frac{e^{-\gamma_{m}|z-z'|}}{\gamma_{m}}$$

$$= \widetilde{G}_{+0}(\bar{r}, \bar{r}') + \frac{1}{a} \sum_{m=1}^{+\infty} \cos(k_{x}x) \cos(k_{x}x') \left(\frac{e^{-\gamma_{m}|z-z'|}}{\gamma_{m}} - \left(\frac{a}{\pi m} + \frac{k^{2}a^{3}}{2(\pi m)^{3}}\right) e^{-\frac{\pi m}{a}|z-z'|}\right)$$

$$+ \underbrace{\frac{1}{a} \sum_{m=1}^{+\infty} \cos(k_{x}x) \cos(k_{x}x') \left(\frac{a}{\pi m} + \frac{k^{2}a^{3}}{2(\pi m)^{3}}\right) e^{-\frac{\pi m}{a}|z-z'|}}_{\widetilde{G}_{e+}} \tag{1.214}$$

The asymptotic part that has to be summed is

$$\widetilde{G}_{e+} = \frac{1}{a} \sum_{m=1}^{+\infty} \cos(k_x x) \cos(k_x x') \left( \frac{a}{\pi m} + \frac{k^2 a^3}{2(\pi m)^3} \right) e^{-\frac{\pi m}{a}|z-z'|}$$

$$= \frac{1}{a} \sum_{m=1}^{+\infty} \cos(k_x x) \cos(k_x x') \left( \frac{a}{\pi m} \right) e^{-\frac{\pi m}{a}|z-z'|}$$

$$+ \frac{1}{a} \sum_{m=1}^{+\infty} \cos(k_x x) \cos(k_x x') \left( \frac{k^2 a^3}{2(\pi m)^3} \right) e^{-\frac{\pi m}{a}|z-z'|}$$
(1.215)

The first series  $\widetilde{G}_{e1+}$  is summed in the previous part (One term: 1.185)

$$\widetilde{G}_{e1+} = \frac{-1}{2\pi} \left[ \mathbb{R}e \left\{ \ln \left[ \left( 1 - e^{-\frac{\pi}{a}[|z-z'| - j(x-x')]} \right) \left( 1 - e^{-\frac{\pi}{a}[|z-z'| - j(x+x')]} \right) \right] \right\} \right]$$
(1.216)

The second series  $\widetilde{G}_{e2+}$  is the subject of study in this part. Using the trigonometric identity written in (1.181),  $\widetilde{G}_{e2+}$  can be summed as follows

$$\widetilde{G}_{e2+} = \frac{1}{a} \sum_{m=1}^{+\infty} \left( \frac{k^2 a^3}{2(\pi m)^3} \right) \frac{1}{2} \left[ \cos(k_x(x - x')) + \cos(k_x(x + x')) \right] e^{-\frac{\pi m}{a}|z - z'|} \\
= \frac{k^2 a^2}{4\pi^3} \sum_{m=1}^{+\infty} \frac{e^{-\frac{\pi m}{a}|z - z'|}}{m^3} \left[ \cos(k_x(x - x')) + \cos(k_x(x + x')) \right] \\
= \frac{k^2 a^2}{4\pi^3} \sum_{m=1}^{+\infty} \cos(k_x(x - x')) \frac{e^{-\frac{\pi m}{a}|z - z'|}}{m^3} \\
+ \frac{k^2 a^2}{4\pi^3} \sum_{m=1}^{+\infty} \cos(k_x(x + x')) \frac{e^{-\frac{\pi m}{a}|z - z'|}}{m^3}$$
(1.217)

where  $k_x = \frac{\pi m}{a}$  and therefore

$$\widetilde{G}_{e2+} = \frac{k^2 a^2}{4\pi^3} \sum_{m=1}^{+\infty} \cos\left(\frac{\pi m}{a}(x - x')\right) \frac{e^{-\frac{\pi m}{a}|z - z'|}}{m^3} + \frac{k^2 a^2}{4\pi^3} \sum_{m=1}^{+\infty} \cos\left(\frac{\pi m}{a}(x + x')\right) \frac{e^{-\frac{\pi m}{a}|z - z'|}}{m^3}$$
(1.218)

In the knowledge that the summations in (1.218) can be expressed in a semi-closed form (see Appendix A.3) as follows

$$\sum_{m=1}^{+\infty} \frac{e^{-nz}}{n^3} \cos(nx) = \mathbb{R}e\left\{ \operatorname{Li}_3\left[e^{(-z+jx)}\right] \right\}$$
 (1.219)

where  $\text{Li}_3(z)$  is the third order polylogarithm of the argument z,  $\widetilde{G}_{e2+}$  can be written as

$$\widetilde{G}_{e2+} = \frac{k^2 a^2}{4\pi^3} \left[ \mathbb{R}e \left\{ \operatorname{Li}_3 \left[ e^{-\frac{\pi}{a} [|z-z'| - j(x-x')]} \right] \right\} + \mathbb{R}e \left\{ \operatorname{Li}_3 \left[ e^{-\frac{\pi}{a} [|z-z'| - j(x+x')]} \right] \right\} \right]$$
(1.220)

Next, we continue applying the same procedure with the series  $\widetilde{G}_{-}(\bar{r},\bar{r}')$ .

$$\widetilde{G}_{-}(\overline{r}, \overline{r}') = \frac{1}{a} \sum_{m=1}^{+\infty} \sin(k_{x}x) \sin(k_{x}x') \frac{e^{-\gamma_{m}|z-z'|}}{\gamma_{m}} 
= \frac{1}{a} \sum_{m=1}^{+\infty} \sin(k_{x}x) \sin(k_{x}x') \left( \frac{e^{-\gamma_{m}|z-z'|}}{\gamma_{m}} - \left( \frac{a}{\pi m} + \frac{k^{2}a^{3}}{2(\pi m)^{3}} \right) e^{-\frac{\pi m}{a}|z-z'|} \right) 
+ \underbrace{\frac{1}{a} \sum_{m=1}^{+\infty} \sin(k_{x}x) \sin(k_{x}x') \left( \frac{a}{\pi m} + \frac{k^{2}a^{3}}{2(\pi m)^{3}} \right) e^{-\frac{\pi m}{a}|z-z'|}}_{\widetilde{G}_{e-}} \tag{1.221}$$

The asymptotic part that has to be summed is

$$\widetilde{G}_{e-} = \frac{1}{a} \sum_{m=1}^{+\infty} \sin(k_x x) \sin(k_x x') \left( \frac{a}{\pi m} + \frac{k^2 a^3}{2(\pi m)^3} \right) e^{-\frac{\pi m}{a}|z-z'|}$$

$$= \frac{1}{a} \sum_{m=1}^{+\infty} \sin(k_x x) \sin(k_x x') \left( \frac{a}{\pi m} \right) e^{-\frac{\pi m}{a}|z-z'|}$$

$$+ \frac{1}{a} \sum_{m=1}^{+\infty} \sin(k_x x) \sin(k_x x') \left( \frac{k^2 a^3}{2(\pi m)^3} \right) e^{-\frac{\pi m}{a}|z-z'|}$$
(1.222)

The first series  $\widetilde{G}_{e1-}$  is summed in the previous part (One term: 1.192)

$$\widetilde{G}_{e1-} = \frac{1}{2\pi} \left[ \mathbb{R}e \left\{ \ln \left( \frac{1 - e^{-\frac{\pi}{a}[|z - z'| - j(x + x')]}}{1 - e^{-\frac{\pi}{a}[|z - z'| - j(x - x')]}} \right) \right\} \right]$$
(1.223)

The second series  $\widetilde{G}_{e2-}$  is the subject of study in this part. Using the trigonometric identity defined in (1.189),  $\widetilde{G}_{e2-}$  can be expressed as follows

$$\widetilde{G}_{e2-} = \frac{1}{a} \sum_{m=1}^{+\infty} \left( \frac{k^2 a^3}{2(\pi m)^3} \right) \frac{1}{2} \left[ \cos(k_x(x - x')) - \cos(k_x(x + x')) \right] e^{-\frac{\pi m}{a}|z - z'|} \\
= \frac{k^2 a^2}{4\pi^3} \sum_{m=1}^{+\infty} \frac{e^{-\frac{\pi m}{a}|z - z'|}}{m^3} \left[ \cos(k_x(x - x')) - \cos(k_x(x + x')) \right] \\
= \frac{k^2 a^2}{4\pi^3} \sum_{m=1}^{+\infty} \cos(k_x(x - x')) \frac{e^{-\frac{\pi m}{a}|z - z'|}}{m^3} \\
- \frac{k^2 a^2}{4\pi^3} \sum_{m=1}^{+\infty} \cos(k_x(x + x')) \frac{e^{-\frac{\pi m}{a}|z - z'|}}{m^3}$$
(1.224)

where  $k_x = \frac{\pi m}{a}$  and therefore

$$\widetilde{G}_{e2-} = \frac{k^2 a^2}{4\pi^3} \sum_{m=1}^{+\infty} \cos\left(\frac{\pi m}{a}(x - x')\right) \frac{e^{-\frac{\pi m}{a}|z - z'|}}{m^3} - \frac{k^2 a^2}{4\pi^3} \sum_{m=1}^{+\infty} \cos\left(\frac{\pi m}{a}(x + x')\right) \frac{e^{-\frac{\pi m}{a}|z - z'|}}{m^3}$$
(1.225)

Assuming that the summations in (1.225) can be expressed in a semi-closed form (see Appendix A.3) by using (1.219),  $\widetilde{G}_{e2-}$  can be written as

$$\widetilde{G}_{e2-} = \frac{k^2 a^2}{4\pi^3} \left[ \mathbb{R}e \left\{ \operatorname{Li}_3 \left[ e^{-\frac{\pi}{a} [|z-z'| - j(x-x')]} \right] \right\} - \mathbb{R}e \left\{ \operatorname{Li}_3 \left[ e^{-\frac{\pi}{a} [|z-z'| - j(x+x')]} \right] \right\} \right]$$
(1.226)

#### • Extraction of Q terms.

The idea in this subsection is to generalize this acceleration technique to the extraction of Q terms. The procedure is the same as the followed previously.

For this purpose, we start from the equation (1.8) where we have obtained the Q retained terms for the general 2-D Green's function with 1-D periodicity.

$$\widetilde{G}_m = \sum_{q=0}^{Q} \frac{\prod_{n=0}^{q-1} (2n+1)}{2^q \, q!} \cdot \frac{k^{2q}}{|k_{xm}|^{2q+1}} \, e^{-|k_{xm}||z-z'|} \tag{1.227}$$

Now, we particularize this expression of the retained terms to the case of parallelplate waveguide, that is,  $\theta = 0^{\circ} \to k_{x0} = 0$  and therefore  $k_{xm} = \frac{\pi m}{a}$ .

$$\widetilde{G}_m = \sum_{q=0}^{Q} \frac{\prod_{n=0}^{q-1} (2n+1)}{2^q \, q!} \cdot \frac{k^{2q}}{\left(\frac{\pi m}{a}\right)^{2q+1}} \, e^{-\left(\frac{\pi m}{a}\right)|z-z'|} \tag{1.228}$$

Using this expression of the asymptotic retained part, we can apply Kummer's transformation to the spectral parallel-plate Green's functions. First, we start with the

series 
$$\widetilde{G}_{+}(\bar{r},\bar{r}')$$
.

$$\widetilde{G}_{+}(\overline{r}, \overline{r}') = \frac{1}{a} \sum_{m=0}^{+\infty} \frac{e^{-\gamma_{m}|z-z'|}}{\gamma_{m}} \cos(k_{x}x) \cos(k_{x}x')$$

$$= \widetilde{G}_{+0}(\overline{r}, \overline{r}') + \frac{1}{a} \sum_{m=1}^{+\infty} \cos(k_{x}x) \cos(k_{x}x') \frac{e^{-\gamma_{m}|z-z'|}}{\gamma_{m}}$$

$$= \widetilde{G}_{+0}(\overline{r}, \overline{r}') + \frac{1}{a} \sum_{m=1}^{+\infty} \cos(k_{x}x) \cos(k_{x}x') \left[ \frac{e^{-\gamma_{m}|z-z'|}}{\gamma_{m}} - \left( \sum_{q=0}^{Q} \frac{\prod_{n=0}^{q-1} (2n+1) k^{2q}}{2^{q} q! \left( \frac{\pi m}{a} \right)^{2q+1}} \right) \right]$$

$$e^{-\frac{\pi m}{a}|z-z'|}$$

$$+ \underbrace{\frac{1}{a} \sum_{m=1}^{+\infty} \cos(k_{x}x) \cos(k_{x}x')}_{\widetilde{G}_{e+}} \left( \sum_{q=0}^{Q} \frac{\prod_{n=0}^{q-1} (2n+1) \cdot k^{2q}}{2^{q} q!} \cdot \frac{k^{2q}}{\left( \frac{\pi m}{a} \right)^{2q+1}} \right) e^{-\frac{\pi m}{a}|z-z'|}$$

$$\widetilde{G}_{e+}$$
(1.229)

The asymptotic part that has to be summed is

$$\widetilde{G}_{e+} = \frac{1}{a} \sum_{m=1}^{+\infty} \cos(k_x x) \cos(k_x x') \left( \sum_{q=0}^{Q} \frac{\prod_{n=0}^{q-1} (2n+1)}{2^q \, q!} \cdot \frac{k^{2q}}{\left(\frac{\pi m}{a}\right)^{2q+1}} \right) e^{-\frac{\pi m}{a}|z-z'|}$$

$$= \frac{1}{a} \sum_{q=0}^{Q} \frac{\prod_{n=0}^{q-1} (2n+1)}{2^q \, q!} \cdot \frac{k^{2q}}{\left(\frac{\pi}{a}\right)^{2q+1}} \sum_{m=1}^{+\infty} \frac{\cos(k_x x) \cos(k_x x')}{m^{2q+1}} e^{-\frac{\pi m}{a}|z-z'|} \tag{1.230}$$

Using the trigonometric identity written in (1.181),  $\widetilde{G}_{e+}$  can be summed as follows

$$\widetilde{G}_{e+} = \sum_{q=0}^{Q} \frac{\prod_{n=0}^{q-1} (2n+1) k^{2q} a^{2q}}{2^{q} q! \pi^{2q+1}} \sum_{m=1}^{+\infty} \frac{\left[\cos(k_{x}(x-x')) + \cos(k_{x}(x+x'))\right]}{2m^{2q+1}} e^{-\frac{\pi m}{a}|z-z'|}$$

$$= \sum_{q=0}^{Q} \frac{\prod_{n=0}^{q-1} (2n+1)}{2^{q+1} q!} \cdot \frac{k^{2q} a^{2q}}{\pi^{2q+1}} \sum_{m=1}^{+\infty} \frac{\left[\cos(k_{x}(x-x')) + \cos(k_{x}(x+x'))\right]}{m^{2q+1}} e^{-\frac{\pi m}{a}|z-z'|}$$

$$(1.231)$$

In the knowledge that the summations in (1.231) can be expressed in a semi-closed form (see Appendix A.3) as follows

$$\sum_{m=1}^{+\infty} \frac{e^{-nz}}{n^{2q+1}} \cos(nx) = \mathbb{R}e \left\{ \text{Li}_{2q+1} \left[ e^{(-z+jx)} \right] \right\}$$
 (1.232)

where  $\text{Li}_{2q+1}(z)$  is the (2q+1)-th order polylogarithm of the argument z,  $\widetilde{G}_{e+}$  can be written as

$$\widetilde{G}_{e+} = \sum_{q=0}^{Q} \frac{\prod_{n=0}^{q-1} (2n+1)}{2^{q+1} q!} \cdot \frac{k^{2q} a^{2q}}{\pi^{2q+1}} \left[ \mathbb{R}e \left\{ \operatorname{Li}_{2q+1} \left[ e^{-\frac{\pi}{a} [|z-z'| - j(x-x')]} \right] \right\} + \mathbb{R}e \left\{ \operatorname{Li}_{2q+1} \left[ e^{-\frac{\pi}{a} [|z-z'| - j(x+x')]} \right] \right\} \right]$$

$$(1.233)$$

Once we have summed efficiently the asymptotic part of  $\widetilde{G}_+$ , we apply the same procedure to the series  $\widetilde{G}_-(\bar{r},\bar{r}')$ .

$$\widetilde{G}_{-}(\overline{r}, \overline{r}') = \frac{1}{a} \sum_{m=1}^{+\infty} \frac{e^{-\gamma_m |z-z'|}}{\gamma_m} \sin(k_x x) \sin(k_x x')$$

$$= \frac{1}{a} \sum_{m=1}^{+\infty} \sin(k_x x) \sin(k_x x') \left[ \frac{e^{-\gamma_m |z-z'|}}{\gamma_m} - \left( \sum_{q=0}^{Q} \frac{\prod_{n=0}^{q-1} (2n+1) k^{2q}}{2^q q! \left( \frac{\pi m}{a} \right)^{2q+1}} \right) \right]$$

$$e^{-\frac{\pi m}{a} |z-z'|}$$

$$+ \underbrace{\frac{1}{a} \sum_{m=1}^{+\infty} \sin(k_x x) \sin(k_x x')}_{m=1} \left( \sum_{q=0}^{Q} \frac{\prod_{n=0}^{q-1} (2n+1)}{2^q q!} \cdot \frac{k^{2q}}{\left( \frac{\pi m}{a} \right)^{2q+1}} \right) e^{-\frac{\pi m}{a} |z-z'|}$$

$$\widetilde{G}_{e-}$$
(1.234)

The asymptotic part that has to be summed is

$$\widetilde{G}_{e-} = \frac{1}{a} \sum_{m=1}^{+\infty} \sin(k_x x) \sin(k_x x') \left( \sum_{q=0}^{Q} \frac{\prod_{n=0}^{q-1} (2n+1)}{2^q q!} \cdot \frac{k^{2q}}{\left(\frac{\pi m}{a}\right)^{2q+1}} \right) e^{-\frac{\pi m}{a}|z-z'|}$$

$$= \frac{1}{a} \sum_{q=0}^{Q} \frac{\prod_{n=0}^{q-1} (2n+1)}{2^q q!} \cdot \frac{k^{2q}}{\left(\frac{\pi}{a}\right)^{2q+1}} \sum_{m=1}^{+\infty} \frac{\sin(k_x x) \sin(k_x x')}{m^{2q+1}} e^{-\frac{\pi m}{a}|z-z'|}$$

$$(1.235)$$

Using the trigonometric identity written in (1.189),  $\widetilde{G}_{e-}$  can be summed as follows

$$\widetilde{G}_{e-} = \sum_{q=0}^{Q} \frac{\prod_{n=0}^{q-1} (2n+1) k^{2q} a^{2q}}{2^{q} q! \pi^{2q+1}} \sum_{m=1}^{+\infty} \frac{\left[\cos(k_{x}(x-x')) - \cos(k_{x}(x+x'))\right]}{2m^{2q+1}} e^{-\frac{\pi m}{a}|z-z'|}$$

$$= \sum_{q=0}^{Q} \frac{\prod_{n=0}^{q-1} (2n+1)}{2^{q+1} q!} \cdot \frac{k^{2q} a^{2q}}{\pi^{2q+1}} \sum_{m=1}^{+\infty} \frac{\left[\cos(k_{x}(x-x')) - \cos(k_{x}(x+x'))\right]}{m^{2q+1}} e^{-\frac{\pi m}{a}|z-z'|}$$

$$(1.236)$$

Assuming that the summations in (1.236) can be expressed in a semi-closed form (see Appendix A.3) using the relation given in (1.232),  $\tilde{G}_{e-}$  can be written as

$$\widetilde{G}_{e-} = \sum_{q=0}^{Q} \frac{\prod_{n=0}^{q-1} (2n+1)}{2^{q+1} q!} \cdot \frac{k^{2q} a^{2q}}{\pi^{2q+1}} \left[ \mathbb{R}e \left\{ \operatorname{Li}_{2q+1} \left[ e^{-\frac{\pi}{a} [|z-z'| - j(x-x')]} \right] \right\} - \mathbb{R}e \left\{ \operatorname{Li}_{2q+1} \left[ e^{-\frac{\pi}{a} [|z-z'| - j(x+x')]} \right] \right\} \right]$$

$$(1.237)$$

In order to summarize, in this section we have accelerated the functions involved in the evaluation of Green's functions in parallel-plate problems. The acceleration technique that has been used for this purpose is the spectral Kummer's transformation. It is important to note that this technique has been reported to the general extraction of Q terms.

Thus, the Q asymptotic retained terms have been expressed in a general form as the summation of polylogarithmic functions which need to be numerically evaluated but are rapidly convergent. This implies a significant improvement thanks to the possibility of particularizing this general technique to the number of terms that we need in each case, as will be shown in Chapter 3.

In addition, it is important to highlight that the polylogarithms that appear in these terms are independent from the frequency, so that, in problems that require a frequency sweep, they do not have to be evaluated at each frequency point. This implies a significant reduction on the computation time in these common problems.

As a general conclusion of this chapter, we have attempted to improve the convergence of the 2-D Green's function with 1-D periodicity as a continuation of our work developed in [11] and apply the acquired knowledge to accelerate the series involved in the practical case of parallel-plate problems.

### Chapter 2

# The 2-D Green's Functions With 2-D Periodicity

The solution of electromagnetic problems in periodic structures, as has been mentioned previously, requires the efficient computation of the periodic Green's functions. In this chapter, we continue dealing with the 2-D Green's functions but with 2-D periodicity.

The 2-D homogeneous Green's functions with 2-D periodicity are the basis of the functions involved in rectangular waveguides and 2-D cavities problems. These functions can also be used to express in closed form the nonperiodic Green's functions of multilayered media as a linear combination of spherical and cylindrical waves in homogeneous media [2]. Because of this, the problem of accelerating the evaluation of the periodic Green's function is addressed here for 2-D configurations.

This chapter is organized as follows. Section 2.1 shows all the theoretical development required to formulate the spatial and the spectral 2-D Green's functions with 2-D periodicity. This formulation has been obtained for both general scenario and particular scenario of phase-shifted array. We also obtain the gradient of the 2-D periodic Green's functions with 2-D periodicity that will be useful in future studies when the integral equation technique will be used for the analysis of microwave devices including dielectric components. The series involved in the computation of this particular Green's functions can be written either as spatial infinite series or as spectral infinite series and can exhibit a very slow convergence. For this reason, once we have formulated these functions both in spectral and spatial domain and their gradient, we apply different acceleration techniques for the efficient computation of these periodic Green's functions. Due to their versatility and good compromise between accuracy and efficiency, the increasingly used acceleration techniques are Ewald's method and Kummer's transformation.

Thus, in Section 2.2 we detail the formulation needed to apply Ewald's method to the 2-D Green's function with 2-D periodicity according to [2]. This technique is also applied to the components of its gradient. In addition, we review the detail about the estimation of the *splitting parameter* for this case.

To compare different techniques of acceleration, in Section 2.3 we show the mathematical formulation involved in the application of Kummer's transformation. Here, we suggest two different strategies to extract the asymptotic terms in this technique. According to this, we outline a study about different procedures to calculate the retained part.

Finally, in Section 2.4 we apply the acquired knowledge about this general Green's function to rectangular waveguide and 2-D cavity problems. In this regard, we carry out the mathematical development to obtain the Green's function of the magnetic and electric scalar and vector potentials involved in cavities and waveguides problems. To accelerate the convergence of these series, we apply Kummer's transformation.

Numerical results from the formulation and the techniques proposed in this document are shown in Chapter 3 and the conclusions are summarized in Chapter 5.

## 2.1 Green's Functions and the Gradient of Green's Functions

In this section, we formulate the spatial and the spectral 2-D Green's functions with 2-D periodicity. This formulation is obtained for both general scenario and particular scenario of phase-shifted array. The case of general scenario can be useful because it can be particularized according to the required topology of particular problems. On the other hand, the case of phase-shifted array can be widely used in rectangular waveguide and cavity problems, which is our intention.

In both cases, the 2-D periodic Green's function will be expressed either as spatial infinite series or as spectral infinite series. It should be noted that these series exhibit a very slow convergence.

Moreover, in this section we also obtain the gradient of the 2-D periodic Green's functions that will be useful in future studies when the integral equation technique will be applied.

#### 2.1.1 Formulation of Green's Functions

Let us consider a two-dimensional spatial array of line sources with 2-D periodicity on x and y-directions which is parallel to the z-direction (see Fig. 2.1). This array is located

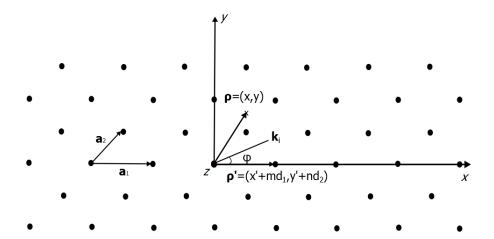


Figure 2.1: Physical configuration of a 2-D infinite distribution with 2-D periodicity on x and y-directions of line sources which are infinite on z-direction.

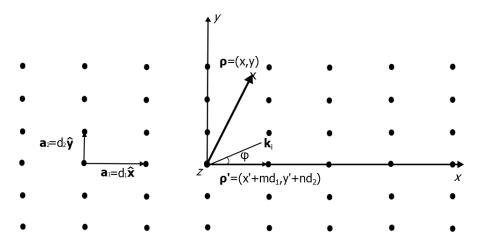


Figure 2.2: Physical configuration of a 2-D infinite distribution with 2-D periodicity on x and y-directions of phase-shifted line sources which are infinite on z-direction.

in an homogeneous media. Consider also, the case of a two-dimensional infinite array of phase-shifted line sources located at (x', y') (see Fig. 2.2). With these scenarios as a starting point, we would like to determine the radiation at an observation point (x, y) from these periodic geometries.

The notation that we are going to use is:

- Position vector for observation point:  $\bar{\rho} = x\hat{x} + y\hat{y}$
- Distance between the observation point and the source:  $|\bar{\rho} \bar{\rho}'| = |\Delta x \hat{x} + \Delta y \hat{y}| = |(x x')\hat{x} + (y y')\hat{y}|$
- $\bullet$  Basis of periodicity:  $\bar{a}_1=a_{1x}\hat{x}+a_{1y}\hat{y}$  and  $\bar{a}_2=a_{2x}\hat{x}+a_{2y}\hat{y}$

- Spatial shift of sources:  $\bar{\rho}_{mn} = m\bar{a}_1 + n\bar{a}_2$
- Position vector for line sources:  $\bar{\rho}' + \bar{\rho}_{mn} = (x' + ma_{1x} + na_{2x})\hat{x} + (y' + ma_{1y} + na_{2y})\hat{y}$

#### Formulation of the Spatial Green's Function

Now, the formulation developed in [11] for the 2-D Green's function with 1-D periodicity is extended to the computation of the double series involved in problems with 2-D periodicity. First, the formulation of the spatial Green's functions is obtained.

In [11] it is reported that the 2-D Green's function in the spatial domain for just one line source located at (x', y') is

$$G(\bar{\rho}, \bar{\rho}') = \frac{1}{4j} H_0^{(2)}(kR)$$
 (2.1)

where  $R = |(x - x')\hat{x} + (y - y')\hat{y}|$  is the spatial distance between the observation point and the source. By superposition theorem, the Green's function produced by a two-dimensional infinite array of line sources can be expressed as

$$G(\bar{\rho}, \bar{\rho}') = \frac{1}{4j} \sum_{m=-\infty}^{+\infty} \sum_{n=-\infty}^{+\infty} H_0^{(2)}(kS_{mn}) e^{-j\bar{k}_{w0} \cdot \bar{\rho}_{mn}}$$
(2.2)

where  $S_{mn} = |\bar{\rho} - \bar{\rho}' - \bar{\rho}_{mn}|$  is the spatial distance between the observation point and the infinite line sources. Using the previous presented notation,  $S_{mn}$  is

$$S_{mn} = |\triangle x \hat{x} + \triangle y \hat{y} - (m\bar{a}_1 + n\bar{a}_2)| = |(x - x')\hat{x} + (y - y')\hat{y} - (m\bar{a}_1 + n\bar{a}_2)|$$
  
=  $|[x - x' - (ma_{1x} + na_{2x})]\hat{x} + [y - y' - (ma_{1y} + na_{2y})]\hat{y}|$  (2.3)

and  $\bar{k}_{w0}$  is the projection on the x-y plane of the wavenumber vector of a wave incident on the array.

$$\bar{k}_{w0} = k \sin \theta \left(\cos \phi \,\hat{x} + \sin \phi \,\hat{y}\right) = k \sin \theta \,\cos \phi \,\hat{x} + k \sin \theta \,\sin \phi \,\hat{y} \tag{2.4}$$

Therefore,  $\bar{k}_{w0} \cdot \bar{\rho}_{mn}$  is

$$\bar{k}_{w0} \cdot \bar{\rho}_{mn} = (k \sin \theta \cos \phi \,\hat{x} + k \sin \theta \sin \phi \,\hat{y}) \cdot (m\bar{a}_1 + n\bar{a}_2)$$

$$= k_{x0}(ma_{1x} + na_{2x}) + k_{y0}(ma_{1y} + na_{2y})$$
(2.5)

The series obtained in (2.2) is the spatial representation of the 2-D Green's function with 2-D periodicity for a generic case. If we are interested in the special case of

two-dimensional infinite array of phase-shifted line sources, the vectors  $\bar{a}_1$  and  $\bar{a}_2$  have to be particularized as  $\bar{a}_1 = d_1\hat{x}$  and  $\bar{a}_2 = d_2\hat{y}$ . According to this, the spatial Green's function is (2.2) where

$$S_{mn} = |(x - x')\hat{x} + (y - y')\hat{y} - (md_1\hat{x} + nd_2\hat{y})| = |(x - x' - md_1)\hat{x} + (y - y' - nd_2)\hat{y}|$$

$$= \sqrt{(x - x' - md_1)^2 + (y - y' - nd_2)^2}$$
(2.6)

and

$$\bar{k}_{w0} \cdot \bar{\rho}_{mn} = (k \sin \theta \cos \phi \hat{x} + k \sin \theta \sin \phi \hat{y}) \cdot (md_1 \hat{x} + nd_2 \hat{y})$$

$$= k \sin \theta \cos \phi \, md_1 + k \sin \theta \sin \phi \, nd_2 = k_{x0} md_1 + k_{v0} nd_2$$
(2.7)

The spatial formulation is extremely slowly convergent, as will be shown in Chapter 3, and therefore its spectral representation will be obtained.

#### Formulation of the Spectral Green's Function

From the spatial representation of the 2-D Green's function with 2-D periodicity obtained previously, we obtain the spectral representation by applying Poisson's formula.

The Sommerfeld identity for 2-D cylindrical radiated fields is given by

$$\frac{1}{4j}H_0^{(2)}(kR) = \frac{1}{2\pi} \int_0^\infty \frac{e^{-R^2s^2 + \frac{k^2}{4s^2}}}{s} ds$$
 (2.8)

Using the spatial definition given in (2.2) and the Sommerfel identity

$$G(\bar{\rho}, \bar{\rho}') = \frac{1}{4j} \sum_{m=-\infty}^{+\infty} \sum_{n=-\infty}^{+\infty} H_0^{(2)}(kS_{mn}) e^{-j\bar{k}_{w0}\cdot\bar{\rho}_{mn}}$$
(2.9)

we can write the spatial series as

$$G(\bar{\rho}, \bar{\rho}') = \frac{1}{2\pi} \sum_{m=-\infty}^{+\infty} \sum_{p=-\infty}^{+\infty} e^{-j\bar{k}_{w0}\cdot\bar{\rho}_{mn}} \int_{0}^{\infty} \frac{e^{-S_{mn}^{2}s^{2} + \frac{k^{2}}{4s^{2}}}}{s} ds$$
 (2.10)

Now, Poisson's formula provides an alternative series for the computation of (2.2) in the spectral domain. Poisson's formula for the case of 2-D non-orthogonal mapping in the Fourier transform is detailed in Appendix A.4. It could suggest that the generic 2-D Poisson's formula is

$$\sum_{m=-\infty}^{+\infty} \sum_{n=-\infty}^{+\infty} f(m\bar{a}_1 + n\bar{a}_2) = \frac{1}{|\bar{a}_1 \times \bar{a}_2|} \sum_{m=-\infty}^{+\infty} \sum_{n=-\infty}^{+\infty} \widetilde{f}\left(\frac{2\pi}{A}m(\bar{a}_2 \times \hat{z}) + \frac{2\pi}{A}n(\hat{z} \times \bar{a}_1)\right)$$
(2.11)

Or in x - y subspace

$$\sum_{m=-\infty}^{+\infty} \sum_{n=-\infty}^{+\infty} f(ma_{1x} + na_{2x}, ma_{1y} + na_{2y})$$

$$= \frac{1}{A} \sum_{m=-\infty}^{+\infty} \sum_{n=-\infty}^{+\infty} \widetilde{f}\left(\frac{2\pi}{A}(ma_{2y} - na_{1y}), \frac{2\pi}{A}(-ma_{2x} + na_{1x})\right)$$
(2.12)

where  $\tilde{f}(k_x, k_y)$  is the Fourier transform of the function  $f(\xi_1, \xi_2)$ , that is

$$\widetilde{f}(k_x, k_y) = \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} f(\xi_1, \xi_2) e^{-jk_x \xi_1} e^{-jk_y \xi_2} d\xi_1 d\xi_2$$
(2.13)

From the equation (2.10), we identify terms so we can write

$$f(ma_{1x} + na_{2x}, ma_{1y} + na_{2y}) = \frac{1}{2\pi} \sum_{m=-\infty}^{+\infty} \sum_{n=-\infty}^{+\infty} e^{-jk_{x0}(ma_{1x} + na_{2x})} e^{-jk_{y0}(ma_{1y} + na_{2y})}$$

$$\times \int_{0}^{\infty} \frac{e^{-[(x-x'-(ma_{1x} + na_{2x}))^{2} + (y-y'-(ma_{1y} + na_{2y}))^{2}]s^{2} + \frac{k^{2}}{4s^{2}}}}{s} ds$$

$$(2.14)$$

And therefore  $\widetilde{f}(k_x, k_y)$  can be written as follows

$$\widetilde{f}(k_x, k_y) = \frac{1}{2\pi} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} d\xi_1 d\xi_2 \times \int_0^{\infty} \frac{e^{-[(x-x'-\xi_1)^2 + (y-y'-\xi_2)^2]s^2 + \frac{k^2}{4s^2}}}{s} e^{-jk_{x0}\xi_1} e^{-jk_{y0}\xi_2} \cdot e^{-jk_x\xi_1} e^{-jk_y\xi_2} ds$$
(2.15)

where we have to replace  $k_x = \frac{2\pi}{A}(ma_{2y} - na_{1y})$  and  $k_y = \frac{2\pi}{A}(-ma_{2x} + na_{1x})$ . According to this, we can define  $k_{xmn}$  and  $k_{ymn}$  as

$$k_{xmn} = k_{x0} + k_x = k_{x0} + \frac{2\pi}{A}(ma_{2y} - na_{1y})$$
 (2.16a)

$$k_{ymn} = k_{y0} + k_y = k_{y0} + \frac{2\pi}{4}(-ma_{2x} + na_{1x})$$
 (2.16b)

and then  $\widetilde{f}(k_x, k_y)$  is

$$\widetilde{f}(k_x, k_y) = \frac{1}{2\pi} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} d\xi_1 d\xi_2 \times \int_0^{\infty} ds \frac{1}{s} e^{\frac{k^2}{4s^2}} e^{-(x-x'-\xi_1)^2 s^2 - jk_{xmn}\xi_1}$$

$$e^{-(y-y'-\xi_2)^2 s^2 - jk_{ymn}\xi_2}$$
(2.17)

Now, we try to find the evaluation of the  $\xi$ -integrals in a closed form using the following formula

$$\int_{-\infty}^{+\infty} e^{-a\xi^2 + b\xi} d\xi = \sqrt{\frac{\pi}{a}} e^{\frac{b^2}{4a}}$$
 (2.18)

For this purpose, we define  $I_1$  and  $I_2$  as the integrals of (2.17) that depend on  $\xi_1$  and  $\xi_2$ , respectively

$$I_1 = \int_{-\infty}^{+\infty} e^{-(x-x'-\xi_1)^2 s^2 - jk_{xmn}\xi_1} d\xi_1$$
 (2.19a)

$$I_2 = \int_{-\infty}^{+\infty} e^{-(y-y'-\xi_2)^2 s^2 - jk_{ymn}\xi_2} d\xi_2$$
 (2.19b)

If we proceed, the relation (2.18) leads to

$$I_{1} = \int_{-\infty}^{+\infty} e^{-(x-x')^{2}s^{2} + 2(x-x')\xi_{1}s^{2} - \xi_{1}^{2}s^{2} - jk_{xmn}\xi_{1}} d\xi_{1}$$

$$= e^{-(x-x')^{2}s^{2}} \int_{-\infty}^{+\infty} e^{-\frac{s^{2}}{2}\xi_{1}^{2} + \frac{(2(x-x')s^{2} - jk_{xmn})\xi_{1}}{b}} d\xi_{1}$$

$$= e^{-(x-x')^{2}s^{2}} \sqrt{\frac{\pi}{s^{2}}} e^{\frac{(2(x-x')s^{2} - jk_{xmn})^{2}}{4s^{2}}} = e^{-\frac{(x-x')^{2}s^{2}}{s^{2}}} \sqrt{\frac{\pi}{s^{2}}} e^{\frac{(x-x')s^{2}}{s^{2}}} e^{-jk_{xmn}(x-x')} e^{\frac{-k_{xmn}^{2}}{4s^{2}}}$$

$$= \sqrt{\frac{\pi}{s^{2}}} e^{-jk_{xm}(x-x')} e^{-\frac{k_{xmn}^{2}}{4s^{2}}}$$

$$(2.20)$$

where  $a = s^2$  and  $b = 2(x - x')s^2 - jk_{xmn}$  have been identified. Equivalently, the integral  $I_2$  is

$$I_2 = \sqrt{\frac{\pi}{s^2}} e^{-jk_{ymn}(y-y')} e^{-\frac{k_{ymn}^2}{4s^2}}$$
 (2.21)

So, interchanging the order of integration and replacing  $I_1$  and  $I_2$  by the previous results,  $\widetilde{f}(k_x, k_y)$  remains

$$\widetilde{f}(k_x, k_y) = \frac{1}{2\pi} \int_0^\infty \sqrt{\frac{\pi}{s^2}} e^{-jk_{xmn}(x-x')} e^{-\frac{k_{xmn}^2}{4s^2}} \sqrt{\frac{\pi}{s^2}} e^{-jk_{ymn}(y-y')} e^{-\frac{k_{ymn}^2}{4s^2}} e^{\frac{k^2}{4s^2}} \frac{1}{s} ds$$
(2.22)

If we define  $\bar{k}_{mn}$  as

$$\bar{k}_{mn} = \bar{k}_{w0} + \frac{2\pi}{A} \left[ m(\bar{a}_2 \times \hat{z}) + n(\hat{z} \times \bar{a}_1) \right] 
= (k_{x0}\hat{x} + k_{y0}\hat{y}) + \frac{2\pi}{A} (ma_{2y} - na_{1y})\hat{x} + \frac{2\pi}{A} (-ma_{2x} + na_{1x})\hat{y} 
= \left( k_{x0} + \frac{2\pi}{A} (ma_{2y} - na_{1y}) \right) \hat{x} + \left( k_{y0} + \frac{2\pi}{A} (-ma_{2x} + na_{1x}) \right) \hat{y} = k_{xmn}\hat{x} + k_{ymn}\hat{y}$$
(2.23)

the exponentials can be merged into

$$e^{-jk_{xmn}(x-x')}e^{-jk_{ymn}(y-y')} = e^{-j[k_{xmn}(x-x')+k_{ymn}(y-y')]} = e^{-j\bar{k}_{mn}\cdot(\bar{\rho}-\bar{\rho}')}$$
(2.24a)

$$e^{-\frac{k_{xmn}^2}{4s^2}}e^{-\frac{k_{ymn}^2}{4s^2}} = e^{-\frac{(k_{xmn}^2 + k_{ymn}^2)}{4s^2}} = e^{-\frac{|\bar{k}_{mn}|^2}{4s^2}}$$
(2.24b)

and  $\widetilde{f}(k_x, k_y)$  can be rewritten as

$$\widetilde{f}(k_x, k_y) = \frac{1}{2} e^{-j\bar{k}_{mn} \cdot (\bar{\rho} - \bar{\rho}')} \int_0^\infty \frac{1}{s^3} e^{-\frac{|\bar{k}_{mn}|^2 - k^2}{4s^2}} ds$$
(2.25)

Now, if we apply this change of variable s'=1/s, the limits change  $s=0 \to s'=\infty$ ,  $s=\infty \to s'=0$  and the differential remains  $ds=-s^2ds'$ .

$$\widetilde{f}(k_x, k_y) = \frac{1}{2} e^{-j\bar{k}_{mn} \cdot (\bar{\rho} - \bar{\rho}')} \int_{\infty}^{0} \frac{-s'^3}{s'^2} e^{-\frac{(|\bar{k}_{mn}|^2 - k^2)s'^2}{4}} ds'$$
(2.26)

Next, we proceed as follows

$$\widetilde{f}(k_{x},k_{y}) = \frac{1}{2}e^{-j\bar{k}_{mn}\cdot(\bar{\rho}-\bar{\rho}')} \int_{\infty}^{0} (-s') \cdot \frac{-2(|\bar{k}_{mn}|^{2}-k^{2})}{4} \cdot e^{-\frac{(|\bar{k}_{mn}|^{2}-k^{2})s'^{2}}{4}} \cdot e^{-\frac{(|\bar{k}_{mn}|^{2}-k^{2})s'^{2}}{4}} \cdot \frac{-4}{2(|\bar{k}_{mn}|^{2}-k^{2})} ds' = e^{-j\bar{k}_{mn}\cdot(\bar{\rho}-\bar{\rho}')} \frac{e^{-\frac{(|\bar{k}_{mn}|^{2}-k^{2})s'^{2}}{4}}}{|\bar{k}_{mn}|^{2}-k^{2}} = \frac{e^{-j\bar{k}_{mn}\cdot(\bar{\rho}-\bar{\rho}')}}{|\bar{k}_{mn}|^{2}-k^{2}}$$

$$(2.27)$$

Once  $\widetilde{f}(k_x, k_y)$  has been obtained, the spectral representation of 2-D Green's function with 2-D periodicity can be written as a function of  $\widetilde{f}(k_x, k_y)$ 

$$\widetilde{G}(\bar{\rho}, \bar{\rho}') = \frac{1}{|\bar{a}_1 \times \bar{a}_2|} \sum_{m=-\infty}^{+\infty} \sum_{n=-\infty}^{+\infty} \widetilde{f}(k_x, k_y) = \frac{1}{A} \sum_{m=-\infty}^{+\infty} \sum_{n=-\infty}^{+\infty} \frac{e^{-j\bar{k}_{mn} \cdot (\bar{\rho} - \bar{\rho}')}}{|\bar{k}_{mn}|^2 - k^2}$$
(2.28)

where  $\bar{k}_{mn}$  is defined as

$$\bar{k}_{mn} = \bar{k}_{w0} + \frac{2\pi}{A} \left[ m(\bar{a}_2 \times \hat{z}) + n(\hat{z} \times \bar{a}_1) \right]$$
 (2.29)

and A is the area of the unit cell of the 2-D lattice

$$A = (\bar{a}_1 \times \bar{a}_2) \cdot \hat{z} = |\bar{a}_1 \times \bar{a}_2| = a_{1x}a_{2y} - a_{2x}a_{1y}$$
 (2.30)

The series obtained in (2.28) is the spectral representation of the 2-D Green's function with 2-D periodicity for a generic case. If we are interested in the special case of two-dimensional infinite array of phase-shifted line sources, the vectors  $\bar{a}_1$  and  $\bar{a}_2$  have to be particularized as  $\bar{a}_1 = d_1\hat{x}$  and  $\bar{a}_2 = d_2\hat{y}$ . In other words,  $a_{1x} = d_1$ ,  $a_{1y} = 0$ ,  $a_{2x} = 0$ ,  $a_{2y} = d_2$  (see Fig. 2.2).

According to this, the spectral Green's function is (2.28) where

$$A = |\bar{a}_1 \times \bar{a}_2| = d_1 \cdot d_2 \tag{2.31}$$

and

$$\bar{k}_{mn} = \bar{k}_{w0} + \frac{2\pi}{A} \left[ md_2 \hat{x} + nd_1 \hat{y} \right] = k \sin \theta \cos \phi \hat{x} + k \sin \theta \sin \phi \, \hat{y} + \frac{2\pi}{A} \left[ md_2 \hat{x} + nd_1 \hat{y} \right] 
= \left( k \sin \theta \cos \phi + \frac{2\pi}{A} md_2 \right) \hat{x} + \left( k \sin \theta \sin \phi + \frac{2\pi}{A} nd_1 \right) \hat{y} 
= \left( k \sin \theta \cos \phi + \frac{2\pi m}{d_1} \right) \hat{x} + \left( k \sin \theta \sin \phi + \frac{2\pi n}{d_2} \right) \hat{y} 
= \left( k_{x0} + \frac{2\pi m}{d_1} \right) \hat{x} + \left( k_{y0} + \frac{2\pi n}{d_2} \right) \hat{y}$$
(2.32)

This spectral formulation exhibits a better convergence than the spatial one, as will be shown in Chapter 3. Nevertheless, it could be possible to obtain faster convergences through applying mathematical methods of series acceleration.

#### 2.1.2 Formulation of the Gradient of Green's Functions

Once the spatial and spectral Green's functions have been obtained, we are interested in the gradient of these functions. It will be necessary to formulate the integral equations where electric and magnetic currents appear in the same problem coupled by differential operators. In this application, not only the potential but also the gradient of the periodic Green's function is required.

The gradient of spectral and spatial Green's functions is obtained by applying the gradient operator to the functions (2.2) and (2.28).

#### Formulation of the Spatial Gradient of Green's Function

To obtain the spatial representation of the gradient of 2-D periodic Green's function we start from the spatial series (2.2)

$$G(\bar{\rho}, \bar{\rho}') = \frac{1}{4j} \sum_{m=-\infty}^{+\infty} \sum_{n=-\infty}^{+\infty} H_0^{(2)}(kS_{mn}) e^{-j\bar{k}_{w0}\cdot\bar{\rho}_{mn}}$$
(2.33)

and we use the 2-D gradient operator

$$\nabla G(\bar{\rho}, \bar{\rho}') = \frac{\partial G(\bar{\rho}, \bar{\rho}')}{\partial x} \cdot \hat{x} + \frac{\partial G(\bar{\rho}, \bar{\rho}')}{\partial y} \cdot \hat{y}$$
 (2.34)

As can be noted, we need the partial derivatives of the function of several variables with respect to each of those variables. Due to the present symmetry in Green's function, we only demonstrate the partial derivative of this function with respect to x. So, we obtain the partial derivative with respect to y by analogy.

$$\frac{\partial G(\bar{\rho}, \bar{\rho}')}{\partial x} = \frac{\partial}{\partial x} \left( \frac{1}{4j} \sum_{m=-\infty}^{+\infty} \sum_{n=-\infty}^{+\infty} H_0^{(2)}(kS_{mn}) e^{-j\bar{k}_{w0} \cdot \bar{\rho}_{mn}} \right)$$
(2.35)

Making use of the following relation

$$\frac{\partial H_0^{(2)}(z)}{\partial z} = -H_1^{(2)}(z) \tag{2.36}$$

and remembering that  $S_{mn}$  is

$$S_{mn} = |[x - x' - (ma_{1x} + na_{2x})]\hat{x} + [y - y' - (ma_{1y} + na_{2y})]\hat{y}|$$

$$= \sqrt{[x - x' - (ma_{1x} + na_{2x})]^2 + [y - y' - (ma_{1y} + na_{2y})]^2}$$
(2.37)

 $\frac{\partial G(\bar{\rho},\bar{\rho}')}{\partial x}$  is calculated using the chain rule as

$$\frac{\partial G(\bar{\rho}, \bar{\rho}')}{\partial x} = \frac{1}{4j} \sum_{m=-\infty}^{+\infty} \sum_{n=-\infty}^{+\infty} H_1^{(2)}(kS_{mn})e^{-j\bar{k}_{w0}\cdot\bar{\rho}_{mn}} 
\cdot \frac{-k 2 \left[x - x' - (ma_{1x} + na_{2x})\right]}{2 \sqrt{[x - x' - (ma_{1x} + na_{2x})]^2 + [y - y' - (ma_{1y} + na_{2y})]^2}} 
= \frac{1}{4j} \sum_{m=-\infty}^{+\infty} \sum_{n=-\infty}^{+\infty} \frac{-k \left[x - x' - (ma_{1x} + na_{2x})\right]}{S_{mn}} H_1^{(2)}(kS_{mn})e^{-j\bar{k}_{w0}\cdot\bar{\rho}_{mn}}$$
(2.38)

Proceeding in a similar way for the other component,  $\frac{\partial G(\bar{\rho},\bar{\rho}')}{\partial y}$  is

$$\frac{\partial G(\bar{\rho}, \bar{\rho}')}{\partial y} = \frac{1}{4j} \sum_{m=-\infty}^{+\infty} \sum_{n=-\infty}^{+\infty} \frac{-k \left[ y - y' - (ma_{1y} + na_{2y}) \right]}{S_{mn}} H_1^{(2)}(kS_{mn}) e^{-j\bar{k}_{w0} \cdot \bar{\rho}_{mn}}$$
(2.39)

The gradient of the spatial 2-D Green's function with 2-D periodicity can be written as

$$\nabla G(\bar{\rho}, \bar{\rho}') = \frac{1}{4j} \sum_{m=-\infty}^{+\infty} \sum_{n=-\infty}^{+\infty} \frac{-k}{S_{mn}} H_1^{(2)}(kS_{mn}) e^{-j\bar{k}_{w0} \cdot \bar{\rho}_{mn}}$$

$$\times \left\{ [x - x' - (ma_{1x} + na_{2x})] \cdot \hat{x} + [y - y' - (ma_{1y} + na_{2y})] \cdot \hat{y} \right\}$$
(2.40)

#### Formulation of the Spectral Gradient of Green's Function

To obtain the spectral representation of the gradient of 2-D periodic Green's function, we start from the spectral series (2.28)

$$\widetilde{G}(\bar{\rho}, \bar{\rho}') = \frac{1}{A} \sum_{m=-\infty}^{+\infty} \sum_{n=-\infty}^{+\infty} \frac{e^{-j\bar{k}_{mn} \cdot (\bar{\rho} - \bar{\rho}')}}{|\bar{k}_{mn}|^2 - k^2}$$
(2.41)

and we use the 2-D gradient operator given by (2.34). We need the partial derivatives of the function with respect to each of those variables. As said before, due to the present symmetry in Green's function, we only demonstrate the partial derivative of this function with respect to x. So, we obtain the partial derivative with respect to y by analogy.

$$\frac{\partial \widetilde{G}(\bar{\rho}, \bar{\rho}')}{\partial x} = \frac{\partial}{\partial x} \left( \frac{1}{A} \sum_{m=-\infty}^{+\infty} \sum_{n=-\infty}^{+\infty} \frac{e^{-j\bar{k}_{mn} \cdot (\bar{\rho} - \bar{\rho}')}}{|\bar{k}_{mn}|^2 - k^2} \right)$$
(2.42)

where

$$\bar{k}_{mn} \cdot (\bar{\rho} - \bar{\rho}') = (k_{xmn}\hat{x} + k_{ymn}\hat{y}) \cdot [(x - x')\hat{x} + (y - y')\hat{y}] = k_{xmn} (x - x') + k_{ymn} (y - y')$$
and then,  $\frac{\partial \tilde{G}(\bar{\rho}, \bar{\rho}')}{\partial x}$  remains

$$\frac{\partial \widetilde{G}(\bar{\rho}, \bar{\rho}')}{\partial x} = \frac{\partial}{\partial x} \left( \frac{1}{A} \sum_{m=-\infty}^{+\infty} \sum_{n=-\infty}^{+\infty} \frac{e^{-jk_{xmn}(x-x')} e^{-jk_{ymn}(y-y')}}{|k_{mn}|^2 - k^2} \right)$$

$$= \frac{1}{A} \sum_{m=-\infty}^{+\infty} \sum_{n=-\infty}^{+\infty} -jk_{xmn} \frac{e^{-j\bar{k}_{mn}\cdot(\bar{\rho}-\bar{\rho}')}}{|\bar{k}_{mn}|^2 - k^2} \tag{2.44}$$

Proceeding in a similar way for the other component,  $\frac{\partial \widetilde{G}(\bar{\rho},\bar{\rho}')}{\partial y}$  is

$$\frac{\partial \widetilde{G}(\bar{\rho}, \bar{\rho}')}{\partial y} = \frac{1}{A} \sum_{m=-\infty}^{+\infty} \sum_{n=-\infty}^{+\infty} -jk_{ymn} \frac{e^{-j\bar{k}_{mn} \cdot (\bar{\rho} - \bar{\rho}')}}{|\bar{k}_{mn}|^2 - k^2}$$
(2.45)

Finally, the gradient of the 2-D Green's function with 2-D periodicity in the spectral domain can be written as

$$\nabla \widetilde{G}(\bar{\rho}, \bar{\rho}') = \frac{1}{A} \sum_{m=-\infty}^{+\infty} \sum_{n=-\infty}^{+\infty} \frac{e^{-j\bar{k}_{mn} \cdot (\bar{\rho} - \bar{\rho}')}}{|\bar{k}_{mn}|^2 - k^2} \left[ -jk_{xmn} \cdot \hat{x} - jk_{ymn} \cdot \hat{y} \right]$$
(2.46)

In order to summarize, in this section we have demonstrated the obtaining of the spatial and spectral 2-D periodic free-space Green's functions with 2-D periodicity and their gradients. These functions will be our starting point in the following sections. This is because the convergence of these series is slow and we will try to improve it through applying widely used techniques of series acceleration.

#### 2.2 Ewald's Method

The spectral and spatial Green's functions formulated in the previous section exhibit extremely slow convergence. A way to avoid this slow convergence is to introduce new transformations that allow the evaluation of these functions with less number of terms, that is, improving their convergences.

According to this, the first acceleration technique that we will apply to 2-D Green's function is Ewald's method [4]. This method consists of splitting the series into two parts, one spectral and the other spatial. Then, each component has to be transformed in its corresponding domain in order to be evaluated as efficiently as possible. The final

expressions of these components are very rapidly convergent. Thus, the advantage of this method is its rapid convergence in comparison to the computation of the direct series. Consequently, its advantages are high accuracy and efficiency. For these reasons, this method has been applied to the 2-D Green's function with 1-D periodicity in [5, 22] and 2-D periodicity in [2].

The idea in this section is to review the formulation needed to obtain the components resulted by the application of Ewald's method. This is because they will be used to compare with future techniques proposed in this project. First, we focus on applying this technique in the Green's function under study. We obtain the components  $G_{spectral}$  and  $G_{spatial}$ , whose sum leads to the total Green's function. It is important to note that the split of these components is addressed by the *splitting parameter*. This parameter has to be optimally adjusted to calculate each component in their optimal region of convergence.

Unlike [11], in this case there is not an equivalent development for the switching method because the observation point does not distance from the source in z-direction. The observation point is always in the x-y plane and therefore near the source. So, the convergence does not depend on the z-direction distance.

Finally, the same procedure will be followed in the gradient components of Green's function.

#### 2.2.1 Green's Function Using Ewald's Method

From the spatial representation of the 2-D Green's function with 2-D periodicity obtained in the previous section, we apply Ewald's method. For this purpose, we start from the Sommerfeld identity for 2-D cylindrical radiated fields, which is given by

$$\frac{1}{4j}H_0^{(2)}(kR) = \frac{1}{2\pi} \int_0^\infty \frac{e^{-R^2s^2 + \frac{k^2}{4s^2}}}{s} ds$$
 (2.47)

Using the spatial definition given by (2.2) and the Sommerfel identity

$$G(\bar{\rho}, \bar{\rho}') = \frac{1}{4j} \sum_{m=-\infty}^{+\infty} \sum_{n=-\infty}^{+\infty} H_0^{(2)}(kS_{mn}) e^{-j\bar{k}_{w0}\cdot\bar{\rho}_{mn}}$$
(2.48)

we can write the spatial series as

$$G(\bar{\rho}, \bar{\rho}') = \frac{1}{2\pi} \sum_{m=-\infty}^{+\infty} \sum_{n=-\infty}^{+\infty} e^{-j\bar{k}_{w0}\cdot\bar{\rho}_{mn}} \int_{0}^{\infty} \frac{e^{-S_{mn}^{2}s^{2} + \frac{k^{2}}{4s^{2}}}}{s} ds$$
 (2.49)

Ewald's method is applied by splitting the previous integral into two parts  $G(\bar{\rho}, \bar{\rho}') = G_{spectral}(\bar{\rho}, \bar{\rho}') + G_{spatial}(\bar{\rho}, \bar{\rho}')$ , where  $\varepsilon$  is the *splitting parameter* and determine where the integral is divided.

Using this parameter, we can consider the total Green's function as the summation of two contributions

$$G_{spectral}(\bar{\rho}, \bar{\rho}') = \frac{1}{2\pi} \sum_{m=-\infty}^{+\infty} \sum_{n=-\infty}^{+\infty} e^{-j\bar{k}_{w0}\cdot\bar{\rho}_{mn}} \int_{0}^{\varepsilon} \frac{e^{-S_{mn}^{2}s^{2} + \frac{k^{2}}{4s^{2}}}}{s} ds$$
 (2.50a)

$$G_{spatial}(\bar{\rho}, \bar{\rho}') = \frac{1}{2\pi} \sum_{m=-\infty}^{+\infty} \sum_{n=-\infty}^{+\infty} e^{-j\bar{k}_{w0} \cdot \bar{\rho}_{mn}} \int_{\varepsilon}^{\infty} \frac{e^{-S_{mn}^2 s^2 + \frac{k^2}{4s^2}}}{s} ds$$
 (2.50b)

The subscripts indicate the domain in which each component will be formulated. According to this, the next step will be transforming each component to obtain the final Ewald's contributions.

#### Spectral Component of Ewald's Method $G_{spectral}$

As the series  $G_{spectral}$  do not exhibit an exponential decay, we transform it into a spectral domain series using the 2-D generic Poisson's formula (see Appendix A.4)

$$\sum_{m=-\infty}^{+\infty} \sum_{n=-\infty}^{+\infty} f(m\bar{a}_1 + n\bar{a}_2) = \frac{1}{|\bar{a}_1 \times \bar{a}_2|} \sum_{m=-\infty}^{+\infty} \sum_{n=-\infty}^{+\infty} \widetilde{f}\left(\frac{2\pi}{A}m(\bar{a}_2 \times \hat{z}) + \frac{2\pi}{A}n(\hat{z} \times \bar{a}_1)\right)$$
(2.51)

Or in x - y subspace

$$\sum_{m=-\infty}^{+\infty} \sum_{n=-\infty}^{+\infty} f(ma_{1x} + na_{2x}, ma_{1y} + na_{2y})$$

$$= \frac{1}{A} \sum_{m=-\infty}^{+\infty} \sum_{n=-\infty}^{+\infty} \widetilde{f}\left(\frac{2\pi}{A}(ma_{2y} - na_{1y}), \frac{2\pi}{A}(-ma_{2x} + na_{1x})\right)$$
(2.52)

where  $\tilde{f}(k_x, k_y)$  is the Fourier transform of the function  $f(\xi_1, \xi_2)$ , that is

$$\widetilde{f}(k_x, k_y) = \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} f(\xi_1, \xi_2) e^{-jk_x \xi_1} e^{-jk_y \xi_2} d\xi_1 d\xi_2$$
(2.53)

From the equation (2.50a), we identify terms so we can write

$$f(ma_{1x} + na_{2x}, ma_{1y} + na_{2y}) = \frac{1}{2\pi} \sum_{m=-\infty}^{+\infty} \sum_{n=-\infty}^{+\infty} e^{-jk_{x0}(ma_{1x} + na_{2x})} e^{-jk_{y0}n(ma_{1y} + na_{2y})}$$

$$\times \int_{0}^{\varepsilon} \frac{e^{-[(x-x'-(ma_{1x} + na_{2x}))^{2} + (y-y'-(ma_{1y} + na_{2y}))^{2}]s^{2} + \frac{k^{2}}{4s^{2}}}}{s} ds$$

$$(2.54)$$

and therefore  $\widetilde{f}(k_x, k_y)$  can be written as follows

$$\widetilde{f}(k_x, k_y) = \frac{1}{2\pi} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} d\xi_1 d\xi_2 \times \int_0^{\varepsilon} \frac{e^{-[(x-x'-\xi_1)^2 + (y-y'-\xi_2)^2]s^2 + \frac{k^2}{4s^2}}}{s} e^{-jk_{x0}\xi_1} e^{-jk_{y0}\xi_2} \cdot e^{-jk_x\xi_1} e^{-jk_y\xi_2} ds$$
(2.55)

where we have to replace  $k_x = \frac{2\pi}{A}(ma_{2y} - na_{1y})$  and  $k_y = \frac{2\pi}{A}(-ma_{2x} + na_{1x})$ . According to this and using the definition of  $k_{xmn}$  and  $k_{ymn}$  written in (2.16b),  $\tilde{f}(k_x, k_y)$  is

$$\widetilde{f}(k_x, k_y) = \frac{1}{2\pi} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} d\xi_1 d\xi_2 \times \int_0^{\varepsilon} ds \, \frac{1}{s} \, e^{\frac{k^2}{4s^2}} \, e^{-(x-x'-\xi_1)^2 s^2 - jk_{xmn}\xi_1}$$

$$e^{-(y-y'-\xi_2)^2 s^2 - jk_{ymn}\xi_2}$$
(2.56)

Now, we try to find the evaluation of the  $\xi$ -integrals in a closed form using the following formula

$$\int_{-\infty}^{+\infty} e^{-a\xi^2 + b\xi} d\xi = \sqrt{\frac{\pi}{a}} e^{\frac{b^2}{4a}}$$
 (2.57)

For this purpose, we define  $I_1$  and  $I_2$  as the integrals of (2.56) that depend on  $\xi_1$  and  $\xi_2$ , respectively

$$I_1 = \int_{-\infty}^{+\infty} e^{-(x-x'-\xi_1)^2 s^2 - jk_{xmn}\xi_1} d\xi_1$$
 (2.58a)

$$I_2 = \int_{-\infty}^{+\infty} e^{-(y-y'-\xi_2)^2 s^2 - jk_{ymn}\xi_2} d\xi_2$$
 (2.58b)

and we use the results obtained in (2.20) and (2.21)

$$I_1 = \sqrt{\frac{\pi}{s^2}} e^{-jk_{xmn}(x-x')} e^{-\frac{k_{xmn}^2}{4s^2}}$$
 (2.59a)

$$I_2 = \sqrt{\frac{\pi}{s^2}} e^{-jk_{ymn}(y-y')} e^{-\frac{k_{ymn}^2}{4s^2}}$$
 (2.59b)

So, interchanging the order of integration and replacing  $I_1$  and  $I_2$  by the previous results,  $\widetilde{f}(k_x, k_y)$  remains

$$\widetilde{f}(k_x, k_y) = \frac{1}{2\pi} \int_0^{\varepsilon} \sqrt{\frac{\pi}{s^2}} e^{-jk_{xmn}(x-x')} e^{-\frac{k_{xmn}^2}{4s^2}} \sqrt{\frac{\pi}{s^2}} e^{-jk_{ymn}(y-y')} e^{-\frac{kymn^2}{4s^2}} e^{\frac{k^2}{4s^2}} \frac{1}{s} ds$$
(2.60)

where we have defined  $\bar{k}_{mn}$  as

$$\bar{k}_{mn} = \bar{k}_{w0} + \frac{2\pi}{A} \left[ m(\bar{a}_2 \times \hat{z}) + n(\hat{z} \times \bar{a}_1) \right] = k_{xmn}\hat{x} + k_{ymn}\hat{y}$$

$$= \left( k_{x0} + \frac{2\pi}{A} (ma_{2y} - na_{1y}) \right) \hat{x} + \left( k_{y0} + \frac{2\pi}{A} (-ma_{2x} + na_{1x}) \right) \hat{y}$$
(2.61)

As has been done in the spectral development, the exponentials can be merged into

$$e^{-jk_{xmn}(x-x')}e^{-jk_{ymn}(y-y')} = e^{-j[k_{xmn}(x-x')+k_{ymn}(y-y')]} = e^{-j\bar{k}_{mn}\cdot(\bar{\rho}-\bar{\rho}')}$$
(2.62a)

$$e^{-\frac{k_{xmn}^2}{4s^2}}e^{-\frac{kymn^2}{4s^2}} = e^{-\frac{(k_{xmn}^2 + kymn^2)}{4s^2}} = e^{-\frac{|\bar{k}_{mn}|^2}{4s^2}}$$
(2.62b)

and  $\widetilde{f}(k_x, k_y)$  can be rewritten as

$$\widetilde{f}(k_x, k_y) = \frac{1}{2} e^{-j\bar{k}_{mn} \cdot (\bar{\rho} - \bar{\rho}')} \int_0^{\varepsilon} \frac{1}{s^3} e^{-\frac{|\bar{k}_{mn}|^2 - k^2}{4s^2}} ds$$
(2.63)

Now, if we apply this change of variable s'=1/s, the limits change  $s=0 \to s'=\infty$ ,  $s=\varepsilon \to s'=1/\varepsilon$  and the differential remains  $ds=-s^2ds'$ .

$$\widetilde{f}(k_x, k_y) = \frac{1}{2} e^{-j\bar{k}_{mn} \cdot (\bar{\rho} - \bar{\rho}')} \int_{2^{n}}^{1/\varepsilon} \frac{-s'^3}{s'^2} e^{-\frac{(|\bar{k}_{mn}|^2 - k^2)s'^2}{4}} ds'$$
(2.64)

Next, we proceed as follows

$$\widetilde{f}(k_{x},k_{y}) = \frac{1}{2}e^{-j\bar{k}_{mn}\cdot(\bar{\rho}-\bar{\rho}')} \int_{\infty}^{1/\varepsilon} (-s') \cdot \frac{-2(|\bar{k}_{mn}|^{2}-k^{2})}{4} \cdot e^{-\frac{(|\bar{k}_{mn}|^{2}-k^{2})s'^{2}}{4}} \cdot e^{-\frac{(|\bar{k}_{mn}|^{2}-k^{2})s'^{2}}{4}} \cdot \frac{-4}{2(|\bar{k}_{mn}|^{2}-k^{2})} ds' = e^{-j\bar{k}_{mn}\cdot(\bar{\rho}-\bar{\rho}')} \frac{e^{-\frac{(|\bar{k}_{mn}|^{2}-k^{2})s'^{2}|_{\infty}^{1/\varepsilon}}}{|\bar{k}_{mn}|^{2}-k^{2}}} = \frac{e^{-j\bar{k}_{mn}\cdot(\bar{\rho}-\bar{\rho}')}}{|\bar{k}_{mn}|^{2}-k^{2}} e^{-\frac{|\bar{k}_{mn}|^{2}-k^{2}}{4\varepsilon^{2}}}$$

$$(2.65)$$

Once  $\widetilde{f}(k_x, k_y)$  has been obtained, the spectral contribution of Ewald's method applied on 2-D Green's function with 2-D periodicity can be written as a function of  $\widetilde{f}(k_x, k_y)$ 

$$G_{spectral}(\bar{\rho}, \bar{\rho}') = \frac{1}{|\bar{a}_1 \times \bar{a}_2|} \sum_{m=-\infty}^{+\infty} \sum_{n=-\infty}^{+\infty} \tilde{f}(k_x, k_y)$$

$$= \frac{1}{A} \sum_{m=-\infty}^{+\infty} \sum_{n=-\infty}^{+\infty} \frac{e^{-j\bar{k}_{mn} \cdot (\bar{\rho} - \bar{\rho}')}}{|\bar{k}_{mn}|^2 - k^2} e^{-\frac{|\bar{k}_{mn}|^2 - k^2}{4\epsilon^2}}$$
(2.66)

where the definition of A and  $\bar{k}_{mn}$  in the generic case and in the case of phase-shifted line sources have been reported in the section 2.1.1.

This spectral formulation of the first contribution resulted by the application of Ewald's method is rapidly convergent, as will be shown in Chapter 3.

#### Spatial Component of Ewald's Method $G_{spatial}$

On the other hand, the second contribution of Ewald's method  $G_{spatial}(\bar{\rho}, \bar{\rho}')$  is transformed in the spatial domain as follows

$$G_{spatial}(\bar{\rho}, \bar{\rho}') = \frac{1}{2\pi} \sum_{m=-\infty}^{+\infty} \sum_{n=-\infty}^{+\infty} e^{-jk_{x0}(ma_{1x} + na_{2x})} e^{-jk_{y0}(ma_{1y} + na_{2y})} \int_{\varepsilon}^{\infty} \frac{e^{-S_{mn}^{2}s^{2} + \frac{k^{2}}{4s^{2}}}}{s} ds$$

$$(2.67)$$

where the exponentials in (2.67) can be merged and therefore  $G_{spatial}(\bar{\rho}, \bar{\rho}')$  remains

$$G_{spatial}(\bar{\rho}, \bar{\rho}') = \frac{1}{2\pi} \sum_{m=-\infty}^{+\infty} \sum_{r=-\infty}^{+\infty} e^{-j\bar{k}_{w0} \cdot \bar{\rho}_{mn}} \int_{\varepsilon}^{\infty} \frac{e^{-S_{mn}^2 s^2 + \frac{k^2}{4s^2}}}{s} ds$$
 (2.68)

If we define I like the integral part of  $G_{spatial}(\bar{\rho}, \bar{\rho}')$ 

$$I = \int_{\varepsilon}^{\infty} \frac{e^{-S_{mn}^2 s^2 + \frac{k^2}{4s^2}}}{s} ds \tag{2.69}$$

and we carry out the following change of variable  $u=s^2$ , the limits of integration change as  $s=\infty \to u=\infty$  and  $s=\varepsilon \to u=\varepsilon^2$ , and the differential remains  $ds=\frac{1}{2\sqrt{u}}du$ .

$$I = \int_{e^2}^{\infty} \frac{1}{2} \frac{e^{-S_{mn}^2 u} e^{\frac{k^2}{4u}}}{u} du$$
 (2.70)

Using the Taylor expansion of an exponential function given by

$$e^{u} = \sum_{q=0}^{+\infty} \frac{u^{q}}{q!}$$
 (2.71)

the integral I can be expressed as

$$I = \int_{\epsilon^2}^{\infty} \frac{1}{2} \frac{e^{-S_{mn}^2 u}}{u} \sum_{q=0}^{+\infty} \frac{\left(\frac{k}{2}\right)^{2q}}{q! u^q} du$$
 (2.72)

Next, we perform another change of variable  $t=u/\varepsilon^2$ , where the limits change  $u=\varepsilon^2\to t=1$  and  $u=\infty\to t=\infty$  and the differential remains  $du=\varepsilon^2 dt$ . This leads to

$$I = \frac{1}{2} \sum_{q=0}^{+\infty} \int_{1}^{\infty} \frac{e^{-S_{mn}^{2} \varepsilon^{2} t}}{\varepsilon^{2} t} \frac{\left(\frac{k}{2}\right)^{2q}}{q! \, \varepsilon^{2q} t^{q}} \, \varepsilon^{2} dt = \frac{1}{2} \sum_{q=0}^{+\infty} \left(\frac{k}{2\varepsilon}\right)^{2q} \frac{1}{q!} \int_{1}^{\infty} \frac{e^{-S_{mn}^{2} \varepsilon^{2} t}}{t^{q+1}} \, dt \qquad (2.73)$$

We make use of the q-th order exponential integral defined as

$$E_q(z) = \int_1^\infty \frac{e^{-zt}}{t^q} dt \tag{2.74}$$

and consequently, I remains

$$I = \frac{1}{2} \sum_{q=0}^{+\infty} \left(\frac{k}{2\varepsilon}\right)^{2q} \frac{1}{q!} \, \mathcal{E}_{q+1}(S_{mn}^2 \varepsilon^2)$$
 (2.75)

The inclusion of (2.75) into (2.68) leads to the following representation of the modified spatial component

$$G_{spatial}(\bar{\rho}, \bar{\rho}') = \frac{1}{4\pi} \sum_{m=-\infty}^{+\infty} \sum_{n=-\infty}^{+\infty} e^{-j\bar{k}_{w0}\cdot\bar{\rho}_{mn}} \times \sum_{q=0}^{+\infty} \left(\frac{k}{2\varepsilon}\right)^{2q} \frac{1}{q!} \operatorname{E}_{q+1}(S_{mn}^2 \varepsilon^2) \quad (2.76)$$

Once we have obtained these two contributions, we can summarize the final formulas resulted by the application of Ewald's method to the 2-D Green's function with 2-D periodicity as

$$G_{Ewald}(\bar{\rho}, \bar{\rho}') = G_{spectral}(\bar{\rho}, \bar{\rho}') + G_{spatial}(\bar{\rho}, \bar{\rho}')$$
(2.77)

where  $G_{spectral}(\bar{\rho}, \bar{\rho}')$  is

$$G_{spectral}(\bar{\rho}, \bar{\rho}') = \frac{1}{A} \sum_{m=-\infty}^{+\infty} \sum_{n=-\infty}^{+\infty} \frac{e^{-j\bar{k}_{mn} \cdot (\bar{\rho} - \bar{\rho}')}}{|\bar{k}_{mn}|^2 - k^2} e^{-\frac{|\bar{k}_{mn}|^2 - k^2}{4\varepsilon^2}}$$
(2.78)

 $G_{spatial}(\bar{\rho}, \bar{\rho}')$  is

$$G_{spatial}(\bar{\rho}, \bar{\rho}') = \frac{1}{4\pi} \sum_{m=-\infty}^{+\infty} \sum_{n=-\infty}^{+\infty} e^{-j\bar{k}_{w0}\cdot\bar{\rho}_{mn}} \times \sum_{q=0}^{+\infty} \left(\frac{k}{2\varepsilon}\right)^{2q} \frac{1}{q!} \operatorname{E}_{q+1}(S_{mn}^2 \varepsilon^2) \quad (2.79)$$

and, as a result, the Green's function calculated by Ewald's method  $G_{Ewald}(\bar{\rho}, \bar{\rho}')$  is

$$G_{Ewald}(\bar{\rho}, \bar{\rho}') = \frac{1}{A} \sum_{m=-\infty}^{+\infty} \sum_{n=-\infty}^{+\infty} \frac{e^{-j\bar{k}_{mn}\cdot(\bar{\rho}-\bar{\rho}')}}{|\bar{k}_{mn}|^2 - k^2} e^{-\frac{|\bar{k}_{mn}|^2 - k^2}{4\varepsilon^2}} + \frac{1}{4\pi} \sum_{m=-\infty}^{+\infty} \sum_{n=-\infty}^{+\infty} e^{-j\bar{k}_{w0}\cdot\bar{\rho}_{mn}} \times \sum_{q=0}^{+\infty} \left(\frac{k}{2\varepsilon}\right)^{2q} \frac{1}{q!} E_{q+1}(S_{mn}^2\varepsilon^2)$$

$$(2.80)$$

Through this technique, we have managed to go from having an infinite series to having two contributions with fast convergence. The improvement obtained by this method will be shown in Chapter 3.

#### 2.2.2 Gradient of Green's Function Using Ewald's Method

The gradient of the periodic 2-D Green's function may be obtained by taking the gradient of the Ewald's method components. Thus, once the spatial and spectral contributions

of Ewald's method have been obtained, we have to apply the gradient operator to these contributions (2.78) and (2.79). Hence, the gradient of Green's function will be expressed as

$$\nabla G_{Ewald}(\bar{\rho}, \bar{\rho}') = \nabla G_{spectral}(\bar{\rho}, \bar{\rho}') + \nabla G_{spatial}(\bar{\rho}, \bar{\rho}')$$
(2.81)

## Spectral Component of Ewald's Method $\nabla G_{spectral}$

The gradient of the spectral component of Ewald's method is

$$\nabla G_{spectral}(\bar{\rho}, \bar{\rho}') = \frac{\partial G_{spectral}(\bar{\rho}, \bar{\rho}')}{\partial x} \cdot \hat{x} + \frac{\partial G_{spectral}(\bar{\rho}, \bar{\rho}')}{\partial y} \cdot \hat{y}$$
 (2.82)

where we have obtained that  $G_{spectral}(\bar{\rho}, \bar{\rho}')$  is

$$G_{spectral}(\bar{\rho}, \bar{\rho}') = \frac{1}{A} \sum_{m=-\infty}^{+\infty} \sum_{n=-\infty}^{+\infty} \frac{e^{-j\bar{k}_{mn}\cdot(\bar{\rho}-\bar{\rho}')}}{|\bar{k}_{mn}|^2 - k^2} e^{-\frac{|\bar{k}_{mn}|^2 - k^2}{4\varepsilon^2}}$$
(2.83)

The partial derivative with respect to x can be calculated as

$$\frac{\partial G_{spectral}(\bar{\rho}, \bar{\rho}')}{\partial x} = \frac{\partial}{\partial x} \left( \frac{1}{A} \sum_{m=-\infty}^{+\infty} \sum_{n=-\infty}^{+\infty} \frac{e^{-j\bar{k}_{mn} \cdot (\bar{\rho} - \bar{\rho}')}}{|\bar{k}_{mn}|^2 - k^2} e^{-\frac{|\bar{k}_{mn}|^2 - k^2}{4\varepsilon^2}} \right)$$

$$= \frac{\partial}{\partial x} \left( \frac{1}{A} \sum_{m=-\infty}^{+\infty} \sum_{n=-\infty}^{+\infty} \frac{e^{-jk_{mn}(x-x')} e^{-jk_{ymn}(y-y')}}{|\bar{k}_{mn}|^2 - k^2} e^{-\frac{|\bar{k}_{mn}|^2 - k^2}{4\varepsilon^2}} \right)$$

$$= \frac{1}{A} \sum_{m=-\infty}^{+\infty} \sum_{n=-\infty}^{+\infty} -jk_{xmn} \frac{e^{-j\bar{k}_{mn} \cdot (\bar{\rho} - \bar{\rho}')}}{|\bar{k}_{mn}|^2 - k^2} e^{-\frac{|\bar{k}_{mn}|^2 - k^2}{4\varepsilon^2}}$$
(2.84)

Similarly, the partial derivative of  $G_{spectral}(\bar{\rho}, \bar{\rho}')$  with respect to y can be calculated as

$$\frac{\partial G_{spectral}(\bar{\rho}, \bar{\rho}')}{\partial y} = \frac{1}{A} \sum_{m=-\infty}^{+\infty} \sum_{n=-\infty}^{+\infty} -jk_{ymn} \frac{e^{-j\bar{k}_{mn}\cdot(\bar{\rho}-\bar{\rho}')}}{|\bar{k}_{mn}|^2 - k^2} e^{-\frac{|\bar{k}_{mn}|^2 - k^2}{4\varepsilon^2}}$$
(2.85)

And therefore,  $\nabla G_{spectral}(\bar{\rho}, \bar{\rho}')$  can be written as

$$\nabla G_{spectral}(\bar{\rho}, \bar{\rho}') = \frac{1}{A} \sum_{m=-\infty}^{+\infty} \sum_{n=-\infty}^{+\infty} \frac{e^{-j\bar{k}_{mn}\cdot(\bar{\rho}-\bar{\rho}')}}{|\bar{k}_{mn}|^2 - k^2} e^{-\frac{|\bar{k}_{mn}|^2 - k^2}{4\varepsilon^2}} \left[ -jk_{xmn} \cdot \hat{x} - jk_{ymn} \cdot \hat{y} \right]$$
(2.86)

## Spatial Component of Ewald's Method $\nabla G_{spatial}$

The gradient of the spatial component of Ewald's method is

$$\nabla G_{spatial}(\bar{\rho}, \bar{\rho}') = \frac{\partial G_{spatial}(\bar{\rho}, \bar{\rho}')}{\partial x} \cdot \hat{x} + \frac{\partial G_{spatial}(\bar{\rho}, \bar{\rho}')}{\partial y} \cdot \hat{y}$$
 (2.87)

where we have obtained that  $G_{spatial}(\bar{\rho}, \bar{\rho}')$  is

$$G_{spatial}(\bar{\rho}, \bar{\rho}') = \frac{1}{4\pi} \sum_{m=-\infty}^{+\infty} \sum_{n=-\infty}^{+\infty} e^{-j\bar{k}_{w0}\cdot\bar{\rho}_{mn}} \times \sum_{q=0}^{+\infty} \left(\frac{k}{2\varepsilon}\right)^{2q} \frac{1}{q!} \operatorname{E}_{q+1}(S_{mn}^2 \varepsilon^2) \quad (2.88)$$

The partial derivative with respect to x can be calculated as

$$\frac{\partial G_{spatial}(\bar{\rho}, \bar{\rho}')}{\partial x} = \frac{\partial}{\partial x} \left( \frac{1}{4\pi} \sum_{m=-\infty}^{+\infty} \sum_{n=-\infty}^{+\infty} e^{-j\bar{k}_{w0} \cdot \bar{\rho}_{mn}} \times \sum_{q=0}^{+\infty} \left( \frac{k}{2\varepsilon} \right)^{2q} \frac{1}{q!} \operatorname{E}_{q+1}(S_{mn}^2 \varepsilon^2) \right)$$
(2.89)

applying the derivative of the q-th order exponential integral

$$\frac{\partial E_{q+1}(z)}{\partial z} = -E_q(z) \tag{2.90}$$

and remembering that  $S_{mn}$  is

$$S_{mn}^{2} = |[x - x' - (ma_{1x} + na_{2x})]\hat{x} + [y - y' - (ma_{1y} + na_{2y})]\hat{y}|^{2}$$

$$= [x - x' - (ma_{1x} + na_{2x})]^{2} + [y - y' - (ma_{1y} + na_{2y})]^{2}$$
(2.91)

$$\frac{\partial G_{spatial}(\bar{\rho},\bar{\rho}')}{\partial x}$$
 remains

$$\frac{\partial G_{spatial}(\bar{\rho}, \bar{\rho}')}{\partial x} = \frac{1}{4\pi} \sum_{m=-\infty}^{+\infty} \sum_{n=-\infty}^{+\infty} e^{-j\bar{k}_{w0}\cdot\bar{\rho}_{mn}} \times \sum_{q=0}^{+\infty} \left(\frac{k}{2\varepsilon}\right)^{2q} \frac{1}{q!} \left(-\operatorname{E}_{q}(S_{mn}^{2}\varepsilon^{2})\right)$$

$$\cdot 2\varepsilon^{2} [x - x' - (ma_{1x} + na_{2x})]$$

$$= \frac{-\varepsilon^{2}}{2\pi} \sum_{m=-\infty}^{+\infty} \sum_{n=-\infty}^{+\infty} [x - x' - (ma_{1x} + na_{2x})] e^{-j\bar{k}_{w0}\cdot\bar{\rho}_{mn}} \times \sum_{q=0}^{+\infty} \left(\frac{k}{2\varepsilon}\right)^{2q} \frac{1}{q!} \operatorname{E}_{q}(S_{mn}^{2}\varepsilon^{2})$$
(2.92)

Similarly, the partial derivative of  $G_{spatial}(\bar{\rho}, \bar{\rho}')$  with respect to y can be calculated as

$$\frac{\partial G_{spatial}(\bar{\rho}, \bar{\rho}')}{\partial y} = \frac{-\varepsilon^2}{2\pi} \sum_{m=-\infty}^{+\infty} \sum_{n=-\infty}^{+\infty} [y - y' - (ma_{1y} + na_{2y})] e^{-j\bar{k}_{w0} \cdot \bar{\rho}_{mn}} \\
\times \sum_{q=0}^{+\infty} \left(\frac{k}{2\varepsilon}\right)^{2q} \frac{1}{q!} \operatorname{E}_{q}(S_{mn}^{2}\varepsilon^{2})$$
(2.93)

And therefore,  $\nabla G_{spatial}(\bar{\rho}, \bar{\rho}')$  can be written as

$$\nabla G_{spatial}(\bar{\rho}, \bar{\rho}') = \frac{-\varepsilon^{2}}{2\pi} \sum_{m=-\infty}^{+\infty} \sum_{n=-\infty}^{+\infty} e^{-j\bar{k}_{w0}\cdot\bar{\rho}_{mn}} \times \sum_{q=0}^{+\infty} \left(\frac{k}{2\varepsilon}\right)^{2q} \frac{1}{q!} \operatorname{E}_{q}(S_{mn}^{2}\varepsilon^{2}) \times \left\{ \left[x - x' - (ma_{1x} + na_{2x})\right] \cdot \hat{x} + \left[y - y' - (ma_{1y} + na_{2y})\right] \cdot \hat{y} \right\}$$
(2.94)

Once we have obtained these two contributions, we can summarize the final gradient of the 2-D Green's function with 2-D periodicity using Ewald's method

$$\nabla G_{Ewald}(\bar{\rho}, \bar{\rho}') = \nabla G_{spectral}(\bar{\rho}, \bar{\rho}') + \nabla G_{spatial}(\bar{\rho}, \bar{\rho}')$$

$$= \frac{1}{A} \sum_{m=-\infty}^{+\infty} \sum_{n=-\infty}^{+\infty} \frac{e^{-j\bar{k}_{mn} \cdot (\bar{\rho} - \bar{\rho}')}}{|\bar{k}_{mn}|^2 - k^2} e^{-\frac{|\bar{k}_{mn}|^2 - k^2}{4\varepsilon^2}} [-jk_{xmn} \cdot \hat{x} - jk_{ymn} \cdot \hat{y}]$$

$$- \frac{\varepsilon^2}{2\pi} \sum_{m=-\infty}^{+\infty} \sum_{n=-\infty}^{+\infty} e^{-j\bar{k}_{w0} \cdot \bar{\rho}_{mn}} \times \sum_{q=0}^{+\infty} \left(\frac{k}{2\varepsilon}\right)^{2q} \frac{1}{q!} E_q(S_{mn}^2 \varepsilon^2)$$

$$\times \left\{ [x - x' - (ma_{1x} + na_{2x})] \cdot \hat{x} + [y - y' - (ma_{1y} + na_{2y})] \cdot \hat{y} \right\}$$

$$(2.95)$$

In order to summarize, in this section we have transformed the original series which are extremely slowly convergent into the sum of two contributions which exhibit a fast convergence. This has been achieved through the application of Ewald's method. In addition, the relation proved in this section  $\tilde{G}(\bar{\rho}, \bar{\rho}') = G_{Ewald}(\bar{\rho}, \bar{\rho}') = G_{spectral}(\bar{\rho}, \bar{\rho}') + G_{spatial}(\bar{\rho}, \bar{\rho}')$  will be decisive in following procedures when we use the components of Ewald's method to sum the spectral Green's function.

The improvement obtained by this technique in the computation of both Green's function and its gradient will be shown in Chapter 3.

## 2.2.3 On the Splitting Parameter in Ewald's Method

The parameter  $\varepsilon$  controls the convergence rate of the two series involved in Ewald's method. A larger  $\varepsilon$  makes the spatial series  $G_{spatial}$  converge faster while a smaller  $\varepsilon$  makes the spectral series  $G_{spectral}$  converge faster. Initially, the *splitting parameter* is an arbitrary number but the *optimum splitting parameter* is used to balance the asymptotic convergence rate between these two series.

The behaviour of the spectral Ewald's method component for a large number of terms is

$$G_{spectral} \sim e^{-\frac{|\bar{k}_{mn}|^2}{4\varepsilon^2}}$$
 (2.96)

$$\sigma_{spectral}^{2} = \left(\frac{\pi}{A\varepsilon}\right)^{2} \left[ (Pa_{2y} - Qa_{1y})^{2} + (-Pa_{2x} + Qa_{1x}) \right]$$
 (2.97)

where P and Q are the numbers of terms needed to achieve the convergence factor  $\sigma_{spectral}^2$ . P is the number of terms in the outer series and Q is the number of terms in the inner series.

On the other hand, the behaviour of the spatial Ewald's method component for a large number of terms is

$$G_{spatial} \sim \frac{e^{S_{mn}^2 \varepsilon^2}}{S_{mn}^2 \varepsilon^2}$$
 (2.98)

$$\sigma_{spatial}^2 = \varepsilon^2 \left[ (Ma_{1x} + Na_{2x})^2 + (Ma_{1y} + Na_{2y})^2 \right]$$
 (2.99)

where M and N are the numbers of terms needed to achieve this convergence factor  $\sigma_{spatial}^2$ . M is the number of terms in the outer series and N is the number of terms in the inner series.

We are interested in balancing the asymptotic convergences of these series. Because of this, we make equal the convergence factor  $\sigma_{spatial}^2 = \sigma_{spectral}^2$ 

$$\varepsilon^{2} \left[ (Ma_{1x} + Na_{2x})^{2} + (Ma_{1y} + Na_{2y})^{2} \right] = \left( \frac{\pi}{A\varepsilon} \right)^{2} \left[ (Pa_{2y} - Qa_{1y})^{2} + (-Pa_{2x} + Qa_{1x}) \right]$$

$$\varepsilon^{2} M^{2} \left[ (a_{1x} + \frac{N}{M}a_{2x})^{2} + (a_{1y} + \frac{N}{M}a_{2y})^{2} \right] = \left( \frac{\pi P}{A\varepsilon} \right)^{2} \left[ (a_{2y} - \frac{Q}{P}a_{1y})^{2} + (-a_{2x} + \frac{Q}{P}a_{1x}) \right]$$
(2.100)

Assuming that the components in Ewald's method are calculated using the same number of terms in the outer series M=P and in the inner series N=Q and defining F as F=N/M=Q/P, the equation (2.100) remains

$$\varepsilon^4 = \frac{\pi^2}{A^2} \frac{\mathcal{P}^2 \left[ (a_{2y} - Fa_{1y})^2 + (-a_{2x} + Fa_{1x}) \right]}{\mathcal{M}^2 \left[ (a_{1x} + Fa_{2x})^2 + (a_{1y} + Fa_{2y})^2 \right]}$$
(2.101)

$$\varepsilon = \sqrt{\frac{\pi}{A}} \sqrt[4]{\frac{\left[ (a_{2y} - Fa_{1y})^2 + (-a_{2x} + Fa_{1x}) \right]}{\left[ (a_{1x} + Fa_{2x})^2 + (a_{1y} + Fa_{2y})^2 \right]}}$$
(2.102)

This general splitting parameter can be particularized depending on the case that we are interested in. This is because the parameter F controls the relation between the number of terms used in the outer and in the inner series. For instance, if the array is not square, that is,  $d_1 \neq d_2$ , it could be worth adjusting the factor F according to the relation between  $d_1$  and  $d_2$ .

On the other hand, if we assume that the number of terms used in the outer and in the inner series is the same, the factor F is F = 1. Being in this case, we can use the following relations

$$|\bar{a}_2 - \bar{a}_1| = \sqrt{(a_{2y} - a_{1y})^2 + (a_{2x} - a_{1x})^2}$$

$$|\bar{a}_1 + \bar{a}_2| = \sqrt{(a_{1x} + a_{2x})^2 + (a_{1y} + a_{2y})^2}$$

$$A = |\bar{a}_1 \times \bar{a}_2|$$
(2.103)

to express the *splitting parameter* as

$$\varepsilon = \sqrt{\frac{\pi |\bar{a}_2 - \bar{a}_1|}{|\bar{a}_1 + \bar{a}_2| |\bar{a}_1 \times \bar{a}_2|}}$$
 (2.104)

This splitting parameter has already been reported in [2]. In addition, in [2] they suggest to choose the splitting parameter as

$$\varepsilon = \max \left\{ \sqrt{\frac{\pi |\bar{a}_2 - \bar{a}_1|}{|\bar{a}_1 + \bar{a}_2| |\bar{a}_1 \times \bar{a}_2|}}, \frac{|\sqrt{k^2 - |\bar{k}_{00}|^2}|}{2H} \right\}$$
 (2.105)

This allows to avoid cancellation errors arising from the addition of very large nearly-equal numbers of opposite sign.

Another way to obtain the *splitting parameter* is following a procedure similar to those reported in [2,5]. We assume that we first order the pairs (m,n) and (p,q) according to their importance in the convergence of the series. This can result in two vectors of pairs of terms, whose lengths are M and P. This allows us to sum in first place the most relevant terms. In this sense, the total number of terms is  $N^{tot} = M + P$ .

$$\sigma = \left(\frac{\pi P}{A\varepsilon}\right) \sqrt{(a_{2y} - a_{1y})^2 + (a_{2x} - a_{1x})}$$
 (2.106)

$$\sigma = \varepsilon M \sqrt{(a_{1x} + a_{2x})^2 + (a_{1y} + a_{2y})^2}$$
 (2.107)

$$N^{tot} = M + P = \underbrace{\varepsilon M \sqrt{(a_{1x} + a_{2x})^2 + (a_{1y} + a_{2y})^2}}_{\sigma} \cdot \frac{1}{\varepsilon \sqrt{(a_{1x} + a_{2x})^2 + (a_{1y} + a_{2y})^2}}$$

$$+ \underbrace{\left(\frac{\pi P}{A\varepsilon}\right) \sqrt{(a_{2y} - a_{1y})^2 + (a_{2x} - a_{1x})}}_{\sigma} \cdot \frac{A\varepsilon}{\pi \sqrt{(a_{2y} - a_{1y})^2 + (a_{2x} - a_{1x})}}$$

$$= \sigma \left(\frac{1}{\varepsilon |\bar{a}_1 + \bar{a}_2|} + \frac{|\bar{a}_1 \times \bar{a}_2|\varepsilon}{\pi |\bar{a}_2 - \bar{a}_1|}\right)$$
(2.108)

As we are interested in minimizing the total number of term, we have to calculate the derivative of  $N^{tot}$  respect to  $\varepsilon$  and make it equal to zero.

$$\frac{\partial N^{tot}}{\partial \varepsilon} = 0$$

$$\frac{\partial}{\partial \varepsilon} \left\{ \sigma \left( \frac{1}{\varepsilon |\bar{a}_1 + \bar{a}_2|} + \frac{|\bar{a}_1 \times \bar{a}_2|\varepsilon}{\pi |\bar{a}_2 - \bar{a}_1|} \right) \right\} = 0$$

$$\sigma \left( \frac{-1}{\varepsilon^2 |\bar{a}_1 + \bar{a}_2|} + \frac{|\bar{a}_1 \times \bar{a}_2|}{\pi |\bar{a}_2 - \bar{a}_1|} \right) = 0$$

$$\frac{|\bar{a}_1 \times \bar{a}_2|}{\pi |\bar{a}_2 - \bar{a}_1|} = \frac{1}{\varepsilon^2 |\bar{a}_1 + \bar{a}_2|}$$
(2.109)

Finally,

$$\varepsilon = \sqrt{\frac{\pi |\bar{a}_2 - \bar{a}_1|}{|\bar{a}_1 \times \bar{a}_2| |\bar{a}_1 + \bar{a}_2|}}$$
 (2.110)

As can be seen, this value of  $\varepsilon$  is equal to the obtained in (2.104) where the same conditions have to be assumed.

The values of the *splitting parameter* reported in this subsection will be used in the implementation of Ewald's method in Chapter 3.

# 2.3 Spectral Kummer's Transformation

As can be appreciated from the previous sections, the spatial and the spectral representations of the 2-D Green's function with 2-D periodicity are slowly convergent. In the particular case of 2-D periodicity, the spatial representation exhibits an extremely slow convergence in all possible scenarios. For this reason, some acceleration technique has to be applied. In addition to Ewald's method, another analytical technique that has been widely used is the spectral Kummer's transformation.

This method consists of extracting the asymptotic part of the series to accelerate the dynamic part and trying to sum it analytically, whenever possible. This technique has been efficiently employed to accelerate the convergence of the 2-D Green's functions with 1-D periodicity in [5,11] and has been reviewed in Section 1.1.

In relation to the 2-D Green's functions with 2-D periodicity, different methods based on the spectral Kummer's technique have been reported before [2, 3] to accelerate the evaluation of the double series involved in these functions.

In this chapter, we apply Kummer's transformation to the spectral 2-D Green's function with 2-D periodicity to accelerate its slow convergence. Our intention is to carry out an in-depth study about the two possible approaches in the extraction of the asymptotic part, as has been done in Chapter 1. It is important to note that, while in the previous sections of this chapter we have worked with both the general and the phase-shifted array 2-D Green's function, from here we are going to deal only with the phase-shifted array 2-D Green's functions. This is because it is the most interesting case for us due to its applicability to the problems which involves rectangular waveguides and 2-D cavities.

For this purpose, we begin with the spectral 2-D Green's function obtained in (2.28)

$$\widetilde{G}(\bar{\rho}, \bar{\rho}') = \frac{1}{A} \sum_{m=-\infty}^{+\infty} \sum_{n=-\infty}^{+\infty} \frac{e^{-j\bar{k}_{mn} \cdot (\bar{\rho} - \bar{\rho}')}}{|\bar{k}_{mn}|^2 - k^2}$$
(2.111)

and we apply Kummer's transformation through the extraction of the asymptotic term  $\widetilde{G}_{mn}$ 

$$\widetilde{G}_{k}(\bar{\rho}, \bar{\rho}') = \frac{1}{A} \sum_{\substack{m = -\infty \\ \forall m, n - \{m = n = 0\}}}^{+\infty} \sum_{\substack{n = -\infty \\ \forall m, n - \{m = n = 0\}}}^{+\infty} \left( \frac{1}{|\bar{k}_{mn}|^{2} - k^{2}} - \widetilde{G}_{mn} \right) e^{-j\bar{k}_{mn} \cdot (\bar{\rho} - \bar{\rho}')} + \widetilde{G}_{00} 
+ \frac{1}{A} \sum_{\substack{m = -\infty \\ \forall m, n - \{m = n = 0\}}}^{+\infty} \sum_{\substack{n = -\infty \\ \forall m, n - \{m = n = 0\}}}^{+\infty} \widetilde{G}_{mn} e^{-j\bar{k}_{mn} \cdot (\bar{\rho} - \bar{\rho}')}$$
(2.112)

 $\widetilde{G}_{00}$  is the contribution of the term m=n=0 in which we do not apply the extraction. The asymptotic retained series  $\widetilde{G}_e(\bar{\rho}, \bar{\rho}')$  has to be efficiently added.

$$\widetilde{G}_e(\bar{\rho}, \bar{\rho}') = \frac{1}{A} \sum_{\substack{m = -\infty \\ \forall m, n - \{m = n = 0\}}}^{+\infty} \sum_{\substack{n = -\infty \\ m = n = 0\}}}^{+\infty} \widetilde{G}_{mn} e^{-j\bar{k}_{mn} \cdot (\bar{\rho} - \bar{\rho}')}$$
(2.113)

As in Chapter 1 for the 2-D Green's function with 1-D periodicity, here we also consider that  $\widetilde{G}_{mn}$  can be obtained by two different ways resulting in two different approaches of formulating the dynamic part. Consequently, two different ways of adding the retained part can be used. The advantages of each approach will be studied in Chapter 3, where we will see that the improvement achieved by each approach is different.

For the first option, we proceed as follows

$$\frac{1}{|\bar{k}_{mn}|^2 - k^2} = \frac{1}{|\bar{k}_{mn}|^2 \left(1 - \underbrace{\left(\frac{k}{|\bar{k}_{mn}|}\right)^2}\right)}$$
(2.114)

and if we use the Taylor expansion when u = 0,

$$\frac{1}{1-u} = \sum_{t=0}^{+\infty} u^t = 1 + u + u^2 + u^3 \dots = \sum_{t=0}^{+\infty} u^t$$
 (2.115)

 $\widetilde{G}_{mn}$  can be written as

$$\widetilde{G}_{mn} = \frac{1}{|\bar{k}_{mn}|^2} \left( 1 + \left( \frac{k}{|\bar{k}_{mn}|} \right)^2 + \left( \frac{k}{|\bar{k}_{mn}|} \right)^4 + \left( \frac{k}{|\bar{k}_{mn}|} \right)^6 + \dots \right)$$

$$= \frac{1}{|\bar{k}_{mn}|^2} + \frac{k^2}{|\bar{k}_{mn}|^4} + \frac{k^4}{|\bar{k}_{mn}|^6} + \frac{k^6}{|\bar{k}_{mn}|^8} + \dots = \sum_{q=0}^{Q} \frac{k^{2q}}{|\bar{k}_{mn}|^{2(q+1)}}$$
(2.116)

where Q is the number of terms that are used in the expansion of the asymptotic series  $\widetilde{G}_{mn}$ . Thus, through the parameter Q we can choose the order of the approximation, that is, the number of terms that we extract in the application of Kummer's transformation.

It is important to note that  $\frac{1}{|\bar{k}_{mn}|^2 - k^2}$  is positive, so in this case the absolute value has been omitted because all these terms are positive due to its own absolute values. Using

this  $\widetilde{G}_{mn}$  approach, the series  $\widetilde{G}_e(\bar{\rho}, \bar{\rho}')$  that has to be efficiently summed is

$$\widetilde{G}_{e}(\bar{\rho}, \bar{\rho}') = \frac{1}{A} \sum_{\substack{m=-\infty\\\forall m,n-\{m=n=0\}}}^{+\infty} \sum_{\substack{n=-\infty\\\forall m,n-\{m=n=0\}}}^{+\infty} \left( \frac{1}{|\bar{k}_{mn}|^{2}} + \frac{k^{2}}{|\bar{k}_{mn}|^{4}} + \frac{k^{4}}{|\bar{k}_{mn}|^{6}} + \frac{k^{6}}{|\bar{k}_{mn}|^{8}} + \dots \right) e^{-j\bar{k}_{mn} \cdot (\bar{\rho} - \bar{\rho}')}$$

$$= \frac{1}{A} \sum_{\substack{m=-\infty\\\forall m,n-\{m=n=0\}}}^{+\infty} \sum_{\substack{n=-\infty\\\forall m,n-\{m=n=0\}}}^{+\infty} \left( \sum_{q=0}^{Q} \frac{k^{2q}}{|\bar{k}_{mn}|^{2(q+1)}} \right) e^{-j\bar{k}_{mn} \cdot (\bar{\rho} - \bar{\rho}')} \tag{2.117}$$

As mentioned in Chapter 1, we can realize that this approach will result in a better approximation of the spectral series. For this reason, this approach provides a faster convergence rate in comparison to the other one. The option that we propose to sum efficiently this series is:

• Option A.1: Sum by Ewald's method.

The formulation of this option will be outlined in the subsection 2.3.1.

The other approach to extract the asymptotic terms is based on the following procedure

$$\frac{1}{|\bar{k}_{mn}|^2 - k^2} = \frac{1}{\left| \left( k_{x0} + \frac{2\pi m}{d_1} \right) \hat{x} + \left( k_{y0} + \frac{2\pi n}{d_2} \right) \hat{y} \right|^2 - k^2} \\
= \frac{1}{\left( k_{x0} + \frac{2\pi m}{d_1} \right)^2 + \left( k_{y0} + \frac{2\pi n}{d_2} \right)^2 - k^2} \\
= \frac{1}{\left( k_{x0}^2 + 2\frac{2\pi m}{d_1} k_{x0} + \left( \frac{2\pi m}{d_1} \right)^2 \right) + \left( k_{y0}^2 + 2\frac{2\pi n}{d_2} k_{y0} + \left( \frac{2\pi n}{d_2} \right)^2 \right) - k^2} \tag{2.118}$$

where we can extract common factor of the terms that we are interested in as

$$\frac{1}{\left|\bar{k}_{mn}\right|^{2} - k^{2}} = \frac{1}{\left(\frac{2\pi m}{d_{1}}\right)^{2} \left(1 + \underbrace{\frac{k_{x0}d_{1}}{\pi m} + \frac{k_{x0}^{2} - k^{2}/2}{\left(\frac{2\pi m}{d_{1}}\right)^{2}}}_{u}\right) + \left(\frac{2\pi n}{d_{2}}\right)^{2} \left(1 + \underbrace{\frac{k_{y0}d_{2}}{\pi n} + \frac{k_{y0}^{2} - k^{2}/2}{\left(\frac{2\pi n}{d_{2}}\right)^{2}}}_{v}\right)}$$

$$(2.119)$$

Naming the factors  $z_u$  and  $z_v$  as

$$z_{u} = \left(\frac{2\pi m}{d_{1}}\right)^{2} \cdot u = \left(\frac{2\pi m}{d_{1}}\right)^{2} \cdot \left(\frac{k_{x0}d_{1}}{\pi m} + \frac{k_{x0}^{2} - k^{2}/2}{\left(\frac{2\pi m}{d_{1}}\right)^{2}}\right) = k_{x0}^{2} - k^{2}/2 + \frac{4\pi m k_{x0}}{d_{1}}$$
(2.120a)

$$z_v = \left(\frac{2\pi n}{d_2}\right)^2 \cdot v = \left(\frac{2\pi n}{d_2}\right)^2 \cdot \left(\frac{k_{y0}d_2}{\pi n} + \frac{k_{y0}^2 - k^2/2}{\left(\frac{2\pi n}{d_2}\right)^2}\right) = k_{y0}^2 - k^2/2 + \frac{4\pi n k_{y0}}{d_2} \quad (2.120b)$$

and carrying out the Taylor expansion using [15] when  $m \to \infty$  and  $n \to \infty$  or, what is the same,  $u \to 0$  and  $v \to 0$ , we have the following approximation  $\widetilde{G}_{mn}$ 

$$\widetilde{G}_{mn} = \frac{1}{\left(\frac{2\pi m}{d_1}\right)^2 + \left(\frac{2\pi n}{d_2}\right)^2} - \frac{z_u + z_v}{\left(\left(\frac{2\pi m}{d_1}\right)^2 + \left(\frac{2\pi n}{d_2}\right)^2\right)^2} + \frac{(z_u + z_v)^2}{\left(\left(\frac{2\pi m}{d_1}\right)^2 + \left(\frac{2\pi n}{d_2}\right)^2\right)^3} + \dots$$

$$= \sum_{q=0}^{Q} \frac{(-1)^q (z_u + z_v)^q}{\left(\left(\frac{2\pi m}{d_1}\right)^2 + \left(\frac{2\pi n}{d_2}\right)^2\right)^{q+1}} \tag{2.121}$$

Using this  $\widetilde{G}_{mn}$  approach, the series  $\widetilde{G}_e(\bar{\rho}, \bar{\rho}')$  that has to be efficiently summed is

$$\widetilde{G}_{e}(\bar{\rho}, \bar{\rho}') = \frac{1}{A} \sum_{\substack{m = -\infty \\ \forall m, n - \{m = n = 0\}}}^{+\infty} \sum_{\substack{n = -\infty \\ \forall m, n - \{m = n = 0\}}}^{+\infty} \left( \frac{1}{\left(\frac{2\pi m}{d_{1}}\right)^{2} + \left(\frac{2\pi n}{d_{2}}\right)^{2}} - \frac{z_{u} + z_{v}}{\left(\left(\frac{2\pi m}{d_{1}}\right)^{2} + \left(\frac{2\pi n}{d_{2}}\right)^{2}\right)^{2}} \right) \\
+ \frac{(z_{u} + z_{v})^{2}}{\left(\left(\frac{2\pi m}{d_{1}}\right)^{2} + \left(\frac{2\pi n}{d_{2}}\right)^{2}\right)^{3}} + \dots \right) e^{-j\bar{k}_{mn} \cdot (\bar{\rho} - \bar{\rho}')} \\
= \frac{1}{A} \sum_{\substack{m = -\infty \\ \forall m, n - \{m = n = 0\}}}^{+\infty} \sum_{\substack{n = -\infty \\ \forall m, n - \{m = n = 0\}}}^{+\infty} \left(\sum_{q = 0}^{Q} \frac{(-1)^{q} (z_{u} + z_{v})^{q}}{\left(\left(\frac{2\pi m}{d_{1}}\right)^{2} + \left(\frac{2\pi n}{d_{2}}\right)^{2}\right)^{q+1}}\right) e^{-j\bar{k}_{mn} \cdot (\bar{\rho} - \bar{\rho}')}$$

$$(2.122)$$

In advance, we can realize that this approach will result in a worse approximation of the spectral series and for this reason in a slower convergence rate in comparison to the previous one. However, the advantage here is that the remaining series is quasi-static so it would be better in the case of problems that require a frequency sweep. The options that we propose to sum efficiently this series are:

- Option B.1: Sum by Ewald's method.
- Option B.2: Lerch transcendent.
- Option B.3: Summation by parts technique.
- Option B.4: Analytical sum in one index.

The formulation of each option will be detailed in the subsections 2.3.2, 2.3.3, 2.3.4 and 2.3.5, respectively.

To summarize, in the option A we are assuming that  $\left(k_{x0} + \frac{2\pi m}{d_1}\right)$  and  $\left(k_{y0} + \frac{2\pi n}{d_2}\right)$  are more significant than k, in the approximation of  $\frac{1}{|\bar{k}_{mn}|^2 - k^2}$  but in the option B we are assuming that not only are  $\left(\frac{2\pi m}{d_1}\right)$  and  $\left(\frac{2\pi n}{d_2}\right)$  more important than k but also than  $k_{x0}$  and  $k_{y0}$ . For this reason, the approximation A is more complete than B and therefore the improvement resulted through the option A would be better. On the contrary, it has the disadvantage of containing the frequency in the terms  $k_{x0}$  and  $k_{y0}$ . Depending on the problem to be solved, we can choose which to use.

In the following sections, we explain how to add efficiently the remaining part of the Kummer's series  $\widetilde{G}_e(\bar{\rho}, \bar{\rho}')$  using both approaches. It is important to note that, whenever possible, we will try to explain the methods in a general way for the extraction of Q asymptotic terms.

# 2.3.1 Option A.1. Approach of $\bar{k}_{mn}$ : Sum by Ewald's Method.

The first alternative to sum the asymptotic retained terms obtained by the application of this first approach of Kummer's transformation is using the corresponding terms in Ewald's method. This can be considered a combination of both techniques. By using this proposed Kummer-Ewald transformation we are able to choose the effort that we want to invest in each technique.

We start with the connection between the first asymptotic term in the spectral domain and the first asymptotic term in Ewald's method. Then, we extract the second term and we extend this formulation to the extraction of Q terms.

• Extraction of one term.

In this case, the series  $\widetilde{G}_e(\bar{\rho}, \bar{\rho}')$  that we have to efficiently sum is

$$\widetilde{G}_{e}(\bar{\rho}, \bar{\rho}') = \frac{1}{A} \sum_{\substack{m = -\infty \\ \forall m, n - \{m = n = 0\}}}^{+\infty} \sum_{\substack{n = -\infty \\ m = n = 0\}}}^{+\infty} \frac{1}{|\bar{k}_{mn}|^{2}} e^{-j\bar{k}_{mn} \cdot (\bar{\rho} - \bar{\rho}')}$$
(2.123)

The idea is to identify this series with an approximation of the spectral one and then use Ewald's transformation to sum the asymptotic series

$$\widetilde{G}_{e}(\bar{\rho}, \bar{\rho}') = \frac{1}{A} \sum_{\substack{m = -\infty \\ \forall m, n - \{m = n = 0\}}}^{+\infty} \sum_{\substack{n = -\infty \\ \forall m, n - \{m = n = 0\}}}^{+\infty} \frac{1}{|\bar{k}_{mn}|^{2}} e^{-j\bar{k}_{mn} \cdot (\bar{\rho} - \bar{\rho}')}$$

$$= \underbrace{\frac{1}{A} \sum_{m = -\infty}^{+\infty} \sum_{n = -\infty}^{+\infty} \frac{1}{|\bar{k}_{mn}|^{2}} e^{-j\bar{k}_{mn} \cdot (\bar{\rho} - \bar{\rho}')} - \frac{1}{A} \frac{1}{|\bar{k}_{00}|^{2}} e^{-j\bar{k}_{00} \cdot (\bar{\rho} - \bar{\rho}')}}$$
(2.124)

Taking into account that the spectral Green's function is

$$\widetilde{G}(\bar{\rho}, \bar{\rho}') = \frac{1}{A} \sum_{m=-\infty}^{+\infty} \sum_{n=-\infty}^{+\infty} \frac{e^{-j\bar{k}_{mn} \cdot (\bar{\rho} - \bar{\rho}')}}{|\bar{k}_{mn}|^2 - k^2}$$
(2.125)

we would like to obtain the approximation of the previous series when  $m \to \infty$  and  $n \to \infty$ 

$$\widetilde{G}(\bar{\rho}, \bar{\rho}')\Big|_{\substack{m \to +\infty \\ n \to +\infty}} = \frac{1}{A} \sum_{m = -\infty}^{+\infty} \sum_{n = -\infty}^{+\infty} \frac{e^{-j\bar{k}_{mn} \cdot (\bar{\rho} - \bar{\rho}')}}{|\bar{k}_{mn}|^2 - k^2} \Big|_{\substack{m \to +\infty \\ n \to +\infty}}$$

$$= \frac{1}{A} \sum_{m = -\infty}^{+\infty} \sum_{n = -\infty}^{+\infty} \frac{e^{-j\bar{k}_{mn} \cdot (\bar{\rho} - \bar{\rho}')}}{|\bar{k}_{mn}|^2}$$
(2.126)

Now, the series S obtained in the retained first term (2.124) can be identified with the previous approximation of the spectral formulation and thus

$$\widetilde{G}_{e}(\bar{\rho}, \bar{\rho}') = \widetilde{G}(\bar{\rho}, \bar{\rho}') \Big|_{\substack{m \to +\infty \\ n \to +\infty}} - \frac{1}{A} \frac{1}{|\bar{k}_{00}|^{2}} e^{-j\bar{k}_{00} \cdot (\bar{\rho} - \bar{\rho}')}$$
(2.127)

Since

$$\widetilde{G}(\bar{\rho}, \bar{\rho}')\Big|_{\substack{m \to +\infty \\ n \to +\infty}} = G_{Ewald}(\bar{\rho}, \bar{\rho}')\Big|_{\substack{m \to +\infty \\ n \to +\infty}} = \left[G_{spectral}(\bar{\rho}, \bar{\rho}') + G_{spatial}(\bar{\rho}, \bar{\rho}')\right]\Big|_{\substack{m \to +\infty \\ n \to +\infty}}$$
(2.128)

we can sum S using Ewald's transformation by the use of the approximation of the Ewald's method components when  $m \to \infty$  and  $n \to \infty$ .

Remembering that the spectral Ewald's method component  $G_{spectral}(\bar{\rho}, \bar{\rho}')$  is obtained in (2.66) as

$$G_{spectral}(\bar{\rho}, \bar{\rho}') = \frac{1}{A} \sum_{m=-\infty}^{+\infty} \sum_{n=-\infty}^{+\infty} \frac{e^{-j\bar{k}_{mn}\cdot(\bar{\rho}-\bar{\rho}')}}{|\bar{k}_{mn}|^2 - k^2} e^{-\frac{|\bar{k}_{mn}|^2 - k^2}{4\varepsilon^2}}$$
(2.129)

The approximation of  $G_{spectral}(\bar{\rho}, \bar{\rho}')$  is given by

$$G_{spectral}(\bar{\rho}, \bar{\rho}')\Big|_{\substack{m \to +\infty \\ n \to +\infty}} = \left(\frac{1}{A} \sum_{m=-\infty}^{+\infty} \sum_{n=-\infty}^{+\infty} \frac{e^{-j\bar{k}_{mn} \cdot (\bar{\rho} - \bar{\rho}')}}{|\bar{k}_{mn}|^2 - k^2} e^{-\frac{|\bar{k}_{mn}|^2 - k^2}{4\varepsilon^2}}\right)\Big|_{\substack{m \to +\infty \\ n \to +\infty}}$$

$$= \frac{1}{A} \sum_{m=-\infty}^{+\infty} \sum_{n=-\infty}^{+\infty} \frac{e^{-j\bar{k}_{mn} \cdot (\bar{\rho} - \bar{\rho}')}}{|\bar{k}_{mn}|^2} e^{-\frac{|\bar{k}_{mn}|^2}{4\varepsilon^2}}$$
(2.130)

We are not interested in summing the term m = n = 0 directly, so we separate it

$$\frac{1}{A} \sum_{m=-\infty}^{+\infty} \sum_{n=-\infty}^{+\infty} \frac{e^{-j\bar{k}_{mn}\cdot(\bar{\rho}-\bar{\rho}')}}{|\bar{k}_{mn}|^2} e^{-\frac{|\bar{k}_{mn}|^2}{4\varepsilon^2}} = \frac{1}{A} \sum_{\substack{m=-\infty\\\forall m,n-\{m=n=0\}}}^{+\infty} \sum_{n=-\infty}^{+\infty} \frac{e^{-j\bar{k}_{mn}\cdot(\bar{\rho}-\bar{\rho}')}}{|\bar{k}_{mn}|^2} e^{-\frac{|\bar{k}_{mn}|^2}{4\varepsilon^2}} + \frac{1}{A} \frac{e^{-j\bar{k}_{00}\cdot(\bar{\rho}-\bar{\rho}')}}{|\bar{k}_{00}|^2} e^{-\frac{|\bar{k}_{00}|^2}{4\varepsilon^2}} \tag{2.131}$$

On the other hand, recalling that the spatial Ewald's method component  $G_{spatial}(\bar{\rho}, \bar{\rho}')$  is obtained in (2.79) as

$$G_{spatial}(\bar{\rho}, \bar{\rho}') = \frac{1}{4\pi} \sum_{m=-\infty}^{+\infty} \sum_{p=-\infty}^{+\infty} e^{-j\bar{k}_{w0}\cdot\bar{\rho}_{mn}} \sum_{q=0}^{+\infty} \left(\frac{k}{2\varepsilon}\right)^{2q} \frac{1}{q!} \operatorname{E}_{q+1}(S_{mn}^2 \varepsilon^2) \qquad (2.132)$$

The approximation when  $m \to \infty$  and  $n \to \infty$  in the spectral domain corresponds to the limit when  $k \to 0$  in the spatial domain. Therefore, the limit of  $G_{spatial}(\bar{\rho}, \bar{\rho}')$  when  $k \to 0$  is given by

$$\lim_{k \to 0} G_{spatial}(\bar{\rho}, \bar{\rho}') = \lim_{k \to 0} \left( \frac{1}{4\pi} \sum_{m = -\infty}^{+\infty} \sum_{n = -\infty}^{+\infty} e^{-j\bar{k}_{w0} \cdot \bar{\rho}_{mn}} \sum_{q = 0}^{+\infty} \left( \frac{k}{2\varepsilon} \right)^{2q} \frac{1}{q!} \operatorname{E}_{q+1}(S_{mn}^2 \varepsilon^2) \right)$$

$$= \frac{1}{4\pi} \sum_{m = -\infty}^{+\infty} \sum_{n = -\infty}^{+\infty} e^{-j\bar{k}_{w0} \cdot \bar{\rho}_{mn}} \operatorname{E}_{1}(S_{mn}^2 \varepsilon^2)$$
(2.133)

The found limits of Ewald's method components can be used to sum the series S

$$S = \frac{1}{A} \sum_{m=-\infty}^{+\infty} \sum_{n=-\infty}^{+\infty} \frac{e^{-j\bar{k}_{mn}\cdot(\bar{\rho}-\bar{\rho}')}}{|\bar{k}_{mn}|^2} = \frac{1}{A} \sum_{\substack{m=-\infty\\\forall m,n-\{m=n=0\}}}^{+\infty} \sum_{\substack{n=-\infty\\\forall m,n-\{m=n=0\}}}^{+\infty} \frac{e^{-j\bar{k}_{mn}\cdot(\bar{\rho}-\bar{\rho}')}}{|\bar{k}_{mn}|^2} e^{-\frac{|\bar{k}_{mn}|^2}{4\varepsilon^2}} + \frac{1}{4\pi} \sum_{m=-\infty}^{+\infty} \sum_{n=-\infty}^{+\infty} e^{-j\bar{k}_{w0}\cdot\bar{\rho}_{mn}} \operatorname{E}_{1}(S_{mn}^{2}\varepsilon^{2})$$

$$(2.134)$$

and using this transformation of S, we can rewrite  $\widetilde{G}_e(\bar{\rho}, \bar{\rho}')$  as follows

$$\widetilde{G}_{e}(\bar{\rho}, \bar{\rho}') = S - \frac{1}{A} \frac{1}{|\bar{k}_{00}|^{2}} e^{-j\bar{k}_{00} \cdot (\bar{\rho} - \bar{\rho}')} 
= \frac{1}{A} \sum_{\substack{m = -\infty \\ \forall m, n - \{m = n = 0\}}}^{+\infty} \sum_{\substack{n = -\infty \\ \forall m, n - \{m = n = 0\}}}^{+\infty} \frac{e^{-j\bar{k}_{mn} \cdot (\bar{\rho} - \bar{\rho}')}}{|\bar{k}_{mn}|^{2}} e^{-\frac{|\bar{k}_{mn}|^{2}}{4\varepsilon^{2}}} + \frac{1}{A} \frac{e^{-j\bar{k}_{00} \cdot (\bar{\rho} - \bar{\rho}')}}{|\bar{k}_{00}|^{2}} e^{-\frac{|\bar{k}_{00}|^{2}}{4\varepsilon^{2}}} 
+ \frac{1}{4\pi} \sum_{m = -\infty}^{+\infty} \sum_{n = -\infty}^{+\infty} e^{-j\bar{k}_{w0} \cdot \bar{\rho}_{mn}} \operatorname{E}_{1}(S_{mn}^{2}\varepsilon^{2}) - \frac{1}{A} \frac{1}{|\bar{k}_{00}|^{2}} e^{-j\bar{k}_{00} \cdot (\bar{\rho} - \bar{\rho}')}$$
(2.135)

Regrouping terms and summing together the residual terms in m = n = 0, the first asymptotic series  $\widetilde{G}_e(\bar{\rho}, \bar{\rho}')$  can be expressed as

$$\widetilde{G}_{e}(\bar{\rho}, \bar{\rho}') = \frac{1}{A} \sum_{\substack{m=-\infty\\\forall m,n-\{m=n=0\}}}^{+\infty} \sum_{\substack{n=-\infty\\\forall m,n-\{m=n=0\}}}^{+\infty} \frac{e^{-j\bar{k}_{mn}\cdot(\bar{\rho}-\bar{\rho}')}}{|\bar{k}_{mn}|^{2}} e^{-\frac{|\bar{k}_{mn}|^{2}}{4\varepsilon^{2}}} + \frac{1}{4\pi} \sum_{\substack{m=-\infty\\m=-\infty}}^{+\infty} \sum_{\substack{n=-\infty\\\forall m,n-\{m=n=0\}}}^{+\infty} e^{-j\bar{k}_{w0}\cdot\bar{\rho}_{mn}} \\
\cdot \operatorname{E}_{1}(S_{mn}^{2}\varepsilon^{2}) + \frac{1}{A} \frac{e^{-j\bar{k}_{00}\cdot(\bar{\rho}-\bar{\rho}')}}{|\bar{k}_{00}|^{2}} e^{-\frac{|\bar{k}_{00}|^{2}}{4\varepsilon^{2}}} - \frac{1}{A} \frac{1}{|\bar{k}_{00}|^{2}} e^{-j\bar{k}_{00}\cdot(\bar{\rho}-\bar{\rho}')} \\
= \frac{1}{A} \sum_{\substack{m=-\infty\\\forall m,n-\{m=n=0\}}}^{+\infty} \sum_{\substack{n=-\infty\\\forall m,n-\{m=n=0\}}}^{+\infty} \frac{e^{-j\bar{k}_{mn}\cdot(\bar{\rho}-\bar{\rho}')}}{|\bar{k}_{mn}|^{2}} e^{-\frac{|\bar{k}_{mn}|^{2}}{4\varepsilon^{2}}} + \frac{1}{4\pi} \sum_{\substack{m=-\infty\\m=-\infty}}^{+\infty} \sum_{\substack{n=-\infty\\n=-\infty}}^{+\infty} e^{-j\bar{k}_{w0}\cdot\bar{\rho}_{mn}} \\
\cdot \operatorname{E}_{1}(S_{mn}^{2}\varepsilon^{2}) + \underbrace{\frac{1}{A} \frac{e^{-j\bar{k}_{00}\cdot(\bar{\rho}-\bar{\rho}')}}{|\bar{k}_{00}|^{2}}}_{[\bar{k}_{00}]^{2}} \left( e^{-\frac{|\bar{k}_{00}|^{2}}{4\varepsilon^{2}}} - 1 \right) }$$

$$(2.136)$$

where the last term T contains the residual value when m = n = 0.

$$T = \frac{1}{A} \frac{e^{-j\bar{k}_{00} \cdot (\bar{\rho} - \bar{\rho}')}}{|\bar{k}_{00}|^2} \left( e^{-\frac{|\bar{k}_{00}|^2}{4\varepsilon^2}} - 1 \right)$$
 (2.137)

Despite there is no problem with T when  $|\bar{k}_{w0}| \neq 0$ , we have to use its limit when  $|\bar{k}_{w0}| = 0$ .

$$\lim_{|\bar{k}_{00}| \to 0} T = \lim_{|\bar{k}_{00}| \to 0} \left\{ \frac{1}{A} \frac{e^{-j\bar{k}_{00} \cdot (\bar{\rho} - \bar{\rho}')}}{|\bar{k}_{00}|^2} \left( e^{-\frac{|\bar{k}_{00}|^2}{4\varepsilon^2}} - 1 \right) \right\} = \frac{1}{A} \frac{1}{|\bar{k}_{00}|^2} \left( 1 - \frac{|\bar{k}_{00}|^2}{4\varepsilon^2} - 1 \right)$$

$$= \frac{1}{A} \frac{1}{|\bar{k}_{00}|^2} \left( -\frac{|\bar{k}_{00}|^2}{4\varepsilon^2} \right) = \frac{-1}{4A\varepsilon^2}$$
(2.138)

#### • Extraction of two terms.

In this part, we extend this procedure for the extraction of one more term in order to accelerate even more the convergence of the spectral 2-D Green's function with 2-D periodicity. In this case, the series  $\widetilde{G}_e(\bar{\rho}, \bar{\rho}')$  that we have to efficiently sum is

$$\widetilde{G}_{e}(\bar{\rho}, \bar{\rho}') = \frac{1}{A} \sum_{\substack{m = -\infty \\ \forall m, n - \{m = n = 0\}}}^{+\infty} \sum_{\substack{n = -\infty \\ m = n = 0}}^{+\infty} \left( \frac{1}{|\bar{k}_{mn}|^{2}} + \frac{k^{2}}{|\bar{k}_{mn}|^{4}} \right) e^{-j\bar{k}_{mn} \cdot (\bar{\rho} - \bar{\rho}')}$$
(2.139)

The first term can be obtained by using the approximation as in the previous section but when we are interested in extracting more than one term, we have to analyse what happens when  $m \to \infty$  and  $n \to \infty$  in the spectral series and in the Ewald's components for higher orders. For this aim, the strategy here is to obtain the retained terms by using the Taylor expansion in these proofs. Thus, the starting point of the spectral development done previously in Subsection 2.1.1 is

$$G(\bar{\rho}, \bar{\rho}') = \frac{1}{2\pi} \sum_{m=-\infty}^{+\infty} \sum_{n=-\infty}^{+\infty} e^{-jk_{x0}m\bar{a}_1} e^{-jk_{y0}n\bar{a}_2} \int_0^\infty \frac{e^{-S_{mn}^2 s^2 + \frac{k^2}{4s^2}}}{s} ds \qquad (2.140)$$

and the starting points of the proofs done in Subsection 2.2.1 of the Ewald's method components are

$$G_{spectral}(\bar{\rho}, \bar{\rho}') = \frac{1}{2\pi} \sum_{m=-\infty}^{+\infty} \sum_{n=-\infty}^{+\infty} e^{-jk_{x0}m\bar{a}_{1}} e^{-jk_{y0}n\bar{a}_{2}} \int_{0}^{\varepsilon} \frac{e^{-S_{mn}^{2}s^{2} + \frac{k^{2}}{4s^{2}}}}{s} ds \quad (2.141a)$$

$$G_{spatial}(\bar{\rho}, \bar{\rho}') = \frac{1}{2\pi} \sum_{m=-\infty}^{+\infty} \sum_{n=-\infty}^{+\infty} e^{-jk_{x0}m\bar{a}_1} e^{-jk_{y0}n\bar{a}_2} \int_{\varepsilon}^{\infty} \frac{e^{-S_{mn}^2 s^2 + \frac{k^2}{4s^2}}}{s} ds \quad (2.141b)$$

All of these components start in the spatial domain, where  $m \to \infty$  and  $n \to \infty$  corresponds to  $k \to 0$ . So we have to calculate the limit of these integrals when  $k \to 0$ . Using the following Taylor expansion when  $u \to 0$ 

$$e^u = \sum_{t=0}^{+\infty} \frac{u^t}{t!} \tag{2.142}$$

we can rewrite the exponential of k in the previous proofs as

$$e^{\frac{k^2}{4s^2}} = \sum_{n=0}^{+\infty} \frac{\left(\frac{k^2}{4s^2}\right)^n}{n!} = 1 + \frac{k^2}{4s^2} + \dots$$
 (2.143)

It can be noted that the first term of the expansion corresponds to the development done when we extract only the first term because it corresponds to the first order approximation of these components. The idea is to use the second order Taylor expansion of  $e^{\frac{k^2}{4s^2}}$  in the equations (2.140), (2.141a) and (2.141b). This will allow us to use the second order expansion of Ewald's method components to sum the second order expansion of the spectral series.

Using this expansion in the equation (2.25) of the spectral development,  $\widetilde{f}(k_x, k_y)$  remains

$$\begin{split} \widetilde{f}(k_{x},k_{y}) &\approx \frac{1}{2}e^{-j\bar{k}_{mn}\cdot(\bar{\rho}-\bar{\rho}')} \int_{0}^{\infty} \frac{1}{s^{3}} e^{-\frac{|\bar{k}_{mn}|^{2}}{4s^{2}}} \left(1 + \frac{k^{2}}{4s^{2}}\right) ds \\ &= \frac{1}{2}e^{-j\bar{k}_{mn}\cdot(\bar{\rho}-\bar{\rho}')} \int_{0}^{\infty} \frac{1}{s^{3}} e^{-\frac{|\bar{k}_{mn}|^{2}}{4s^{2}}} ds + \frac{1}{2}e^{-j\bar{k}_{mn}\cdot(\bar{\rho}-\bar{\rho}')} \int_{0}^{\infty} \frac{1}{s^{3}} e^{-\frac{|\bar{k}_{mn}|^{2}}{4s^{2}}} \frac{k^{2}}{4s^{2}} ds \\ &= \underbrace{\frac{1}{2}e^{-j\bar{k}_{mn}\cdot(\bar{\rho}-\bar{\rho}')} \int_{0}^{\infty} \frac{1}{s^{3}} e^{-\frac{|\bar{k}_{mn}|^{2}}{4s^{2}}} ds}_{S_{1}} + \underbrace{\frac{k^{2}}{2}e^{-j\bar{k}_{mn}\cdot(\bar{\rho}-\bar{\rho}')} \int_{0}^{\infty} \frac{1}{4s^{5}} e^{-\frac{|\bar{k}_{mn}|^{2}}{4s^{2}}} ds}_{S_{2}} \end{split}$$

$$(2.144)$$

In the knowledge that the previous integrals can be solved using [15] as

$$\int_0^\infty \frac{e^{-\frac{a}{s^2}}}{s^3} \, ds = \frac{1}{2a} \tag{2.145a}$$

$$\int_0^\infty \frac{e^{-\frac{a}{s^2}}}{s^5} \, ds = \frac{1}{2a^2} \tag{2.145b}$$

where in this case  $a = \frac{|\bar{k}_{mn}|^2}{4}$ , the equation (2.144) remains as

$$\widetilde{f}(k_x, k_y) \approx \frac{1}{2} e^{-j\bar{k}_{mn} \cdot (\bar{\rho} - \bar{\rho}')} \left( \frac{4}{2|\bar{k}_{mn}|^2} + \frac{16k^2}{8|\bar{k}_{mn}|^4} \right) = e^{-j\bar{k}_{mn} \cdot (\bar{\rho} - \bar{\rho}')} \left( \frac{1}{|\bar{k}_{mn}|^2} + \frac{k^2}{|\bar{k}_{mn}|^4} \right)$$
(2.146)

Thus, the second order approximation of the spectral series  $\widetilde{G}(\bar{\rho}, \bar{\rho}')$  when  $m \to \infty$  and  $n \to \infty$  is

$$\widetilde{G}(\bar{\rho}, \bar{\rho}')\big|_{\substack{m \to +\infty \\ n \to +\infty}} = \frac{1}{A} \sum_{m = -\infty}^{+\infty} \sum_{n = -\infty}^{+\infty} \left( \frac{1}{|\bar{k}_{mn}|^2} + \frac{k^2}{|\bar{k}_{mn}|^4} \right) e^{-j\bar{k}_{mn} \cdot (\bar{\rho} - \bar{\rho}')}$$
(2.147)

Using this, we can write the asymptotic spectral series  $\widetilde{G}_e(\bar{\rho}, \bar{\rho}')$  used in Kummer's transformation with the expansion of two terms as

$$\widetilde{G}_{e}(\bar{\rho}, \bar{\rho}') = \frac{1}{A} \sum_{\substack{m = -\infty \\ \forall m, n - \{m = n = 0\}}}^{+\infty} \sum_{\substack{n = -\infty \\ \forall m, n - \{m = n = 0\}}}^{+\infty} \left( \frac{1}{|\bar{k}_{mn}|^{2}} + \frac{k^{2}}{|\bar{k}_{mn}|^{4}} \right) e^{-j\bar{k}_{mn} \cdot (\bar{\rho} - \bar{\rho}')}$$

$$= \underbrace{\frac{1}{A} \sum_{m = -\infty}^{+\infty} \sum_{n = -\infty}^{+\infty} \left( \frac{1}{|\bar{k}_{mn}|^{2}} + \frac{k^{2}}{|\bar{k}_{mn}|^{4}} \right) e^{-j\bar{k}_{mn} \cdot (\bar{\rho} - \bar{\rho}')} - \frac{1}{A} \left( \frac{1}{|\bar{k}_{00}|^{2}} + \frac{k^{2}}{|\bar{k}_{00}|^{4}} \right) (2.148)}$$

$$\cdot e^{-j\bar{k}_{00} \cdot (\bar{\rho} - \bar{\rho}')}$$

where S has been identified with the approximation of the spectral series when  $m \to +\infty$  and  $n \to +\infty$ . The idea is to sum this series using Ewald's method as equation (2.128). Through this proposed Kummer-Ewald transformation, the asymptotic retained series  $\widetilde{G}_e(\bar{\rho}, \bar{\rho}')$  can be efficiently calculated by using the rapidly convergent components of Ewald's method.

The proof of spectral component of Ewald's method has been reported in Subsection 2.2.1. In this development we have to use the expansion of the exponential that depends on k when  $k \to 0$ , as we have done in the spectral asymptotic expansion. For this purpose, we start from (2.63) and we replace  $e^{\frac{k^2}{4s^2}}$  by  $1 + \frac{k^2}{4s^2}$ 

$$\widetilde{f}(k_x, k_y) \approx \frac{1}{2} e^{-j\bar{k}_{mn} \cdot (\bar{\rho} - \bar{\rho}')} \int_0^{\varepsilon} \frac{1}{s^3} e^{-\frac{|\bar{k}_{mn}|^2}{4s^2}} \left( 1 + \frac{k^2}{4s^2} \right) ds$$

$$= \frac{1}{2} e^{-j\bar{k}_{mn} \cdot (\bar{\rho} - \bar{\rho}')} \int_0^{\varepsilon} \frac{1}{s^3} e^{-\frac{|\bar{k}_{mn}|^2}{4s^2}} ds + \frac{1}{2} e^{-j\bar{k}_{mn} \cdot (\bar{\rho} - \bar{\rho}')} \int_0^{\varepsilon} \frac{1}{s^3} e^{-\frac{|\bar{k}_{mn}|^2}{4s^2}} \frac{k^2}{4s^2} ds \quad (2.149)$$

$$= \frac{1}{2} e^{-j\bar{k}_{mn} \cdot (\bar{\rho} - \bar{\rho}')} \int_0^{\varepsilon} \frac{1}{s^3} e^{-\frac{|\bar{k}_{mn}|^2}{4s^2}} ds + \frac{k^2}{2} e^{-j\bar{k}_{mn} \cdot (\bar{\rho} - \bar{\rho}')} \int_0^{\varepsilon} \frac{1}{4s^5} e^{-\frac{|\bar{k}_{mn}|^2}{4s^2}} ds$$

In the knowledge that the previous integrals can be solved using [15] as

$$\int_0^\varepsilon \frac{e^{-\frac{a}{s^2}}}{s^3} ds = \frac{1}{2a} e^{-\frac{a}{\varepsilon^2}} \tag{2.150a}$$

$$\int_0^\varepsilon \frac{e^{-\frac{a}{s^2}}}{s^5} ds = \frac{a+\varepsilon^2}{2a^2\varepsilon^2} e^{-\frac{a}{\varepsilon^2}}$$
 (2.150b)

where in this case  $a = \frac{|\bar{k}_{mn}|^2}{2}$ , the equation (2.149) remains

$$\widetilde{f}(k_{x}, k_{y}) \approx \frac{1}{2} e^{-j\bar{k}_{mn} \cdot (\bar{\rho} - \bar{\rho}')} e^{-\frac{|\bar{k}_{mn}|^{2}}{4\varepsilon^{2}}} \left[ \frac{4}{2|\bar{k}_{mn}|^{2}} + \frac{16k^{2}}{8|\bar{k}_{mn}|^{4}\varepsilon^{2}} \left( \frac{|\bar{k}_{mn}|^{2}}{4} + \varepsilon^{2} \right) \right] 
= e^{-j\bar{k}_{mn} \cdot (\bar{\rho} - \bar{\rho}')} e^{-\frac{|\bar{k}_{mn}|^{2}}{4\varepsilon^{2}}} \left( \frac{\left(1 + \frac{k^{2}}{4\varepsilon^{2}}\right)}{|\bar{k}_{mn}|^{2}} + \frac{k^{2}}{|\bar{k}_{mn}|^{4}} \right)$$
(2.151)

Using this, we can write the asymptotic spectral component using the expansion of two terms as

$$G_{spectral}(\bar{\rho}, \bar{\rho}')\big|_{\substack{m \to +\infty \\ n \to +\infty}} = \frac{1}{A} \sum_{m=-\infty}^{+\infty} \sum_{n=-\infty}^{+\infty} \left( \frac{\left(1 + \frac{k^2}{4\varepsilon^2}\right)}{\left|\bar{k}_{mn}\right|^2} + \frac{k^2}{\left|\bar{k}_{mn}\right|^4} \right) e^{-\frac{|\bar{k}_{mn}|^2}{4\varepsilon^2}} e^{-j\bar{k}_{mn} \cdot (\bar{\rho} - \bar{\rho}')}$$

$$(2.152)$$

If we separate the term in m=n=0, the expansion of  $G_{spectral}(\bar{\rho},\bar{\rho}')$  is

$$G_{spectral}(\bar{\rho}, \bar{\rho}')\Big|_{\substack{m \to +\infty \\ n \to +\infty}} = \frac{1}{A} \sum_{m=-\infty}^{+\infty} \sum_{n=-\infty}^{+\infty} \left( \frac{\left(1 + \frac{k^2}{4\varepsilon^2}\right)}{|\bar{k}_{mn}|^2} + \frac{k^2}{|\bar{k}_{mn}|^4} \right) e^{-\frac{|\bar{k}_{mn}|^2}{4\varepsilon^2}} e^{-j\bar{k}_{mn} \cdot (\bar{\rho} - \bar{\rho}')}$$

$$= \frac{1}{A} \sum_{\substack{m=-\infty \\ \forall m,n-\{m=n=0\}}}^{+\infty} \sum_{\substack{n=-\infty \\ \forall m,n-\{m=n=0\}}}^{+\infty} \left( \frac{\left(1 + \frac{k^2}{4\varepsilon^2}\right)}{|\bar{k}_{mn}|^2} + \frac{k^2}{|\bar{k}_{mn}|^4} \right) e^{-\frac{|\bar{k}_{mn}|^2}{4\varepsilon^2}} e^{-j\bar{k}_{mn} \cdot (\bar{\rho} - \bar{\rho}')}$$

$$+ \frac{1}{A} \left( \frac{\left(1 + \frac{k^2}{4\varepsilon^2}\right)}{|\bar{k}_{00}|^2} + \frac{k^2}{|\bar{k}_{00}|^4} \right) e^{-\frac{|\bar{k}_{00}|^2}{4\varepsilon^2}} e^{-j\bar{k}_{00} \cdot (\bar{\rho} - \bar{\rho}')}$$

$$(2.153)$$

On the other hand, the spatial Ewald's method component  $G_{spatial}(\bar{\rho}, \bar{\rho}')$  is obtained in Subsection 2.2.1. In this component, the summation in q corresponds to the expansion of  $e^{\frac{k^2}{4s^2}}$  previously done in the proof of the spectral series and in the proof of the spectral Ewald's component. This expansion is originally carried out in the development of the spatial Ewald's method component so the second order expansion of  $G_{spatial}(\bar{\rho}, \bar{\rho}')$  when  $k \to 0$  corresponds to the use of two terms in the q-summation.

$$\lim_{k \to 0} G_{spatial}(\bar{\rho}, \bar{\rho}') = \lim_{k \to 0} \left( \frac{1}{4\pi} \sum_{m = -\infty}^{\infty} \sum_{n = -\infty}^{\infty} e^{-j\bar{k}_{w0}\cdot\bar{\rho}_{mn}} \sum_{q = 0}^{+\infty} \left( \frac{k}{2\varepsilon} \right)^{2q} \frac{1}{q!} \operatorname{E}_{q+1}(S_{mn}^{2}\varepsilon^{2}) \right)$$

$$= \frac{1}{4\pi} \sum_{m = -\infty}^{\infty} \sum_{n = -\infty}^{\infty} e^{-j\bar{k}_{w0}\cdot\bar{\rho}_{mn}} \left[ \operatorname{E}_{1}(S_{mn}^{2}\varepsilon^{2}) + \left( \frac{k^{2}}{4\varepsilon^{2}} \right) \operatorname{E}_{2}(S_{mn}^{2}\varepsilon^{2}) \right]$$

$$(2.154)$$

Once we have the second order expansion of the Ewald's method components, we can summarize how to sum the asymptotic retained part through Ewald's method.

$$\widetilde{G}_{e}(\bar{\rho}, \bar{\rho}') = \widetilde{G}(\bar{\rho}, \bar{\rho}') \Big|_{\substack{m \to +\infty \\ n \to +\infty}} - \frac{1}{A} \left( \frac{1}{|\bar{k}_{00}|^{2}} + \frac{k^{2}}{|\bar{k}_{00}|^{4}} \right) e^{-j\bar{k}_{00} \cdot (\bar{\rho} - \bar{\rho}')}$$

$$= \frac{1}{A} \sum_{\substack{m = -\infty \\ \forall m, n - \{m = n = 0\}}}^{+\infty} \sum_{\substack{l = -\infty \\ \forall m, n - \{m = n = 0\}}}^{+\infty} \left( \frac{\left( 1 + \frac{k^{2}}{4\varepsilon^{2}} \right)}{|\bar{k}_{mn}|^{2}} + \frac{k^{2}}{|\bar{k}_{mn}|^{4}} \right) e^{-\frac{|\bar{k}_{mn}|^{2}}{4\varepsilon^{2}}} e^{-j\bar{k}_{mn} \cdot (\bar{\rho} - \bar{\rho}')}$$

$$+ \frac{1}{A} \left( \frac{\left( 1 + \frac{k^{2}}{4\varepsilon^{2}} \right)}{|\bar{k}_{00}|^{2}} + \frac{k^{2}}{|\bar{k}_{00}|^{4}} \right) e^{-\frac{|\bar{k}_{00}|^{2}}{4\varepsilon^{2}}} e^{-j\bar{k}_{00} \cdot (\bar{\rho} - \bar{\rho}')} + \frac{1}{4\pi} \sum_{m = -\infty}^{+\infty} \sum_{n = -\infty}^{+\infty} e^{-j\bar{k}_{w0} \cdot \bar{\rho}_{mn}}$$

$$\cdot \left[ E_{1}(S_{mn}^{2}\varepsilon^{2}) + \left( \frac{k^{2}}{4\varepsilon^{2}} \right) E_{2}(S_{mn}^{2}\varepsilon^{2}) \right] - \frac{1}{A} \left( \frac{1}{|\bar{k}_{00}|^{2}} + \frac{k^{2}}{|\bar{k}_{00}|^{4}} \right) e^{-j\bar{k}_{00} \cdot (\bar{\rho} - \bar{\rho}')}$$

$$(2.155)$$

Regrouping terms,  $\widetilde{G}_e(\bar{\rho}, \bar{\rho}')$  remains

$$\widetilde{G}_{e}(\bar{\rho}, \bar{\rho}') = \frac{1}{A} \sum_{\substack{m = -\infty \\ \forall m, n - \{m = n = 0\}}}^{+\infty} \sum_{\substack{n = -\infty \\ \forall m, n - \{m = n = 0\}}}^{+\infty} \left( \frac{\left( 1 + \frac{k^{2}}{4\varepsilon^{2}} \right)}{|\bar{k}_{mn}|^{2}} + \frac{k^{2}}{|\bar{k}_{mn}|^{4}} \right) e^{-\frac{|\bar{k}_{mn}|^{2}}{4\varepsilon^{2}}} e^{-j\bar{k}_{mn} \cdot (\bar{\rho} - \bar{\rho}')} \\
+ \frac{1}{4\pi} \sum_{m = -\infty}^{+\infty} \sum_{n = -\infty}^{+\infty} \sum_{n = -\infty}^{+\infty} e^{-j\bar{k}_{w0} \cdot \bar{\rho}_{mn}} \left[ E_{1}(S_{mn}^{2}\varepsilon^{2}) + \left( \frac{k^{2}}{4\varepsilon^{2}} \right) E_{2}(S_{mn}^{2}\varepsilon^{2}) \right] \\
+ \underbrace{\frac{1}{A}}_{T} e^{-j\bar{k}_{00} \cdot (\bar{\rho} - \bar{\rho}')} \left[ \left( \frac{\left( 1 + \frac{k^{2}}{4\varepsilon^{2}} \right)}{|\bar{k}_{00}|^{2}} + \frac{k^{2}}{|\bar{k}_{00}|^{4}} \right) e^{-\frac{|\bar{k}_{00}|^{2}}{4\varepsilon^{2}}} - \left( \frac{1}{|\bar{k}_{00}|^{2}} + \frac{k^{2}}{|\bar{k}_{00}|^{4}} \right) \right]$$

$$(2.156)$$

where the last term T contains the residual value when m = n = 0.

$$T = \frac{1}{A} e^{-j\bar{k}_{00} \cdot (\bar{\rho} - \bar{\rho}')} \left[ \left( \frac{\left(1 + \frac{k^2}{4\bar{\epsilon}^2}\right)}{|\bar{k}_{00}|^2} + \frac{k^2}{|\bar{k}_{00}|^4} \right) e^{-\frac{|\bar{k}_{00}|^2}{4\bar{\epsilon}^2}} - \left( \frac{1}{|\bar{k}_{00}|^2} + \frac{k^2}{|\bar{k}_{00}|^4} \right) \right]$$

$$(2.157)$$

As said before, despite there is no problem with T when  $|\bar{k}_{w0}| \neq 0$ , we have to use its limit when  $|\bar{k}_{w0}| = 0$ .

$$\lim_{|\bar{k}_{00}| \to 0} T = \lim_{|\bar{k}_{00}| \to 0} \left\{ \frac{1}{A} e^{-j\bar{k}_{00} \cdot (\bar{\rho} - \bar{\rho}')} \left[ \left( \frac{\left(1 + \frac{k^2}{4\varepsilon^2}\right)}{|\bar{k}_{00}|^2} + \frac{k^2}{|\bar{k}_{00}|^4} \right) e^{-\frac{|\bar{k}_{00}|^2}{4\varepsilon^2}} - \left( \frac{1}{|\bar{k}_{00}|^2} + \frac{k^2}{|\bar{k}_{00}|^4} \right) \right] \right\} = -\frac{8\varepsilon^2 + k^2}{32A\varepsilon^4} = -\frac{1}{4A\varepsilon^2} - \frac{k^2}{32A\varepsilon^4}$$
(2.158)

#### $\bullet$ Extraction of Q terms.

The intention in this subsection is to generalize this acceleration technique to the extraction of Q terms. The procedure is the same as the one followed previously. In this general case, the series  $\widetilde{G}_e(\bar{\rho}, \bar{\rho}')$  that has to be efficiently summed is

$$\widetilde{G}_{e}(\bar{\rho}, \bar{\rho}') = \frac{1}{A} \sum_{\substack{m = -\infty \\ \forall m, n - \{m = n = 0\}}}^{+\infty} \sum_{\substack{n = -\infty \\ m = n = 0}}^{+\infty} \left( \sum_{q = 0}^{Q} \frac{k^{2q}}{|\bar{k}_{mn}|^{2(q+1)}} \right) e^{-j\bar{k}_{mn} \cdot (\bar{\rho} - \bar{\rho}')}$$
(2.159)

As discussed earlier in this section, the idea is to identify this series with an approximation of the spectral one and then use Ewald's transformation to sum the asymptotic terms.

$$\widetilde{G}_{e}(\bar{\rho}, \bar{\rho}') = \underbrace{\frac{1}{A} \sum_{m=-\infty}^{+\infty} \sum_{n=-\infty}^{+\infty} \left( \sum_{q=0}^{Q} \frac{k^{2q}}{|\bar{k}_{mn}|^{2(q+1)}} \right) e^{-j\bar{k}_{mn} \cdot (\bar{\rho} - \bar{\rho}')}}_{S_{Q}} - \frac{1}{A} \left( \sum_{q=0}^{Q} \frac{k^{2q}}{|\bar{k}_{00}|^{2(q+1)}} \right) e^{-j\bar{k}_{00} \cdot (\bar{\rho} - \bar{\rho}')} \tag{2.160}$$

For this purpose, we replace in (2.25) the exponential  $e^{\frac{k^2}{4s^2}}$  by its Taylor expansion reported in (2.143)

$$\widetilde{f}(k_x, k_y) = \frac{1}{2} e^{-j\bar{k}_{mn} \cdot (\bar{\rho} - \bar{\rho}')} \int_0^\infty \frac{1}{s^3} e^{-\frac{|\bar{k}_{mn}|^2}{4s^2}} \left( \sum_{q=0}^{+\infty} \left( \frac{k}{2s} \right)^{2q} \frac{1}{q!} \right) ds$$

$$\approx \left( \sum_{q=0}^Q \frac{k^{2q}}{|\bar{k}_{mn}|^{2(q+1)}} \right) e^{-j\bar{k}_{mn} \cdot (\bar{\rho} - \bar{\rho}')}$$
(2.161)

Using this, we can write the asymptotic spectral series with the expansion of Q terms as

$$\widetilde{G}(\bar{\rho}, \bar{\rho}')\big|_{\substack{m \to +\infty \\ n \to +\infty}} = \frac{1}{A} \sum_{m=-\infty}^{+\infty} \sum_{n=-\infty}^{+\infty} \left( \sum_{q=0}^{Q} \frac{k^{2q}}{|\bar{k}_{mn}|^{2(q+1)}} \right) e^{-j\bar{k}_{mn} \cdot (\bar{\rho} - \bar{\rho}')}$$
(2.162)

We can identify the series  $S_Q$  in the equation (2.160) with the previous approximation of the spectral series when  $k \to 0$ . Thus, we can sum this series  $S_Q$  using Ewald's method by carrying out the same expansion  $(k \to 0)$  in the proofs of its components. Through this proposed Kummer-Ewald transformation, the asymptotic retained part can be efficiently calculated by using the rapidly convergent components of Ewald's method.

Replacing in the spectral Ewald's method component the exponential  $e^{\frac{k^2}{4s^2}}$  by its Taylor expansion reported in (2.143), (2.63) remains

$$\widetilde{f}(k_x, k_y) = \frac{1}{2} e^{-j\bar{k}_{mn} \cdot (\bar{\rho} - \bar{\rho}')} \int_0^{\varepsilon} \frac{1}{s^3} e^{-\frac{|\bar{k}_{mn}|^2}{4s^2}} \left( \sum_{q=0}^{+\infty} \left( \frac{k}{2s} \right)^{2q} \frac{1}{q!} \right) ds$$

$$\approx \left( \sum_{q=0}^{Q} \frac{k^{2q} \sum_{t=0}^{Q-q} \left( \frac{k}{2\varepsilon} \right)^{2t} \frac{1}{t!}}{|\bar{k}_{mn}|^{2(q+1)}} \right) e^{-j\bar{k}_{mn} \cdot (\bar{\rho} - \bar{\rho}')} e^{-\frac{|\bar{k}_{mn}|^2}{4\varepsilon^2}}$$
(2.163)

Using this, we can write the asymptotic spectral component using the expansion of Q terms as

$$G_{spectral}(\bar{\rho}, \bar{\rho}')|_{\substack{m \to +\infty \\ n \to +\infty}} = \frac{1}{A} \sum_{m=-\infty}^{+\infty} \sum_{n=-\infty}^{+\infty} \left( \sum_{q=0}^{Q} \frac{k^{2q} \sum_{t=0}^{Q-q} \left(\frac{k}{2\varepsilon}\right)^{2t} \frac{1}{t!}}{|\bar{k}_{mn}|^{2(q+1)}} \right) e^{-j\bar{k}_{mn} \cdot (\bar{\rho} - \bar{\rho}')} e^{-\frac{|\bar{k}_{mn}|^2}{4\varepsilon^2}}$$
(2.164)

If we separate the term m=n=0, the expansion of  $G_{spectral}(\bar{\rho}, \bar{\rho}')$  is

$$G_{spectral}(\bar{\rho}, \bar{\rho}') = \frac{1}{A} \sum_{m=-\infty}^{+\infty} \sum_{n=-\infty}^{+\infty} \left( \sum_{q=0}^{Q} \frac{k^{2q} \sum_{t=0}^{Q-q} \left(\frac{k}{2\varepsilon}\right)^{2t} \frac{1}{t!}}{|\bar{k}_{mn}|^{2(q+1)}} \right) e^{-j\bar{k}_{mn} \cdot (\bar{\rho} - \bar{\rho}')} e^{-\frac{|\bar{k}_{mn}|^{2}}{4\varepsilon^{2}}}$$

$$= \frac{1}{A} \sum_{\substack{m=-\infty\\ \forall m,n-\{m=n=0\}}}^{+\infty} \sum_{n=-\infty}^{+\infty} \left( \sum_{q=0}^{Q} \frac{k^{2q} \sum_{t=0}^{Q-q} \left(\frac{k}{2\varepsilon}\right)^{2t} \frac{1}{t!}}{|\bar{k}_{mn}|^{2(q+1)}} \right) e^{-j\bar{k}_{mn} \cdot (\bar{\rho} - \bar{\rho}')} e^{-\frac{|\bar{k}_{mn}|^{2}}{4\varepsilon^{2}}}$$

$$+ \frac{1}{A} \left( \sum_{q=0}^{Q} \frac{k^{2q} \sum_{t=0}^{Q-q} \left(\frac{k}{2\varepsilon}\right)^{2t} \frac{1}{t!}}{|\bar{k}_{00}|^{2(q+1)}} \right) e^{-j\bar{k}_{00} \cdot (\bar{\rho} - \bar{\rho}')} e^{-\frac{|\bar{k}_{00}|^{2}}{4\varepsilon^{2}}}$$

$$(2.165)$$

On the other hand, the spatial Ewald's method component  $G_{spatial}(\bar{\rho}, \bar{\rho}')$  is obtained in Subsection 2.2.1. As was pointed out, the summation in q corresponds to the expansion of  $e^{\frac{k^2}{4s^2}}$ . So, the q-th order expansion of  $G_{spatial}(\bar{\rho}, \bar{\rho}')$  when  $k \to 0$  corresponds directly to the use of Q terms in the q-summation.

$$\lim_{k \to 0} G_{spatial}(\bar{\rho}, \bar{\rho}') = \frac{1}{4\pi} \sum_{m = -\infty}^{+\infty} \sum_{n = -\infty}^{+\infty} e^{-j\bar{k}_{w0} \cdot \bar{\rho}_{mn}} \sum_{q = 0}^{Q} \left(\frac{k}{2\varepsilon}\right)^{2q} \frac{1}{q!} \, \mathrm{E}_{q+1}(S_{mn}^2 \varepsilon^2) \quad (2.166)$$

Once we have the q-th order expansion of the Ewald's method components, we can summarize how to sum the asymptotic retained part through Ewald's method as follows

$$\widetilde{G}_{e}(\bar{\rho}, \bar{\rho}') = \frac{1}{A} \sum_{\substack{m = -\infty \\ \forall m, n - \{m = n = 0\}}}^{+\infty} \sum_{\substack{n = -\infty \\ \forall m, n - \{m = n = 0\}}}^{+\infty} \left( \sum_{q = 0}^{Q} \frac{k^{2q} \sum_{t = 0}^{Q - q} \left(\frac{k}{2\varepsilon}\right)^{2t} \frac{1}{t!}}{|\bar{k}_{mn}|^{2(q+1)}} \right) e^{-j\bar{k}_{mn} \cdot (\bar{\rho} - \bar{\rho}')} e^{-\frac{|\bar{k}_{mn}|^{2}}{4\varepsilon^{2}}} \\
+ \frac{1}{4\pi} \sum_{m = -\infty}^{+\infty} \sum_{n = -\infty}^{+\infty} \sum_{n = -\infty}^{+\infty} e^{-j\bar{k}_{w0} \cdot \bar{\rho}_{mn}} \sum_{q = 0}^{Q} \left(\frac{k}{2\varepsilon}\right)^{2q} \frac{1}{q!} \operatorname{E}_{q+1}(S_{mn}^{2}\varepsilon^{2}) \\
+ \underbrace{\frac{1}{A} \left(\sum_{q = 0}^{Q} \frac{k^{2q} \sum_{t = 0}^{Q - q} \left(\frac{k}{2\varepsilon}\right)^{2t} \frac{1}{t!}}{|\bar{k}_{00}|^{2(q+1)}}\right) e^{-j\bar{k}_{00} \cdot (\bar{\rho} - \bar{\rho}')} e^{-\frac{|\bar{k}_{00}|^{2}}{4\varepsilon^{2}}} - \frac{1}{A} \left(\sum_{q = 0}^{Q} \frac{k^{2q}}{|\bar{k}_{00}|^{2(q+1)}}\right) e^{-j\bar{k}_{00} \cdot (\bar{\rho} - \bar{\rho}')} e^{-j\bar{k}_{00} \cdot (\bar{$$

where the last term  $T_Q$  contains the residual value when m=n=0.

$$T_{Q} = \frac{1}{A} \left( \sum_{q=0}^{Q} \frac{k^{2q} \sum_{t=0}^{Q-q} \left( \frac{k}{2\varepsilon} \right)^{2t} \frac{1}{t!}}{|\bar{k}_{00}|^{2(q+1)}} \right) e^{-j\bar{k}_{00} \cdot (\bar{\rho} - \bar{\rho}')} e^{-\frac{|\bar{k}_{00}|^{2}}{4\varepsilon^{2}}} - \frac{1}{A} \left( \sum_{q=0}^{Q} \frac{k^{2q}}{|\bar{k}_{00}|^{2(q+1)}} \right)$$

$$e^{-j\bar{k}_{00} \cdot (\bar{\rho} - \bar{\rho}')} = \frac{1}{A} e^{-j\bar{k}_{00} \cdot (\bar{\rho} - \bar{\rho}')} \left[ \sum_{q=0}^{Q} \frac{k^{2q}}{|\bar{k}_{00}|^{2(q+1)}} \left( e^{-\frac{|\bar{k}_{00}|^{2}}{4\varepsilon^{2}}} \sum_{t=0}^{Q-q} \left( \frac{k}{2\varepsilon} \right)^{2t} \frac{1}{t!} - 1 \right) \right]$$

$$(2.168)$$

Despite there is no problem with  $T_Q$  when  $|\bar{k}_{w0}| \neq 0$ , we have to use its limit when  $|\bar{k}_{w0}| = 0$ .

$$\lim_{|\bar{k}_{00}| \to 0} T_Q = \lim_{|\bar{k}_{00}| \to 0} \left\{ \frac{1}{A} \left( \sum_{q=0}^{Q} \frac{k^{2q}}{|\bar{k}_{00}|^{2(q+1)}} \right) e^{-j\bar{k}_{00} \cdot (\bar{\rho} - \bar{\rho}')} \left[ e^{-\frac{|\bar{k}_{00}|^2}{4\varepsilon^2}} \sum_{t=0}^{Q-q} \left( \frac{k}{2\varepsilon} \right)^{2t} \frac{1}{t!} - 1 \right] \right\}$$

$$= \frac{-1}{A} \sum_{q=0}^{Q} \frac{k^{2q}}{(q+1)! (2\varepsilon)^{2(q+1)}} \tag{2.169}$$

To summarize, in this section we have accelerated the spectral 2-D Green's function with 2-D periodicity by using Kummer's transformation and summing efficiently the asymptotic retained part through Ewald's method.

We have obtained the connection between the first, the second and the q-th order asymptotic terms in the spectral series and the summation of these with Ewald's method. This approach has been generalized to Q terms. These Q asymptotic retained terms can be summed using the rapidly convergent components of Ewald's method. By using this proposed Kummer-Ewald transformation, we are able to choose the effort that we want to invest in each technique through the parameter Q.

In this regard, the more Q terms we extract, the higher improvement we obtain through Kummer's transformation but more and more terms we have to sum by Ewald's method. Theoretically, there is not any problem with the use of more terms in Ewald's method because its components are rapidly convergent. The extreme case would be extract an infinite number of terms, where we subtract the total spectral series to the spectral series (null) and we sum the total Ewald's component, that is, we would be evaluating the Green's function by Ewald's method. On the contrary, if we do not extract any term, we would be evaluating the Green's function through its spectral form.

The development done in this approach implies a significant improvement over the slow convergence of the original series, as will be shown in Chapter 3.

# 2.3.2 Option B.1. Approach of $\left(\frac{2\pi m}{d_1}, \frac{2\pi n}{d_2}\right)$ : Sum by Ewald's Method.

The first alternative to sum the asymptotic retained terms obtained by the application of this second approach of Kummer's transformation is using the corresponding terms in Ewald's method. The strategy is similar to the one followed in the previous subsection 2.3.1 but using the other approach in the extraction of the asymptotic terms.

In this subsection, we report the connection between the first asymptotic term in the spectral domain and the first asymptotic term in Ewald's method. Then, we extract the second term and we show how to sum it using Ewald's method.

#### • Extraction of one term.

Here we suggest summing the static first term through Ewald's method. In this case, the series  $\widetilde{G}_e(\bar{\rho}, \bar{\rho}')$  that we have to efficiently sum is

$$\widetilde{G}_{e}(\bar{\rho}, \bar{\rho}') = \frac{1}{A} \sum_{\substack{m = -\infty \\ \forall m, n - \{m = n = 0\}}}^{+\infty} \sum_{\substack{n = -\infty \\ m = n = 0\}}}^{+\infty} \left( \frac{1}{\left(\frac{2\pi m}{d_{1}}\right)^{2} + \left(\frac{2\pi n}{d_{2}}\right)^{2}} \right) e^{-j\bar{k}_{mn} \cdot (\bar{\rho} - \bar{\rho}')}$$
(2.170)

The idea is to identify this series with an approximation of the spectral one and then use Ewald's transformation to sum the asymptotic term. For this purpose, we have to remember that the spectral Green's function is

$$\widetilde{G}(\bar{\rho}, \bar{\rho}') = \frac{1}{A} \sum_{m=-\infty}^{+\infty} \sum_{n=-\infty}^{+\infty} \frac{e^{-j\bar{k}_{mn} \cdot (\bar{\rho} - \bar{\rho}')}}{|\bar{k}_{mn}|^2 - k^2}$$
(2.171)

where we name

$$\bar{k}_{xy} = \frac{2\pi m}{d_1}\hat{x} + \frac{2\pi n}{d_2}\hat{y} \tag{2.172}$$

and then

$$|\bar{k}_{mn}|^2 = |\bar{k}_{w0} + \bar{k}_{xy}|^2 = \left(k_{x0} + \frac{2\pi m}{d_1}\right)^2 + \left(k_{y0} + \frac{2\pi n}{d_2}\right)^2$$
 (2.173)

We want to obtain the approximation of the previous series when  $m \to \infty$  and  $n \to \infty$  using this second approach. It is important to note that in this second approach we are assuming that  $\frac{1}{|\bar{k}_{mn}|^2 - k^2}$  is approximated through  $\left(\frac{2\pi m}{d_1}\right)^2 + \left(\frac{2\pi n}{d_2}\right)^2$ , that is

$$\frac{1}{|\bar{k}_{mn}|^2 - k^2} \bigg|_{\substack{m \to +\infty \\ n \to +\infty}} = \frac{1}{\left(k_{10} + \frac{2\pi m}{d_1}\right)^2 + \left(k_{10} + \frac{2\pi n}{d_2}\right)^2 - k^2} = \frac{1}{\left(\frac{2\pi m}{d_1}\right)^2 + \left(\frac{2\pi n}{d_2}\right)^2} \tag{2.174}$$

Therefore, we are assuming not only is  $\left(k_{x0} + \frac{2\pi m}{d_1}\right)^2 + \left(k_{y0} + \frac{2\pi n}{d_2}\right)^2$  more important than k (like the other option) but also  $\left(\frac{2\pi m}{d_1}\right)^2 + \left(\frac{2\pi n}{d_2}\right)^2$  is more important than  $k_{x0}$  and  $k_{y0}$ . This leads to believe that both k,  $k_{x0}$  and  $k_{y0}$  tend to 0. For this reason, in m=n=0, where we only have  $|\bar{k}_{w0}|$ , we will use the static limit of this term when  $|\bar{k}_{w0}| \to 0$ . Thus,  $\widetilde{G}_e(\bar{\rho}, \bar{\rho}')$  can be written as

$$\widetilde{G}_{e}(\bar{\rho}, \bar{\rho}') = \frac{e^{-j\bar{k}_{w0}\cdot(\bar{\rho}-\bar{\rho}')}}{A} \sum_{\substack{m=-\infty\\\forall m,n-\{m=n=0\}}}^{+\infty} \sum_{\substack{n=-\infty\\m=n=0\}}}^{+\infty} \left(\frac{1}{\left(\frac{2\pi m}{d_{1}}\right)^{2} + \left(\frac{2\pi n}{d_{2}}\right)^{2}}\right) e^{-j\bar{k}_{xy}\cdot(\bar{\rho}-\bar{\rho}')}$$

$$= e^{-j\bar{k}_{w0}\cdot(\bar{\rho}-\bar{\rho}')} \left[\underbrace{\frac{1}{A} \sum_{m=-\infty}^{+\infty} \sum_{n=-\infty}^{+\infty} \left(\frac{1}{\left(\frac{2\pi m}{d_{1}}\right)^{2} + \left(\frac{2\pi n}{d_{2}}\right)^{2}}\right) e^{-j\bar{k}_{mn}\cdot(\bar{\rho}-\bar{\rho}')}}_{S} - \frac{1}{A} \lim_{|\bar{k}_{00}| \to 0} \left(\frac{1}{|\bar{k}_{00}|^{2}} e^{-j\bar{k}_{00}\cdot(\bar{\rho}-\bar{\rho}')}\right)\right] \tag{2.175}$$

and the approximation of the spectral Green's function is

$$\widetilde{G}(\bar{\rho}, \bar{\rho}')\Big|_{\substack{m \to +\infty \\ n \to +\infty}} = \frac{1}{A} \sum_{m = -\infty}^{+\infty} \sum_{n = -\infty}^{+\infty} \frac{e^{-j\bar{k}_{mn} \cdot (\bar{\rho} - \bar{\rho}')}}{|\bar{k}_{mn}|^2 - k^2} \Big|_{\substack{m \to +\infty \\ n \to +\infty}}$$

$$= \underbrace{\frac{1}{A} \sum_{m = -\infty}^{+\infty} \sum_{n = -\infty}^{+\infty} \frac{e^{-j\bar{k}_{xy} \cdot (\bar{\rho} - \bar{\rho}')}}{\left(\frac{2\pi m}{d_1}\right)^2 + \left(\frac{2\pi n}{d_2}\right)^2}}_{S} \tag{2.176}$$

As seen, we can identify the series S as this approximation and therefore we can write  $\widetilde{G}_e(\bar{\rho}, \bar{\rho}')$  as a function of the approximation of the spectral Green's function when  $m \to \infty$  and  $n \to \infty$ .

$$\widetilde{G}_{e}(\bar{\rho}, \bar{\rho}') = e^{-j\bar{k}_{w0}(\bar{\rho} - \bar{\rho}')} \left[ S - \frac{1}{A} \lim_{|\bar{k}_{00}| \to 0} \left( \frac{1}{|\bar{k}_{00}|^{2}} e^{-j\bar{k}_{00} \cdot (\bar{\rho} - \bar{\rho}')} \right) \right]$$
(2.177)

where the idea is to sum S rapidly by using the approximation of the Ewald's method components when  $m \to \infty$  and  $n \to \infty$ .

$$S = \widetilde{G}(\bar{\rho}, \bar{\rho}')\Big|_{\substack{m \to +\infty \\ n \to +\infty}} = G_{spectral}(\bar{\rho}, \bar{\rho}')\Big|_{\substack{m \to +\infty \\ n \to +\infty}} + G_{spatial}(\bar{\rho}, \bar{\rho}')\Big|_{\substack{m \to +\infty \\ n \to +\infty}}$$
(2.178)

Remembering that the spectral Ewald's method component  $G_{spectral}(\bar{\rho}, \bar{\rho}')$  is obtained in (2.66) as

$$G_{spectral}(\bar{\rho}, \bar{\rho}') = \frac{1}{A} \sum_{m=-\infty}^{+\infty} \sum_{n=-\infty}^{+\infty} \frac{e^{-j\bar{k}_{mn} \cdot (\bar{\rho} - \bar{\rho}')}}{|\bar{k}_{mn}|^2 - k^2} e^{-\frac{|\bar{k}_{mn}|^2 - k^2}{4\varepsilon^2}}$$
(2.179)

the approximation of  $G_{spectral}(\bar{\rho}, \bar{\rho}')$  is given by

$$G_{spectral}(\bar{\rho}, \bar{\rho}')\Big|_{\substack{m \to +\infty \\ n \to +\infty}} = \left(\frac{1}{A} \sum_{m=-\infty}^{+\infty} \sum_{n=-\infty}^{+\infty} \frac{e^{-j\bar{k}_{mn} \cdot (\bar{\rho} - \bar{\rho}')}}{|\bar{k}_{mn}|^2 - k^2} e^{-\frac{|\bar{k}_{mn}|^2 - k^2}{4\varepsilon^2}}\right)\Big|_{\substack{m \to +\infty \\ n \to +\infty}}$$

$$= \frac{1}{A} \sum_{m=-\infty}^{+\infty} \sum_{n=-\infty}^{+\infty} e^{-j\bar{k}_{xy} \cdot (\bar{\rho} - \bar{\rho}')} \left(\frac{1}{\left(\frac{2\pi m}{d_1}\right)^2 + \left(\frac{2\pi n}{d_2}\right)^2}\right) e^{-\frac{|\bar{k}_{xy}|^2}{4\varepsilon^2}}$$

$$(2.180)$$

where we sum separately the term m=n=0 because we are not interested in summing it directly

$$\frac{1}{A} \sum_{m=-\infty}^{+\infty} \sum_{n=-\infty}^{+\infty} \frac{e^{-j\bar{k}_{xy} \cdot (\bar{\rho} - \bar{\rho}')} e^{-\frac{|\bar{k}_{xy}|^2}{4\varepsilon^2}}}{\left(\frac{2\pi m}{d_1}\right)^2 + \left(\frac{2\pi n}{d_2}\right)^2} = \frac{1}{A} \sum_{\substack{m=-\infty\\\forall m,n-\{m=n=0\}}}^{+\infty} \sum_{\substack{n=-\infty\\\forall m,n-\{m=n=0\}}}^{+\infty} \frac{e^{-j\bar{k}_{xy} \cdot (\bar{\rho} - \bar{\rho}')} e^{-\frac{|\bar{k}_{xy}|^2}{4\varepsilon^2}}}{\left(\frac{2\pi n}{d_1}\right)^2 + \left(\frac{2\pi n}{d_2}\right)^2} + \frac{1}{A} \lim_{|\bar{k}_{00}| \to 0} \left(\frac{e^{-j\bar{k}_{00} \cdot (\bar{\rho} - \bar{\rho}')}}{|\bar{k}_{00}|^2} e^{-\frac{|\bar{k}_{00}|^2}{4\varepsilon^2}}\right) \tag{2.181}$$

As said before, in m=n=0 we have to calculate the limit of  $|\bar{k}_{w0}|$  because we are using the approximation  $|\bar{k}_{mn}|^2 \approx \left(\frac{2\pi m}{d_1}\right)^2 + \left(\frac{2\pi n}{d_2}\right)^2$  ignoring not only k but also  $k_{x0}$  and  $k_{y0}$ .

On the other hand, recalling that the spatial Ewald's method component  $G_{spatial}(\bar{\rho}, \bar{\rho}')$  is given in (2.79) as

$$G_{spatial}(\bar{\rho}, \bar{\rho}') = \frac{1}{4\pi} \sum_{m=-\infty}^{+\infty} \sum_{n=-\infty}^{+\infty} e^{-j\bar{k}_{w0}\cdot\bar{\rho}_{mn}} \sum_{q=0}^{+\infty} \left(\frac{k}{2\varepsilon}\right)^{2q} \frac{1}{q!} \operatorname{E}_{q+1}(S_{mn}^2 \varepsilon^2) \qquad (2.182)$$

the approximation when  $m \to \infty$  and  $n \to \infty$  in the spectral domain corresponds to  $k \to 0$  in the spatial domain. Therefore, the limit of  $G_{spatial}(\bar{\rho}, \bar{\rho}')$  when  $k \to 0$  is given by

$$\lim_{\substack{k \to 0 \\ \bar{k}_{w0} \to 0}} G_{spatial}(\bar{\rho}, \bar{\rho}') = \lim_{\substack{k \to 0 \\ \bar{k}_{w0} \to 0}} \left( \frac{1}{4\pi} \sum_{m=-\infty}^{+\infty} \sum_{n=-\infty}^{+\infty} e^{-j\bar{k}_{w0} \cdot \bar{\rho}_{mn}} \sum_{q=0}^{+\infty} \left( \frac{k}{2\varepsilon} \right)^{2q} \frac{1}{q!} \operatorname{E}_{q+1}(S_{mn}^2 \varepsilon^2) \right)$$

$$= \frac{1}{4\pi} \sum_{m=-\infty}^{+\infty} \sum_{n=-\infty}^{+\infty} \operatorname{E}_{1}(S_{mn}^2 \varepsilon^2)$$
(2.183)

The found limits of Ewald's method components can be used to sum the series S as

$$S = \frac{1}{A} \sum_{m=-\infty}^{+\infty} \sum_{n=-\infty}^{+\infty} \frac{e^{-j\bar{k}_{xy}\cdot(\bar{\rho}-\bar{\rho}')}}{\left(\frac{2\pi m}{d_1}\right)^2 + \left(\frac{2\pi n}{d_2}\right)^2} = \frac{1}{A} \sum_{\substack{m=-\infty\\\forall m,n-\{m=n=0\}}}^{+\infty} \sum_{\substack{n=-\infty\\\forall m,n-\{m=n=0\}}}^{+\infty} e^{-j\bar{k}_{xy}\cdot(\bar{\rho}-\bar{\rho}')}$$

$$\frac{e^{-\frac{|\bar{k}_{xy}|^2}{4\varepsilon^2}}}{\left(\frac{2\pi m}{d_1}\right)^2 + \left(\frac{2\pi n}{d_2}\right)^2} + \frac{1}{A} \lim_{|\bar{k}_{00}|\to 0} \left(\frac{e^{-j\bar{k}_{00}\cdot(\bar{\rho}-\bar{\rho}')}}{|\bar{k}_{00}|^2} e^{-\frac{|\bar{k}_{00}|^2}{4\varepsilon^2}}\right) + \frac{1}{4\pi} \sum_{m=-\infty}^{+\infty} \sum_{n=-\infty}^{+\infty} \text{E}_1(S_{mn}^2\varepsilon^2)$$

$$(2.184)$$

Using this transformation, we can rewrite  $\widetilde{G}_e(\bar{\rho}, \bar{\rho}')$  as follows

$$\widetilde{G}_{e}(\bar{\rho}, \bar{\rho}') = e^{-j\bar{k}_{w0}\cdot(\bar{\rho}-\bar{\rho}')} \left[ S - \lim_{|\bar{k}_{00}|\to 0} \left( \frac{1}{A} \frac{1}{|\bar{k}_{00}|^{2}} e^{-j\bar{k}_{00}\cdot(\bar{\rho}-\bar{\rho}')} \right) \right] \\
= e^{-j\bar{k}_{w0}\cdot(\bar{\rho}-\bar{\rho}')} \left[ \frac{1}{A} \sum_{\substack{m=-\infty\\\forall m,n-\{m=n=0\}}}^{+\infty} \sum_{\substack{n=-\infty\\\forall m,n-\{m=n=0\}}}^{+\infty} e^{-j\bar{k}_{xy}\cdot(\bar{\rho}-\bar{\rho}')} \frac{e^{-\frac{|\bar{k}_{xy}|^{2}}{4\varepsilon^{2}}}}{\left(\frac{2\pi m}{d_{1}}\right)^{2} + \left(\frac{2\pi n}{d_{2}}\right)^{2}} \right] \\
+ \frac{1}{A} \lim_{|\bar{k}_{00}|\to 0} \left( \frac{e^{-j\bar{k}_{00}\cdot(\bar{\rho}-\bar{\rho}')}}{|\bar{k}_{00}|^{2}} e^{-\frac{|\bar{k}_{00}|^{2}}{4\varepsilon^{2}}} \right) + \frac{1}{4\pi} \sum_{m=-\infty}^{+\infty} \sum_{n=-\infty}^{+\infty} E_{1}(S_{mn}^{2}\varepsilon^{2}) \\
- \frac{1}{A} \lim_{|\bar{k}_{00}|\to 0} \left( \frac{1}{|\bar{k}_{00}|^{2}} e^{-j\bar{k}_{00}\cdot(\bar{\rho}-\bar{\rho}')} \right) \right] \tag{2.185}$$

If we regroup terms and sum together the values of the series in m = n = 0,  $\widetilde{G}_e(\bar{\rho}, \bar{\rho}')$  remains

$$\widetilde{G}_{e}(\bar{\rho}, \bar{\rho}') = e^{-j\bar{k}_{w0}\cdot(\bar{\rho}-\bar{\rho}')} \left[ \frac{1}{A} \sum_{\substack{m=-\infty\\\forall m,n-\{m=n=0\}}}^{+\infty} \sum_{\substack{n=-\infty\\\forall m,n-\{m=n=0\}}}^{+\infty} \frac{e^{-j\bar{k}_{xy}\cdot(\bar{\rho}-\bar{\rho}')} e^{-\frac{|\bar{k}_{xy}|^{2}}{4\varepsilon^{2}}}}{\left(\frac{2\pi m}{d_{1}}\right)^{2} + \left(\frac{2\pi n}{d_{2}}\right)^{2}} + \frac{1}{4\pi} \sum_{m=-\infty}^{+\infty} \sum_{n=-\infty}^{+\infty} E_{1}(S_{mn}^{2}\varepsilon^{2}) + \underbrace{\frac{1}{A} \lim_{|\bar{k}_{00}| \to 0} \left(\frac{e^{-j\bar{k}_{00}\cdot(\bar{\rho}-\bar{\rho}')}}{|\bar{k}_{00}|^{2}} \left(e^{-\frac{|\bar{k}_{00}|^{2}}{4\varepsilon^{2}}} - 1\right)\right)}_{T} \right] (2.186)$$

where the last term T contains the residual value when m=n=0. As discussed before, in this approach we have to calculate and use the limit when  $|\bar{k}_{w0}| \to 0$  in all cases.

$$T = \frac{1}{A} \lim_{|\bar{k}_{00}| \to 0} \left( \frac{e^{-j\bar{k}_{00} \cdot (\bar{\rho} - \bar{\rho}')}}{|\bar{k}_{00}|^2} \left( e^{-\frac{|\bar{k}_{00}|^2}{4\varepsilon^2}} - 1 \right) \right) = \frac{1}{A} \frac{1}{|\bar{k}_{00}|^2} \left( 1 - \frac{|\bar{k}_{00}|^2}{4\varepsilon^2} - 1 \right)$$

$$= \frac{1}{A} \frac{1}{|\bar{k}_{00}|^2} \left( -\frac{|\bar{k}_{00}|^2}{4\varepsilon^2} \right) = \frac{-1}{4A\varepsilon^2}$$
(2.187)

Introducing (2.187) in (2.186),  $\widetilde{G}_e(\bar{\rho}, \bar{\rho}')$  can be finally written as

$$\widetilde{G}_{e}(\bar{\rho}, \bar{\rho}') = e^{-j\bar{k}_{w0}\cdot(\bar{\rho}-\bar{\rho}')} \left[ \frac{1}{A} \sum_{\substack{m=-\infty\\\forall m,n-\{m=n=0\}}}^{+\infty} \sum_{\substack{n=-\infty\\\forall m,n-\{m=n=0\}}}^{+\infty} e^{-j\bar{k}_{xy}\cdot(\bar{\rho}-\bar{\rho}')} \frac{e^{-\frac{|\bar{k}_{xy}|^{2}}{4\varepsilon^{2}}}}{\left(\frac{2\pi m}{d_{1}}\right)^{2} + \left(\frac{2\pi n}{d_{2}}\right)^{2}} \right]$$

$$+ \frac{1}{4\pi} \sum_{m=-\infty}^{+\infty} \sum_{n=-\infty}^{+\infty} E_{1}(S_{mn}^{2}\varepsilon^{2}) - \frac{1}{4A\varepsilon^{2}}$$
(2.188)

#### • Extraction of two terms.

The first term can be obtained by using the previous first order approximation but when we are interested in extracting more than one term, we have to analyse what happens in higher orders when  $m \to \infty$  and  $n \to \infty$  in the spectral series and in the Ewald's components. For this aim, the strategy here is to obtain the retained terms by using the Taylor expansion not only for  $e^{\frac{k^2}{4s^2}}$  but also for  $e^{-jk_{x0}md_1}$  and  $e^{-jk_{y0}nd_2}$ .

The starting point of the spectral development done previously in Subsection 2.1.1 is

$$G(\bar{\rho}, \bar{\rho}') = \frac{1}{2\pi} \sum_{m=-\infty}^{+\infty} \sum_{n=-\infty}^{+\infty} e^{-j\bar{k}_{w0}\cdot\bar{\rho}_{mn}} \int_0^\infty \frac{e^{-S_{mn}^2 s^2 + \frac{k^2}{4s^2}}}{s} ds$$
 (2.189)

and the starting points of the proofs done in Subsection 2.2.1 of the Ewald's components are

$$G_{spectral}(\bar{\rho}, \bar{\rho}') = \frac{1}{2\pi} \sum_{m=-\infty}^{+\infty} \sum_{n=-\infty}^{+\infty} e^{-j\bar{k}_{w0}\cdot\bar{\rho}_{mn}} \int_{0}^{\varepsilon} \frac{e^{-S_{mn}^{2}s^{2} + \frac{k^{2}}{4s^{2}}}}{s} ds$$
 (2.190a)

$$G_{spatial}(\bar{\rho}, \bar{\rho}') = \frac{1}{2\pi} \sum_{m=-\infty}^{+\infty} \sum_{n=-\infty}^{+\infty} e^{-j\bar{k}_{w0}\cdot\bar{\rho}_{mn}} \int_{\varepsilon}^{\infty} \frac{e^{-S_{mn}^2 s^2 + \frac{k^2}{4s^2}}}{s} ds \qquad (2.190b)$$

All of these components start in the spatial domain, where  $m \to \infty$  and  $n \to \infty$  is  $k \to 0$ . In addition, in this second approach we have to force  $\bar{k}_{w0}$  to be zero. Thus, we have to calculate the limit of these integrals when  $k \to 0$  and  $\bar{k}_{w0} \to 0$ . Using the Taylor expansion when  $u \to 0$  we can rewrite the exponential of k in the previous proofs as in the equation (2.143) and the exponential of  $\bar{k}_{w0}$  as

$$e^{-j\bar{k}_{w0}\cdot\bar{\rho}_{mn}} = \sum_{n=0}^{+\infty} \frac{\left(-j\bar{k}_{w0}\cdot\bar{\rho}_{mn}\right)^{n}}{n!} = 1 - j\bar{k}_{w0}\cdot\bar{\rho}_{mn} + \frac{\left(-j\bar{k}_{w0}\cdot\bar{\rho}_{mn}\right)^{2}}{2} + \dots$$

$$= 1 - jk_{x0}md_{1} - jk_{y0}nd_{2} - \frac{(k_{x0}md_{1})^{2}}{2} - \frac{(k_{y0}nd_{2})^{2}}{2} + \dots$$
(2.191)

It can be noted that the first term of these expansions corresponds to the development done previously when we extract only the first term. The idea is to use the second order Taylor expansions of  $e^{\frac{k^2}{4s^2}}$  and  $e^{-j\bar{k}_{w0}\cdot\bar{\rho}_{mn}}$  in the equations (2.189), (2.190a) and (2.190b). This will allow us to use the second order expansion of Ewald's method components to sum the second order expansion of the spectral series.

As introduction to this procedure, we have the product of three Taylor expansions. To extract what we have called the second term, we use the following combination of terms summing together: The second order expansion of the k-integral with the first order expansion of the  $\bar{k}_{w0}$ -integral and the second order expansion of the  $\bar{k}_{w0}$ -integral with the first order expansion of the k-integral.

Firstly, we start with the second order expansion of the k-integral with the first order expansion of the  $\bar{k}_{w0}$ -integral. For this purpose, we assume the first order expansion in the  $\bar{k}_{w0}$ -integral and we use the expansion given in (2.143) in the equation (2.15) of the spectral development.

Thus, we start from the equation (2.15) and we assume  $e^{-jk_{x0}\xi_1} \approx 1$  and  $e^{-jk_{y0}\xi_2} \approx 1$ 

$$\widetilde{f}(k_x, k_y) \approx \frac{1}{2\pi} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} d\xi_1 d\xi_2 \times \int_0^{\infty} \frac{e^{-[(x-x'-\xi_1)^2 + (y-y'-n\xi_2)^2]s^2 + \frac{k^2}{4s^2}}}{s} e^{-jk_{x0}\xi_1} e^{-jk_{y0}\xi_2} ds$$

$$(2.192)$$

Now, we have to replace  $k_x = \frac{2\pi}{A}(ma_{2y} - na_{1y})$  and  $k_y = \frac{2\pi}{A}(-ma_{2x} + na_{1x})$ . Following the same procedure as Subsection 2.1.1, if we resolve the  $\xi$ -integrals and if we interchange the order of integration,  $\widetilde{f}(k_x, k_y)$  remains

$$\widetilde{f}(k_x, k_y) \approx \frac{1}{2\pi} \int_0^\infty \sqrt{\frac{\pi}{s^2}} e^{-jk_x(x-x')} e^{-\frac{k_x^2}{4s^2}} \sqrt{\frac{\pi}{s^2}} e^{-jk_y(y-y')} e^{-\frac{k_y^2}{4s^2}} e^{\frac{k^2}{4s^2}} \frac{1}{s} ds \quad (2.193)$$

Using the definition of  $\bar{k}_{xy}$ 

$$\bar{k}_{xy} = \frac{2\pi}{A} \left[ m(\bar{a}_2 \times \hat{z}) + n(\hat{z} \times \bar{a}_1) \right] = \frac{2\pi}{A} (ma_{2y} - na_{1y})\hat{x} + \frac{2\pi}{A} (-ma_{2x} + na_{1x})\hat{y}$$

$$= k_x \hat{x} + k_y \hat{y}$$
(2.194)

the exponentials can be merged into

$$e^{-jk_x(x-x')}e^{-jk_y(y-y')} = e^{-j[k_x(x-x')+k_y(y-y')]} = e^{-j\bar{k}_{xy}\cdot(\bar{\rho}-\bar{\rho}')}$$
(2.195a)

$$e^{-\frac{k_x^2}{4s^2}}e^{-\frac{k_y^2}{4s^2}} = e^{-\frac{(k_x^2 + k_y^2)}{4s^2}} = e^{-\frac{|\bar{k}_{xy}|^2}{4s^2}}$$
(2.195b)

and  $\widetilde{f}(k_x, k_y)$  can be rewritten using the Taylor expansion of the k-exponential as

$$\widetilde{f}(k_x, k_y) \approx \frac{1}{2} e^{-j\bar{k}_{xy}\cdot(\bar{\rho}-\bar{\rho}')} \int_0^\infty \frac{1}{s^3} \left(1 + \frac{k^2}{4s^2}\right) e^{-\frac{|\bar{k}_{xy}|^2}{4s^2}} ds$$
 (2.196)

In the knowledge that the previous integrals can be solved using the relations given in (2.145a) and (2.145b) where in this case  $a = \frac{|\bar{k}_{xy}|^2}{4}$ , the equation (2.196) remains

$$\widetilde{f}(k_x, k_y) \approx \frac{1}{2} e^{-j\bar{k}_{xy} \cdot (\bar{\rho} - \bar{\rho}')} \left( \frac{4}{2|\bar{k}_{xy}|^2} + \frac{16k^2}{8|\bar{k}_{xy}|^4} \right) = e^{-j\bar{k}_{xy} \cdot (\bar{\rho} - \bar{\rho}')} \left( \frac{1}{|\bar{k}_{xy}|^2} + \frac{k^2}{|\bar{k}_{xy}|^4} \right)$$
(2.197)

Now, we continue with the second order expansion of the  $\bar{k}_{w0}$ -integral with the first order expansion of the k-integral. For this purpose, we start from (2.15) and we assume the first order expansion in the k-integral and we use the expansion given in (2.191) in the equation (2.15) of the spectral development. That is, we write  $e^{\frac{k^2}{4s^2}} \approx 1$ ,  $e^{-jk_{x0}\xi_1} \approx 1 - jk_{x0}\xi_1 - (k_{x0}\xi_1)^2/2$  and  $e^{-jk_{y0}\xi_2} \approx 1$  in the following equation

$$\widetilde{f}(k_x, k_y) \approx \frac{1}{2\pi} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} d\xi_1 d\xi_2 \times \int_{0}^{\infty} \frac{e^{-[(x-x'-\xi_1)^2 + (y-y'-n\xi_2)^2]s^2} e^{\frac{k^2}{4s^2}}}{s} \times \left[1 - jk_{x0}\xi_1 - (k_{x0}\xi_1)^2/2\right] e^{-jk_y0\xi_2} e^{-jk_x\xi_1} e^{-jk_y\xi_2} ds$$
(2.198)

where we have to replace  $k_x = \frac{2\pi}{A}(ma_{2y} - na_{1y})$  and  $k_y = \frac{2\pi}{A}(-ma_{2x} + na_{1x})$ .

$$\widetilde{f}(k_x, k_y) \approx \frac{1}{2\pi} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} d\xi_1 d\xi_2 \times \int_{0}^{\infty} ds \, \frac{1}{s} \, e^{-(x-x'-\xi_1)^2 s^2 - jk_x \xi_1} e^{-(y-y'-\xi_2)^2 s^2 - jk_y \xi_2} \\
\times \left[ 1 - jk_{x0}\xi_1 - (k_{x0}\xi_1)^2 / 2 \right] = \frac{1}{2\pi} \int_{0}^{\infty} ds \, \frac{1}{s} \int_{-\infty}^{\infty} e^{-(x-x'-\xi_1)^2 s^2 - jk_x \xi_1} \\
\times \left[ 1 - jk_{x0}\xi_1 - \frac{(k_{x0}\xi_1)^2}{2} \right] d\xi_1 \times \int_{-\infty}^{\infty} e^{-(y-y'-\xi_2)^2 s^2 - jk_y \xi_2} d\xi_2$$
(2.199)

As before, we try to find the evaluation in a closed form of the  $\xi$ -integrals. For this purpose, we define  $I_1$  and  $I_2$  as the integrals of (2.17) that depend on  $\xi_1$  and  $\xi_2$ , respectively.

The integral  $I_2$  can be solved as previously

$$I_2 = \int_{-\infty}^{\infty} e^{-(y-y'-\xi_2)^2 s^2 - jk_y \xi_2} d\xi_2 = \sqrt{\frac{\pi}{s^2}} e^{-jk_y(y-y')} e^{-\frac{k_y^2}{4s^2}}$$
(2.200)

On the other hand, the integral  $I_1$  can be divided into three integrals

$$I_{1} = \int_{-\infty}^{+\infty} \left[ 1 - jk_{x0}\xi_{1} - (k_{x0}\xi_{1})^{2}/2 \right] e^{-(x-x')^{2}s^{2} + 2(x-x')\xi_{1}s^{2} - \xi_{1}^{2}s^{2} - jk_{x}\xi_{1}} d\xi_{1}$$

$$= \int_{-\infty}^{+\infty} e^{-(x-x')^{2}s^{2} + 2(x-x')\xi_{1}s^{2} - \xi_{1}^{2}s^{2} - jk_{x}\xi_{1}} d\xi_{1}$$

$$+ \int_{-\infty}^{+\infty} \left( -jk_{x0}\xi_{1} \right) e^{-(x-x')^{2}s^{2} + 2(x-x')\xi_{1}s^{2} - \xi_{1}^{2}s^{2} - jk_{x}\xi_{1}} d\xi_{1}$$

$$+ \int_{-\infty}^{+\infty} \left[ \frac{-(k_{x0}\xi_{1})^{2}}{2} \right] e^{-(x-x')^{2}s^{2} + 2(x-x')\xi_{1}s^{2} - \xi_{1}^{2}s^{2} - jk_{x}\xi_{1}} d\xi_{1}$$

$$(2.201)$$

The first has already been computed previously so we only have to take into account the second and the third one. In the knowledge that the previous integral can be solved using [15] as

$$\int_{-\infty}^{+\infty} \xi \, e^{-a\xi^2 + b\xi} d\xi = \frac{b\sqrt{\pi}}{2a^{3/2}} e^{\frac{b^2}{4a}} \tag{2.202}$$

$$\int_{-\infty}^{+\infty} \xi^2 e^{-a\xi^2 + b\xi} d\xi = \frac{(2a + b^2)\sqrt{\pi}}{4a^{5/2}} e^{\frac{b^2}{4a}}$$
 (2.203)

where  $a = s^2$  and  $b = 2(x - x')s^2 - jk_x$  have been identified, the integral  $I_1$  can be written as

$$I_{1} = \int_{-\infty}^{+\infty} \left[ \mathcal{I} - jk_{x0}\xi_{1} - (k_{x0}\xi_{1})^{2} \right] e^{-(x-x')^{2}s^{2} + 2(x-x')\xi_{1}s^{2} - \xi_{1}^{2}s^{2} - jk_{x}\xi_{1}} d\xi_{1}$$

$$= -jk_{x0} \left[ \frac{(x-x')\sqrt{\pi}}{s} - \frac{jk_{x}\sqrt{\pi}}{2s^{3}} \right] e^{-\frac{k_{x}^{2}}{4s^{2}}} e^{-jk_{x}(x-x')}$$

$$- \frac{k_{x0}^{2}}{2} \left[ \frac{\sqrt{\pi}}{2s^{3}} + \frac{(x-x')^{2}\sqrt{\pi}}{s} - \frac{jk_{x}(x-x')\sqrt{\pi}}{s^{3}} - \frac{k_{x}^{2}\sqrt{\pi}}{4s^{5}} \right] e^{-\frac{k_{x}^{2}}{4s^{2}}} e^{-jk_{x}(x-x')}$$

$$(2.204)$$

The expression of  $I_1$  and  $I_2$  given in (2.204) and (2.200) respectively lead to

$$\widetilde{f}(k_{x}, k_{y}) \approx \frac{-jk_{x0} e^{-j\overline{k}_{xy} \cdot (\bar{\rho} - \bar{\rho}')}}{2\pi} \int_{0}^{\infty} ds \frac{1}{s} \sqrt{\pi} \left[ \frac{(x - x')}{s} - \frac{jk_{x}}{2s^{3}} \right] \frac{\sqrt{\pi}}{s} e^{-\frac{|\bar{k}_{xy}|^{2}}{4s^{2}}} 
+ \frac{-\frac{k_{x0}^{2}}{2} e^{-j\overline{k}_{xy} \cdot (\bar{\rho} - \bar{\rho}')}}{2\pi} \int_{0}^{\infty} ds \frac{1}{s} \sqrt{\pi} \left[ \frac{1}{2s^{3}} + \frac{(x - x')^{2}}{s} - \frac{jk_{x}(x - x')}{s^{3}} - \frac{k_{x}^{2}}{4s^{5}} \right] \frac{\sqrt{\pi}}{s} e^{-\frac{|\bar{k}_{xy}|^{2}}{4s^{2}}}$$
(2.205)

Solving these integrals using the relations given in (2.145a) and (2.145b),  $\tilde{f}(k_x, k_y)$  remains

$$\widetilde{f}(k_{x},k_{y}) \approx e^{-j\bar{k}_{xy}\cdot(\bar{\rho}-\bar{\rho}')} \left[ \frac{-jk_{x0}(x-x')}{|\bar{k}_{xy}|^{2}} - \frac{2k_{x0}k_{x}}{|\bar{k}_{xy}|^{4}} + \frac{-k_{x0}^{2}}{|\bar{k}_{xy}|^{4}} - \frac{(x-x')^{2}k_{x0}^{2}/2}{|\bar{k}_{xy}|^{2}} + \frac{2jk_{x0}^{2}k_{x}(x-x')}{|\bar{k}_{xy}|^{4}} + \frac{4k_{x0}^{2}k_{x}^{2}}{|\bar{k}_{xy}|^{6}} \right]$$
(2.206)

where  $k_x = \frac{2\pi}{A}(ma_{2y} - na_{1y})$  and  $k_y = \frac{2\pi}{A}(-ma_{2x} + na_{1x})$ .

The last group of terms that we have to obtain results from doing  $e^{\frac{k^2}{4s^2}} \approx 1$ ,  $e^{-jk_{x0}\xi_1} \approx 1$  and  $e^{-jk_{y0}\xi_2} \approx 1 - jk_{y0}\xi_2 - (k_{y0}\xi_2)^2/2$  in the following equation

$$\widetilde{f}(k_x, k_y) \approx \frac{1}{2\pi} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} d\xi_1 d\xi_2 \times \int_{0}^{\infty} \frac{e^{-[(x-x'-\xi_1)^2 + (y-y'-n\xi_2)^2]s^2} e^{\frac{k^2}{4s^2}}}{s} \times \left[1 - jk_{y0}\xi_2 - (k_{y0}\xi_2)^2/2\right] e^{-jk_x 0\xi_1} e^{-jk_x \xi_1} e^{-jk_y \xi_2} ds$$
(2.207)

This can be solved in a similar way to the previous development. Thus, we can conclude that in this case  $\tilde{f}(k_x, k_y)$  is

$$\widetilde{f}(k_{x},k_{y}) \approx e^{-j\bar{k}_{xy}\cdot(\bar{\rho}-\bar{\rho}')} \left[ \frac{-jk_{y0}(y-y')}{|\bar{k}_{xy}|^{2}} - \frac{2k_{y0}k_{y}}{|\bar{k}_{xy}|^{4}} + \frac{-k_{y0}^{2}}{|\bar{k}_{xy}|^{4}} - \frac{(y-y')^{2}k_{y0}^{2}/2}{|\bar{k}_{xy}|^{2}} + \frac{2jk_{y0}^{2}k_{y}(y-y')}{|\bar{k}_{xy}|^{4}} + \frac{4k_{y0}^{2}k_{y}^{2}}{|\bar{k}_{xy}|^{6}} \right]$$
(2.208)

Now, we can use together the three groups of terms and write the asymptotic term  $\widetilde{G}_{mn}$  as

$$\widetilde{G}_{mn} = \frac{1 - jk_{x0}(x - x') - jk_{y0}(y - y') - (x - x')^{2}k_{x0}^{2}/2 - (y - y')^{2}k_{y0}^{2}/2}{|\bar{k}_{xy}|^{2}} + \frac{k^{2} - 2k_{x0}k_{x} - 2k_{y0}k_{y} - k_{x0}^{2} - k_{y0}^{2} + 2jk_{x0}^{2}k_{x}(x - x') + 2jk_{y0}^{2}k_{y}(y - y')}{|\bar{k}_{xy}|^{4}} + \frac{4k_{x0}^{2}k_{x}^{2} + 4k_{y0}^{2}k_{y}^{2}}{|\bar{k}_{xy}|^{6}}$$

$$(2.209)$$

It should be pointed out that the complex terms correspond to the expansion of the complex exponential that originally is  $e^{-j\bar{k}_{w0}\cdot(\bar{\rho}-\bar{\rho}')}$ . Thus, the application of Kummer's transformation in this case is

$$\widetilde{G}_{k}(\bar{\rho}, \bar{\rho}') = \frac{1}{A} \sum_{\substack{m = -\infty \\ \forall m, n - \{m = n = 0\}}}^{+\infty} \sum_{\substack{n = -\infty \\ \forall m, n - \{m = n = 0\}}}^{+\infty} \left( \frac{e^{-j\bar{k}_{w0} \cdot (\bar{\rho} - \bar{\rho}')}}{|\bar{k}_{mn}|^{2} - k^{2}} - \widetilde{G}_{mn} \right) e^{-j\bar{k}_{xy} \cdot (\bar{\rho} - \bar{\rho}')} + \widetilde{G}_{00} 
+ \frac{1}{A} \sum_{\substack{m = -\infty \\ \forall m, n - \{m = n = 0\}}}^{+\infty} \sum_{\substack{n = -\infty \\ \forall m, n - \{m = n = 0\}}}^{+\infty} \widetilde{G}_{mn} e^{-j\bar{k}_{xy} \cdot (\bar{\rho} - \bar{\rho}')}$$
(2.210)

where  $\widetilde{G}_{00}$  is the term in m=n=0 and  $\widetilde{G}_e(\bar{\rho},\bar{\rho}')$  is the remaining part that has to be efficiently summed.

$$\widetilde{G}_{e}(\bar{\rho}, \bar{\rho}') = \frac{1}{A} \sum_{\substack{m = -\infty \\ \forall m, n - \{m = n = 0\}}}^{+\infty} \sum_{\substack{n = -\infty \\ m = n = 0}}^{+\infty} \widetilde{G}_{mn} e^{-j\bar{k}_{xy}(\bar{\rho} - \bar{\rho}')} = \frac{1}{A} \sum_{m = -\infty}^{+\infty} \sum_{n = -\infty}^{+\infty} \widetilde{G}_{mn} e^{-j\bar{k}_{xy}\cdot(\bar{\rho} - \bar{\rho}')} - \widetilde{G}_{e0}$$

$$= \widetilde{G}(\bar{\rho}, \bar{\rho}')\Big|_{\substack{m \to +\infty \\ n \to +\infty}} - \widetilde{G}_{e0}$$
(2.211)

 $\widetilde{G}_{e0}$  is the asymptotic part in m=n=0 and the other part can be seen as the approximation of the spectral series obtained before. The idea is to sum this series using Ewald's method. Through this proposed Kummer-Ewald transformation, the asymptotic retained part  $\widetilde{G}_e(\bar{\rho}, \bar{\rho}')$  can be efficiently calculated using the rapidly convergent components of Ewald's method.

Firstly, we start with the spectral Ewald's component. The proof of spectral component of Ewald's method has been reported in Subsection 2.2.1. In this development we have to use the same expansions done in the previous one for the spectral series.

We first carry out the second order expansion of the k-integral with the first order expansion of the  $\bar{k}_{w0}$ -integral. For this purpose, we assume the first order expansion in the  $\bar{k}_{w0}$ -integral and we use the expansion given in (2.143) in the equation (2.60) of the spectral development.

Thus, we start from the equation (2.60) and we assume  $e^{-jk_{x0}\xi_1} \approx 1$  and  $e^{-jk_{y0}\xi_2} \approx 1$ 

$$\widetilde{f}(k_x, k_y) = \frac{1}{2\pi} \int_0^{\varepsilon} \sqrt{\frac{\pi}{s^2}} e^{-jk_x(x-x')} e^{-\frac{k_x^2}{4s^2}} \sqrt{\frac{\pi}{s^2}} e^{-jk_y(y-y')} e^{-\frac{k_y^2}{4s^2}} e^{\frac{k^2}{4s^2}} \frac{1}{s} ds \qquad (2.212)$$

where using the definition of  $\bar{k}_{xy}$  and the second order expansion of the k-exponential,  $\tilde{f}(k_x, k_y)$  remains

$$\widetilde{f}(k_x, k_y) \approx \frac{1}{2} e^{-j\bar{k}_{xy} \cdot (\bar{\rho} - \bar{\rho}')} \int_0^{\varepsilon} \frac{1}{s^3} \left( 1 + \frac{k^2}{4s^2} \right) e^{-\frac{|\bar{k}_{xy}|^2}{4s^2}} ds$$
 (2.213)

In the knowledge that the previous integrals can be solved using [15] using the relations given in (2.150a) and (2.150b) where in this case  $a = \frac{|\bar{k}_{xy}|^2}{4}$ , the equation (2.213) remains

$$\widetilde{f}(k_x, k_y) \approx e^{-j\bar{k}_{xy}\cdot(\bar{\rho}-\bar{\rho}')}e^{-\frac{|\bar{k}_{xy}|^2}{4\varepsilon^2}} \left[ \frac{1}{|\bar{k}_{xy}|^2} + \frac{k^2}{|\bar{k}_{xy}|^4} + \frac{k^2}{4\varepsilon^2|\bar{k}_{xy}|^2} \right]$$
 (2.214)

Now, we continue with the second order expansion of the  $\bar{k}_{w0}$ -integral with the first order expansion of the k-integral. For this purpose, we start from (2.55) and we assume the first order expansion in the k-integral and we use the expansion given in (2.191) in the equation (2.55) of the spectral Ewald's development. That is, we assume  $e^{\frac{k^2}{4s^2}} \approx 1$ ,  $e^{-jk_{x0}\xi_1} \approx 1 - jk_{x0}\xi_1 - (k_{x0}\xi_1)^2/2$  and  $e^{-jk_{y0}\xi_2} \approx 1$  in the following equation

$$\widetilde{f}(k_x, k_y) \approx \frac{1}{2\pi} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} d\xi_1 d\xi_2 \times \int_0^{\varepsilon} \frac{e^{-[(x-x'-\xi_1)^2 + (y-y'-n\xi_2)^2]s^2} e^{\frac{k^2}{4s^2}}}{s} \times \left[1 - jk_{x0}\xi_1 - (k_{x0}\xi_1)^2/2\right] e^{-jk_{y0}\xi_2} e^{-jk_x\xi_1} e^{-jk_y\xi_2} ds$$
(2.215)

$$\widetilde{f}(k_x, k_y) = \frac{1}{2\pi} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} d\xi_1 d\xi_2 \times \int_0^{\varepsilon} ds \, \frac{1}{s} \, e^{-(x-x'-\xi_1)^2 s^2 - jk_x \xi_1} e^{-(y-y'-\xi_2)^2 s^2 - jk_y \xi_2} \\
\times \left[ 1 - jk_{x0}\xi_1 - (k_{x0}\xi_1)^2 / 2 \right] \\
= \frac{1}{2\pi} \int_0^{\varepsilon} ds \, \frac{1}{s} \int_{-\infty}^{\infty} e^{-(x-x'-\xi_1)^2 s^2 - jk_x \xi_1} \left[ 1 - jk_{x0}\xi_1 - \frac{(k_{x0}\xi_1)^2}{2} \right] d\xi_1 \\
\times \int_{-\infty}^{\infty} e^{-(y-y'-\xi_2)^2 s^2 - jk_y \xi_2} d\xi_2 \tag{2.216}$$

Proceeding as previously, we can solve the  $\varepsilon$ -integrals as (2.204) and (2.200). This leads to

$$\widetilde{f}(k_{x},k_{y}) \approx \frac{-j\bar{k}_{x0}}{2\pi} \frac{e^{-j\bar{k}_{xy}\cdot(\bar{\rho}-\bar{\rho}')}}{2\pi} \int_{0}^{\varepsilon} ds \, \frac{1}{s} \sqrt{\pi} \left[ \frac{(x-x')}{s} - \frac{jk_{x}}{2s^{3}} \right] \frac{\sqrt{\pi}}{s} \, e^{-\frac{|\bar{k}_{xy}|^{2}}{4s^{2}}} \\
+ \frac{-\frac{\bar{k}_{x0}^{2}}{2}}{2\pi} \frac{e^{-jk_{xy}\cdot(\bar{\rho}-\bar{\rho}')}}{2\pi} \int_{0}^{\varepsilon} ds \, \frac{1}{s} \sqrt{\pi} \left[ \frac{1}{2s^{3}} + \frac{(x-x')^{2}}{s} - \frac{jk_{x}(x-x')}{s^{3}} - \frac{k_{x}^{2}}{4s^{5}} \right] \frac{\sqrt{\pi}}{s} \, e^{-\frac{|\bar{k}_{xy}|^{2}}{4s^{2}}} \tag{2.217}$$

Solving these integral by using the relation given in (2.150a) and (2.150b),  $\widetilde{f}(k_x, k_y)$  remains

$$\begin{split} \widetilde{f}(k_{x},k_{y}) &\approx e^{-j\bar{k}_{xy}\cdot(\bar{\rho}-\bar{\rho}')}e^{-\frac{|\bar{k}_{xy}|^{2}}{4\varepsilon^{2}}}\left[\frac{-jk_{x0}(x-x')}{|\bar{k}_{xy}|^{2}} - \frac{2k_{x0}k_{x}}{|\bar{k}_{xy}|^{4}} - \frac{2k_{x0}k_{x}}{4\varepsilon^{2}|\bar{k}_{xy}|^{2}} - \frac{k_{x0}^{2}}{|\bar{k}_{xy}|^{4}}\right. \\ &- \frac{k_{x0}^{2}}{4\varepsilon^{2}|\bar{k}_{xy}|^{2}} - \frac{(x-x')^{2}k_{x0}^{2}/2}{|\bar{k}_{xy}|^{2}} + \frac{2jk_{x0}^{2}k_{x}(x-x')}{|\bar{k}_{xy}|^{4}} + \frac{2jk_{x0}^{2}k_{x}(x-x')}{4\varepsilon^{2}|\bar{k}_{xy}|^{2}} \\ &+ \frac{4k_{x0}^{2}k_{x}^{2}}{|\bar{k}_{xy}|^{6}} + \frac{4k_{x0}^{2}k_{x}^{2}}{4\varepsilon^{2}|\bar{k}_{xy}|^{4}} + \frac{4k_{x0}^{2}k_{x}^{2}}{32\varepsilon^{4}|\bar{k}_{xy}|^{2}} \right] \end{split}$$

where  $k_x = \frac{2\pi}{A}(ma_{2y} - na_{1y})$  and  $k_y = \frac{2\pi}{A}(-ma_{2x} + na_{1x})$ .

The last group of terms that we have to obtain results from doing  $e^{\frac{k^2}{4s^2}} \approx 1$ ,  $e^{-jk_{x0}\xi_1} \approx 1$  and  $e^{-jk_{y0}\xi_2} \approx 1 - jk_{y0}\xi_2 - (k_{y0}\xi_2)^2/2$  in the following equation

$$\widetilde{f}(k_x, k_y) \approx \frac{1}{2\pi} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} d\xi_1 d\xi_2 \times \int_0^{\varepsilon} \frac{e^{-[(x-x'-\xi_1)^2 + (y-y'-n\xi_2)^2]s^2} e^{\frac{k^2}{4s^2}}}{s} \times \left[1 - jk_{y0}\xi_2 - (k_{y0}\xi_2)^2/2\right] e^{-jk_{x0}\xi_1} e^{-jk_x\xi_1} e^{-jk_y\xi_2} ds$$
(2.219)

This can be solved in a similar way to the previous development. Thus, we can conclude that in this case  $\tilde{f}(k_x, k_y)$  is

$$\begin{split} \widetilde{f}(k_{x},k_{y}) &\approx e^{-j\bar{k}_{xy}\cdot(\bar{\rho}-\bar{\rho}')}e^{-\frac{|\bar{k}_{xy}|^{2}}{4\varepsilon^{2}}}\left[\frac{-jk_{y0}(y-y')}{|\bar{k}_{xy}|^{2}} - \frac{2k_{y0}k_{y}}{|\bar{k}_{xy}|^{4}} - \frac{2k_{y0}k_{y}}{4\varepsilon^{2}|\bar{k}_{xy}|^{2}} - \frac{k_{y0}^{2}}{|\bar{k}_{xy}|^{4}}\right. \\ &- \frac{k_{y0}^{2}}{4\varepsilon^{2}|\bar{k}_{xy}|^{2}} - \frac{(y-y')^{2}k_{y0}^{2}/2}{|\bar{k}_{xy}|^{2}} + \frac{2jk_{y0}^{2}k_{y}(y-y')}{|\bar{k}_{xy}|^{4}} + \frac{2jk_{y0}^{2}k_{y}(y-y')}{4\varepsilon^{2}|\bar{k}_{xy}|^{2}} \\ &+ \frac{4k_{y0}^{2}k_{y}^{2}}{|\bar{k}_{xy}|^{6}} + \frac{4k_{y0}^{2}k_{y}^{2}}{4\varepsilon^{2}|\bar{k}_{xy}|^{4}} + \frac{4k_{y0}^{2}k_{y}^{2}}{32\varepsilon^{4}|\bar{k}_{xy}|^{2}} \right] \end{split}$$

Now, we can use together the three groups of terms and write the asymptotic spectral Ewald's method component  $G_{spectral}$  as

$$G_{spectral}|_{\substack{m \to +\infty \\ n \to +\infty}} = \frac{1}{A} \sum_{m = -\infty}^{+\infty} \sum_{n = -\infty}^{+\infty} e^{-j\bar{k}_{xy} \cdot (\bar{\rho} - \bar{\rho}')} e^{-\frac{|\bar{k}_{xy}|^2}{4\varepsilon^2}}$$

$$\times \left[ \frac{1 - jk_{x0}(x - x') - jk_{y0}(y - y') - (x - x')^2 k_{x0}^2 / 2 - (y - y')^2 k_{y0}^2 / 2}{|\bar{k}_{xy}|^2} \right]$$

$$+ \frac{k^2 - 2k_{x0}k_x - 2k_{y0}k_y - k_{x0}^2 - k_{y0}^2 + 2jk_{x0}^2 k_x (x - x') + 2jk_{y0}^2 k_y (y - y')}{|\bar{k}_{xy}|^4}$$

$$+ \frac{k^2 - 2k_{x0}k_x - 2k_{y0}k_y - k_{x0}^2 - k_{y0}^2 + 2jk_{x0}^2 k_x (x - x') + 2jk_{y0}^2 k_y (y - y')}{4\varepsilon^2 |\bar{k}_{xy}|^2}$$

$$+ \frac{4k_{x0}^2 k_x^2 + 4k_{y0}^2 k_y^2}{|\bar{k}_{xy}|^6} + \frac{4k_{x0}^2 k_x^2 + 4k_{y0}^2 k_y^2}{4\varepsilon^2 |\bar{k}_{xy}|^4} + \frac{4k_{x0}^2 k_x^2 + 4k_{y0}^2 k_y^2}{32\varepsilon^4 |\bar{k}_{xy}|^2}$$

If we sum apart the term  $G_{spectral-0}$ , which correspond to the value in m = n = 0,  $G_{spectral}$  remains

$$G_{spectral}|_{\substack{n \to +\infty \\ n \to +\infty}} = \frac{1}{A} \sum_{\substack{m = -\infty \\ \forall m, n - \{m = n = 0\}}}^{+\infty} \sum_{\substack{n = -\infty \\ \forall m, n - \{m = n = 0\}}}^{+\infty} e^{-j\bar{k}_{xy}\cdot(\bar{\rho} - \bar{\rho}')} e^{-\frac{|\bar{k}_{xy}|^2}{4\varepsilon^2}}$$

$$\times \left[ \frac{1 - jk_{x0}(x - x') - jk_{y0}(y - y') - (x - x')^2k_{x0}^2/2 - (y - y')^2k_{y0}^2/2}{|\bar{k}_{xy}|^2} \right]$$

$$+ \frac{k^2 - 2k_{x0}k_x - 2k_{y0}k_y - k_{x0}^2 - k_{y0}^2 + 2jk_{x0}^2k_x(x - x') + 2jk_{y0}^2k_y(y - y')}{|\bar{k}_{xy}|^4}$$

$$+ \frac{k^2 - 2k_{x0}k_x - 2k_{y0}k_y - k_{x0}^2 - k_{y0}^2 + 2jk_{x0}^2k_x(x - x') + 2jk_{y0}^2k_y(y - y')}{4\varepsilon^2|\bar{k}_{xy}|^2}$$

$$+ \frac{4k_{x0}^2k_x^2 + 4k_{y0}^2k_y^2}{|\bar{k}_{xy}|^6} + \frac{4k_{x0}^2k_x^2 + 4k_{y0}^2k_y^2}{4\varepsilon^2|\bar{k}_{xy}|^4} + \frac{4k_{x0}^2k_x^2 + 4k_{y0}^2k_y^2}{32\varepsilon^4|\bar{k}_{xy}|^2} + G_{spectral-0}$$

On the other hand, we have to proceed in the same way with the spatial Ewald's component  $G_{spatial}(\bar{\rho}, \bar{\rho}')$ . It might be easier because the summation in q corresponds to the expansion of the k-exponential so we have to use 2 terms in the q-summation. The  $k_{x0}$ -exponential and  $k_{y0}$ -exponential appear as are so, we have to use the second

order expansion as

$$\lim_{\substack{k \to 0 \\ \bar{k}_{w0} \to 0}} G_{spatial}(\bar{\rho}, \bar{\rho}') = \lim_{\substack{k \to 0 \\ \bar{k}_{w0} \to 0}} \left( \frac{1}{4\pi} \sum_{m=-\infty}^{+\infty} \sum_{n=-\infty}^{+\infty} e^{-j\bar{k}_{w0} \cdot \bar{\rho}_{mn}} \sum_{q=0}^{+\infty} \left( \frac{k}{2\varepsilon} \right)^{2q} \frac{1}{q!} \operatorname{E}_{q+1}(S_{mn}^2 \varepsilon^2) \right)$$

$$= \frac{1}{4\pi} \sum_{m=-\infty}^{+\infty} \sum_{n=-\infty}^{+\infty} \left[ \left( 1 - jk_{x0}md_1 - jk_{y0}nd_2 - \frac{(k_{x0}md_1)^2}{2} - \frac{(k_{y0}nd_2)^2}{2} \right) \times \operatorname{E}_1(S_{mn}^2 \varepsilon^2) + \left( \frac{k^2}{4\varepsilon^2} \right) \operatorname{E}_2(S_{mn}^2 \varepsilon^2) \right]$$

$$\times \left[ \operatorname{E}_1(S_{mn}^2 \varepsilon^2) + \left( \frac{k^2}{4\varepsilon^2} \right) \operatorname{E}_2(S_{mn}^2 \varepsilon^2) \right]$$

$$(2.223)$$

Once we have the second order expansion of the Ewald's method components obtained in (2.222) and (2.223), we can summarize how to sum the asymptotic retained part through Ewald's method.

$$\begin{split} \widetilde{G}_{e}(\bar{\rho},\bar{\rho}') &= \widetilde{G}(\bar{\rho},\bar{\rho}') \Big|_{\substack{m \to +\infty \\ n \to +\infty}} - \widetilde{G}_{e0} = \frac{1}{A} \sum_{\substack{m = -\infty \\ \forall m,n - \{m = n = 0\}}}^{+\infty} \sum_{\substack{n = -\infty \\ m = n = 0\}}}^{+\infty} e^{-j\bar{k}_{xy}\cdot(\bar{\rho}-\bar{\rho}')} e^{-\frac{|\bar{k}_{xy}|^{2}}{4\varepsilon^{2}}} \\ &\times \left[ \frac{1 - jk_{x0}(x - x') - jk_{y0}(y - y') - (x - x')^{2}k_{x0}^{2}/2 - (y - y')^{2}k_{y0}^{2}/2}{|\bar{k}_{xy}|^{2}} \right. \\ &+ \frac{k^{2} - 2k_{x0}k_{x} - 2k_{y0}k_{y} - k_{x0}^{2} - k_{y0}^{2} + 2jk_{x0}^{2}k_{x}(x - x') + 2jk_{y0}^{2}k_{y}(y - y')}{|\bar{k}_{xy}|^{4}} \\ &+ \frac{k^{2} - 2k_{x0}k_{x} - 2k_{y0}k_{y} - k_{x0}^{2} - k_{y0}^{2} + 2jk_{x0}^{2}k_{x}(x - x') + 2jk_{y0}^{2}k_{y}(y - y')}{4\varepsilon^{2}|\bar{k}_{xy}|^{2}} \\ &+ \frac{4k_{x0}^{2}k_{x}^{2} + 4k_{y0}^{2}k_{y}^{2}}{|\bar{k}_{xy}|^{6}} + \frac{4k_{x0}^{2}k_{x}^{2} + 4k_{y0}^{2}k_{y}^{2}}{4\varepsilon^{2}|\bar{k}_{xy}|^{4}} + \frac{4k_{x0}^{2}k_{x}^{2} + 4k_{y0}^{2}k_{y}^{2}}{32\varepsilon^{4}|\bar{k}_{xy}|^{2}} \right] \\ &+ \frac{1}{4\pi} \sum_{m = -\infty}^{\infty} \sum_{n = -\infty}^{\infty} \left[ \left. \left( 1 - jk_{x0}md_{1} - jk_{y0}nd_{2} - \frac{(k_{x0}md_{1})^{2}}{2} - \frac{(k_{y0}nd_{2})^{2}}{2} \right) \right. \\ &\times E_{1}(S_{mn}^{2}\varepsilon^{2}) + \left( \frac{k^{2}}{4\varepsilon^{2}} \right) E_{2}(S_{mn}^{2}\varepsilon^{2}) \right] + \underbrace{G_{spectral-0} - \widetilde{G}_{e0}}_{T} \end{split}$$

where the last term T contains the residual value when m = n = 0. As discussed before, in this approach we have to calculate and use the limit when  $|k_{w0}| \to 0$  in all cases. Thus, T can be calculated using [15] as

$$T = \frac{(-1 + jk_{x0}(x - x') + jk_{y0}(y - y') + (x - x')^2 k_{x0}^2 / 2 + (y - y')^2 k_{y0}^2 / 2)}{4A\varepsilon^2} + \frac{(-k^2 + k_{x0}^2 + k_{y0}^2)}{32A\varepsilon^4}$$
(2.225)

Introducing (2.225) in (2.224),  $\widetilde{G}_e(\bar{\rho}, \bar{\rho}')$  can be finally written as

$$\begin{split} \widetilde{G}_{e}(\bar{\rho},\bar{\rho}') &= \widetilde{G}(\bar{\rho},\bar{\rho}') \Big|_{\substack{m \to +\infty \\ n \to +\infty}} - \widetilde{G}_{e0} = \frac{1}{A} \sum_{\substack{m = -\infty \\ \forall m,n - \{m = n = 0\}}}^{+\infty} \sum_{\substack{n = -\infty \\ \forall m,n - \{m = n = 0\}}}^{+\infty} e^{-j\bar{k}_{xy} \cdot (\bar{\rho} - \bar{\rho}')} e^{-\frac{|\bar{k}_{xy}|^{2}}{4\varepsilon^{2}}} \\ &\times \left[ \frac{1 - jk_{x0}(x - x') - jk_{y0}(y - y') - (x - x')^{2}k_{x0}^{2}/2 - (y - y')^{2}k_{y0}^{2}/2}{|\bar{k}_{xy}|^{2}} \right. \\ &+ \frac{k^{2} - 2k_{x0}k_{x} - 2k_{y0}k_{y} - k_{x0}^{2} - k_{y0}^{2} + 2jk_{x0}^{2}k_{x}(x - x') + 2jk_{y0}^{2}k_{y}(y - y')}{|\bar{k}_{xy}|^{4}} \\ &+ \frac{k^{2} - 2k_{x0}k_{x} - 2k_{y0}k_{y} - k_{x0}^{2} - k_{y0}^{2} + 2jk_{x0}^{2}k_{x}(x - x') + 2jk_{y0}^{2}k_{y}(y - y')}{4\varepsilon^{2}|\bar{k}_{xy}|^{2}} \\ &+ \frac{4k_{x0}^{2}k_{x}^{2} + 4k_{y0}^{2}k_{y}^{2}}{|\bar{k}_{xy}|^{6}} + \frac{4k_{x0}^{2}k_{x}^{2} + 4k_{y0}^{2}k_{y}^{2}}{4\varepsilon^{2}|\bar{k}_{xy}|^{4}} + \frac{4k_{x0}^{2}k_{x}^{2} + 4k_{y0}^{2}k_{y}^{2}}{32\varepsilon^{4}|\bar{k}_{xy}|^{2}} \right] \\ &+ \frac{1}{4\pi} \sum_{m = -\infty}^{\infty} \sum_{n = -\infty}^{\infty} \left[ \left( 1 - jk_{x0}(x - x') - jk_{y0}(y - y') - \frac{(k_{x0}md_{1})^{2}}{2} - \frac{(k_{y0}nd_{2})^{2}}{2} \right) \right. \\ &\times E_{1}(S_{mn}^{2}\varepsilon^{2}) + \left( \frac{k^{2}}{4\varepsilon^{2}} \right) E_{2}(S_{mn}^{2}\varepsilon^{2}) \right] + \frac{(-k^{2} + k_{x0}^{2} + k_{y0}^{2})}{32A\varepsilon^{4}} \\ &+ \frac{(-1 + jk_{x0}(x - x') + jk_{y0}(y - y') + (x - x')^{2}k_{x0}^{2}/2 + (y - y')^{2}k_{y0}^{2}/2)}{4A\varepsilon^{2}} \end{split}$$

The generalization to Q terms is not carried out due to the difficulty that arises from the Ewald's integrals when we extract more than two terms with this approach. This is because we have the product of three Taylor expansions and the integrals resulted by this product become complicated. Nevertheless, the procedures followed in this subsection will be useful in the acceleration of the 2-D Green's function with 2-D periodicity, as will be shown in Chapter 3.

To summarize, in this subsection we have accelerated the spectral Green's function by using the second proposed approach in Kummer's transformation and summing efficiently the asymptotic retained part through Ewald's method.

## 2.3.3 Option B.2. Approach of $\left(\frac{2\pi m}{d_1}, \frac{2\pi n}{d_2}\right)$ : Lerch Transcendent.

The strategy of this second alternative is to develop the formulation without applying any transformation on it. For this aim, the final expression of this procedure will be expressed in a semi-closed form using the Lerch transcendent.

In this case, the series  $\widetilde{G}_e(\bar{\rho}, \bar{\rho}')$  that has to be efficiently summed is

$$\widetilde{G}_{e}(\bar{\rho}, \bar{\rho}') = \frac{1}{A} \sum_{\substack{m = -\infty \\ \forall m, n - \{m = n = 0\}}}^{+\infty} \sum_{\substack{n = -\infty \\ m = n = 0\}}}^{+\infty} \frac{1}{\left(\frac{2\pi m}{d_{1}}\right)^{2} + \left(\frac{2\pi n}{d_{2}}\right)^{2}} e^{-j\bar{k}_{mn} \cdot (\bar{\rho} - \bar{\rho}')}$$
(2.227)

To transform this series and use the Lerch transcendent, we proceed as follows

$$\widetilde{G}_{e}(\bar{\rho}, \bar{\rho}') = \frac{e^{-j\bar{k}_{w0}\cdot(\bar{\rho}-\bar{\rho}')}}{A} \sum_{\substack{m=-\infty\\\forall m,n-\{m=n=0\}}}^{+\infty} \sum_{\substack{n=-\infty\\m=n=0\}}}^{+\infty} \frac{1}{\left(\frac{2\pi m}{d_{1}}\right)^{2} + \left(\frac{2\pi n}{d_{2}}\right)^{2}} e^{-j\frac{2\pi m}{d_{1}}(x-x')} e^{-j\frac{2\pi n}{d_{2}}(y-y')}$$

$$= \frac{e^{-j\bar{k}_{w0}(\rho-\rho')}}{A} \sum_{m=-\infty}^{+\infty} \frac{e^{-j\frac{2\pi m}{d_{1}}(x-x')}}{\left(\frac{2\pi}{d_{2}}\right)^{2}} \sum_{n=-\infty}^{+\infty} \frac{e^{-j\frac{2\pi n}{d_{2}}(y-y')}}{\left(\frac{md_{2}}{d_{1}}\right)^{2} + n^{2}} \tag{2.228}$$

Now, we separate the total series into the sum of two different ones, according to the positive and negative m

$$\widetilde{G}_{e}(\bar{\rho}, \bar{\rho}') = \frac{e^{-j\bar{k}_{w0}\cdot(\bar{\rho}-\bar{\rho}')}}{A} \left( \sum_{m=1}^{+\infty} \frac{e^{-j\frac{2\pi m}{d_{1}}(x-x')}}{\left(\frac{2\pi}{d_{2}}\right)^{2}} \sum_{n=-\infty}^{+\infty} \frac{e^{-j\frac{2\pi n}{d_{2}}(y-y')}}{\left(\frac{md_{2}}{d_{1}}\right)^{2} + n^{2}} + \sum_{m=1}^{+\infty} \frac{e^{j\frac{2\pi m}{d_{1}}(x-x')}}{\left(\frac{2\pi}{d_{2}}\right)^{2}} \sum_{n=-\infty}^{+\infty} \frac{e^{-j\frac{2\pi n}{d_{2}}(y-y')}}{\left(\frac{md_{2}}{d_{1}}\right)^{2} + n^{2}} + \sum_{n=-\infty}^{+\infty} \frac{e^{-j\frac{2\pi n}{d_{2}}(y-y')}}{\left(\frac{2\pi n}{d_{2}}\right)^{2}} \right)$$
(2.229)

Then, we take out common factor as

$$\widetilde{G}_{e}(\bar{\rho}, \bar{\rho}') = \frac{e^{-j\bar{k}_{w0}\cdot(\bar{\rho}-\bar{\rho}')}}{A} \left[ \sum_{m=1}^{+\infty} \frac{1}{\left(\frac{2\pi}{d_{2}}\right)^{2}} \sum_{n=-\infty}^{+\infty} \frac{e^{-j\frac{2\pi n}{d_{2}}(y-y')}}{\left(\frac{md_{2}}{d_{1}}\right)^{2} + n^{2}} \left( e^{-j\frac{2\pi m}{d_{1}}(x-x')} + e^{j\frac{2\pi m}{d_{1}}(x-x')} \right) \right] \\
+ \sum_{n=-\infty}^{+\infty} \frac{e^{-j\frac{2\pi n}{d_{2}}(y-y')}}{\left(\frac{2\pi n}{d_{2}}\right)^{2}} \right] \\
= \frac{e^{-j\bar{k}_{w0}\cdot(\bar{\rho}-\bar{\rho}')}}{A} \left[ \sum_{m=1}^{+\infty} \frac{2\cos\left(\frac{2\pi m}{d_{1}}(x-x')\right)}{\left(\frac{2\pi}{d_{2}}\right)^{2}} \underbrace{\sum_{n=-\infty}^{+\infty} \frac{e^{-j\frac{2\pi n}{d_{2}}(y-y')}}{\left(\frac{md_{2}}{d_{1}}\right)^{2} + n^{2}}}_{S_{1}} + \underbrace{\sum_{n=-\infty}^{+\infty} \frac{e^{-j\frac{2\pi n}{d_{1}}(y-y')}}{\left(\frac{2\pi n}{d_{2}}\right)^{2}}}_{S_{2}} \right]$$

$$(2.230)$$

The series  $S_1$  and  $S_2$  have to be optimally summed in order to calculate efficiently the series  $\widetilde{G}_e(\bar{\rho}, \bar{\rho}')$  as

$$\widetilde{G}_{e}(\bar{\rho}, \bar{\rho}') = \frac{e^{-j\bar{k}_{w0}\cdot(\bar{\rho}-\bar{\rho}')}}{A} \left( \sum_{m=1}^{+\infty} \frac{2\cos\left(\frac{2\pi m}{d_{1}}(x-x')\right)}{\left(\frac{2\pi}{d_{2}}\right)^{2}} S_{1} + S_{2} \right)$$
(2.231)

For this purpose, we start by transforming the series  $S_1$  to use the Lerch transcendent. It is important to note that this function is defined as

$$\Phi(z, s, a) = \sum_{k=0}^{+\infty} \frac{z^k}{(a+k)^s}$$
 (2.232)

Through the Lerch transcendent, the following identity can be obtained using [15]

$$S = \sum_{n=-\infty}^{+\infty} \frac{e^{xn}}{a^2 + n^2} = \frac{-j}{2a} e^{-x} \left[ \Phi\left(e^{-x}, 1, 1 - aj\right) - \Phi\left(e^{-x}, 1, 1 + aj\right) + e^x \Phi\left(e^x, 1, -aj\right) - e^x \Phi\left(e^x, 1, aj\right) \right]$$

$$(2.233)$$

Thus, we can rewrite the series  $S_1$  as

$$S_{1} = \sum_{n=-\infty}^{+\infty} \frac{e^{-j\frac{2\pi n}{d_{2}}(y-y')}}{\left(\frac{md_{2}}{d_{1}}\right)^{2} + n^{2}} = \frac{-jd_{1}}{2md_{2}} e^{j\frac{2\pi}{d_{2}}(y-y')} \left[ \Phi\left(e^{j\frac{2\pi}{d_{2}}(y-y')}, 1, 1 - \left(\frac{md_{2}}{d_{1}}\right)j\right) - \Phi\left(e^{j\frac{2\pi}{d_{2}}(y-y')}, 1, 1 + \left(\frac{md_{2}}{d_{1}}\right)j\right) + e^{-j\frac{2\pi}{d_{2}}(y-y')} \Phi\left(e^{-j\frac{2\pi}{d_{2}}(y-y')}, 1, -\left(\frac{md_{2}}{d_{1}}\right)j\right) - e^{j\frac{-2\pi}{d_{2}}(y-y')} \Phi\left(e^{-j\frac{2\pi}{d_{2}}(y-y')}, 1, \left(\frac{md_{2}}{d_{1}}\right)j\right) \right]$$

$$(2.234)$$

On the other hand, we can transform the series  $\mathcal{S}_2$  as follows

$$S_{2} = \sum_{\substack{n = -\infty \\ n \neq 0}}^{+\infty} \frac{e^{-j\frac{2\pi n}{d_{2}}(y - y')}}{\left(\frac{2\pi n}{d_{2}}\right)^{2}} = \sum_{n=1}^{+\infty} \frac{e^{-j\frac{2\pi n}{d_{2}}(y - y')}}{\left(\frac{2\pi n}{d_{2}}\right)^{2}} + \sum_{n=-\infty}^{-1} \frac{e^{-j\frac{2\pi n}{d_{2}}(y - y')}}{\left(\frac{2\pi n}{d_{2}}\right)^{2}}$$

$$= \sum_{n=1}^{+\infty} \frac{e^{-j\frac{2\pi n}{d_{2}}(y - y')}}{\left(\frac{2\pi n}{d_{2}}\right)^{2}} + \sum_{n=1}^{+\infty} \frac{e^{j\frac{2\pi n}{d_{2}}(y - y')}}{\left(\frac{2\pi n}{d_{2}}\right)^{2}}$$

$$(2.235)$$

Remembering that the polylogarithm, which is a particular case of the Lerch transcendent, is defined as

$$\operatorname{Li}_{s}(z) = \sum_{k=0}^{+\infty} \frac{z^{k}}{k^{s}} \tag{2.236}$$

we can write the series  $S_2$ , which is a particular case of the series  $S_1$  when m = 0, as

$$S_2 = \frac{1}{\left(\frac{2\pi}{d_2}\right)^2} \left[ \text{Li}_2(e^{-j\frac{2\pi}{d_2}(y-y')}) + \text{Li}_2(e^{j\frac{2\pi}{d_2}(y-y')}) \right]$$
(2.237)

An alternative to sum this series  $S_2$  is achieved using the summation of a cosine series

$$S_2 = \sum_{n=1}^{+\infty} \frac{1}{\left(\frac{2\pi n}{d_2}\right)^2} \left( e^{-j\frac{2\pi n}{d_2}(y-y')} + e^{j\frac{2\pi n}{d_2}(y-y')} \right) = \sum_{n=1}^{+\infty} \frac{2\cos\left(\frac{2\pi n}{d_2}(y-y')\right)}{\left(\frac{2\pi n}{d_2}\right)^2}$$
(2.238)

Thus, if the following relation is used,

$$\sum_{n=1}^{+\infty} \frac{\cos(nx)}{n^2} = \frac{x^2}{4} - \frac{\pi x}{2} + \frac{\pi^2}{6}$$
 (2.239)

the series  $S_2$  remains

$$S_{2} = \frac{2}{\left(\frac{2\pi}{d_{2}}\right)^{2}} \sum_{n=1}^{+\infty} \frac{\cos\left(\frac{2\pi(y-y')}{d_{2}}n\right)}{n^{2}} = \frac{2}{\left(\frac{2\pi}{d_{2}}\right)^{2}} \left[\frac{\left(\frac{2\pi(y-y')}{d_{2}}\right)^{2}}{4} - \frac{\pi\left(\frac{2\pi(y-y')}{d_{2}}\right)}{2} + \frac{\pi^{2}}{6}\right]$$

$$= \frac{(y-y')^{2}}{2} - \frac{(y-y')d_{2}}{2} + \frac{d_{2}^{2}}{12}$$

$$(2.240)$$

Once we have summed the series  $S_1$  and  $S_2$ , we can conclude that the spectral Green's function has been accelerated by retaining the first term in Kummer's transformation. This asymptotic retained term can be efficiently summed using this method in a semi-closed form with the Lerch transcendent formulation combined with either the polylogarithm or the closed form defined in (2.239). This alternative reduces the dimensionality of the original series.

# 2.3.4 Option B.3. Approach of $\left(\frac{2\pi m}{d_1}, \frac{2\pi n}{d_2}\right)$ : Summation by Parts.

In this subsection, we study an alternative to sum the remaining part using the summation by parts technique [9]. By using this technique, the series  $\widetilde{G}_e(\bar{\rho}, \bar{\rho}')$  can be written as the sum of two parts, one analytical and the other numerical but finite.

In this case, the series  $\widetilde{G}_e(\bar{\rho}, \bar{\rho}')$  that we have to sum efficiently is

$$\widetilde{G}_{e}(\bar{\rho}, \bar{\rho}') = \frac{1}{A} \sum_{\substack{m = -\infty \\ \forall m, n - \{m = n = 0\}}}^{+\infty} \sum_{\substack{n = -\infty \\ d_{1}}}^{+\infty} \frac{1}{\left(\frac{2\pi m}{d_{1}}\right)^{2} + \left(\frac{2\pi n}{d_{2}}\right)^{2}} e^{-j\bar{k}_{mn} \cdot (\bar{\rho} - \bar{\rho}')}$$
(2.241)

This series can be transformed as in Subsection 2.3.3 and can be written as the equation (2.229) as

$$\widetilde{G}_{e}(\bar{\rho}, \bar{\rho}') = \frac{e^{-j\bar{k}_{w0}\cdot(\bar{\rho}-\bar{\rho}')}}{A} \left( \sum_{m=1}^{+\infty} \frac{e^{-j\frac{2\pi m}{d_{1}}(x-x')}}{\left(\frac{2\pi}{d_{2}}\right)^{2}} \sum_{n=-\infty}^{+\infty} \frac{e^{-j\frac{2\pi n}{d_{2}}(y-y')}}{\left(\frac{md_{2}}{d_{1}}\right)^{2} + n^{2}} + \sum_{m=1}^{+\infty} \frac{e^{j\frac{2\pi m}{d_{1}}(x-x')}}{\left(\frac{2\pi}{d_{2}}\right)^{2}} \sum_{n=-\infty}^{+\infty} \frac{e^{-j\frac{2\pi n}{d_{2}}(y-y')}}{\left(\frac{md_{2}}{d_{1}}\right)^{2} + n^{2}} + \sum_{n=-\infty}^{+\infty} \frac{e^{-j\frac{2\pi n}{d_{2}}(y-y')}}{\left(\frac{2\pi n}{d_{2}}\right)^{2}} \right)$$
(2.242)

Now, the summations are separated according to positive and negative n

$$\widetilde{G}_{e}(\bar{\rho}, \bar{\rho}') = \frac{e^{-j\bar{k}_{w0}\cdot(\bar{\rho}-\bar{\rho}')}}{A} \left[ \sum_{m=1}^{+\infty} \frac{e^{-j\frac{2\pi m}{d_{1}}(x-x')}}{\left(\frac{2\pi}{d_{2}}\right)^{2}} \left( \sum_{n=1}^{+\infty} \frac{e^{-j\frac{2\pi n}{d_{2}}(y-y')}}{\left(\frac{md_{2}}{d_{1}}\right)^{2} + n^{2}} + \sum_{n=-\infty}^{-1} \frac{e^{-j\frac{2\pi n}{d_{2}}(y-y')}}{\left(\frac{md_{2}}{d_{1}}\right)^{2} + n^{2}} + \frac{1}{n} \right] + \sum_{n=-\infty}^{+\infty} \frac{e^{-j\frac{2\pi n}{d_{2}}(y-y')}}{\left(\frac{2\pi}{d_{1}}\right)^{2}} \left( \sum_{n=1}^{+\infty} \frac{e^{-j\frac{2\pi n}{d_{2}}(y-y')}}{\left(\frac{md_{2}}{d_{1}}\right)^{2} + n^{2}} + \sum_{n=-\infty}^{-1} \frac{e^{-j\frac{2\pi n}{d_{2}}(y-y')}}{\left(\frac{md_{2}}{d_{1}}\right)^{2} + n^{2}} + \frac{1}{\left(\frac{md_{2}}{d_{1}}\right)^{2}} \right) + \sum_{n=-\infty}^{+\infty} \frac{e^{-j\frac{2\pi n}{d_{2}}(y-y')}}{\left(\frac{2\pi n}{d_{2}}\right)^{2}} \right]$$

$$(2.243)$$

and we proceed as follows

$$\widetilde{G}_{e}(\bar{\rho}, \bar{\rho}') = \frac{e^{-j\bar{k}_{w0} \cdot (\bar{\rho} - \bar{\rho}')}}{A} \left[ \sum_{m=1}^{+\infty} \frac{e^{-j\frac{2\pi m}{d_1}(x - x')}}{\left(\frac{2\pi}{d_2}\right)^2} \left( \sum_{n=1}^{+\infty} \frac{e^{-j\frac{2\pi n}{d_2}(y - y')}}{\left(\frac{md_2}{d_1}\right)^2 + n^2} + \sum_{n=1}^{+\infty} \frac{e^{j\frac{2\pi n}{d_2}(y - y')}}{\left(\frac{md_2}{d_1}\right)^2 + n^2} \right] + \sum_{n=1}^{+\infty} \frac{e^{j\frac{2\pi n}{d_2}(x - x')}}{\left(\frac{2\pi}{d_2}\right)^2} \left( \sum_{n=1}^{+\infty} \frac{e^{-j\frac{2\pi n}{d_2}(y - y')}}{\left(\frac{md_2}{d_1}\right)^2 + n^2} + \sum_{n=1}^{+\infty} \frac{e^{j\frac{2\pi n}{d_2}(y - y')}}{\left(\frac{md_2}{d_1}\right)^2 + n^2} + \sum_{n=1}^{+\infty} \frac{e^{j\frac{2\pi n}{d_2}(y - y')}}{\left(\frac{md_2}{d_1}\right)^2} + n^2} \right) + \sum_{n=-\infty}^{+\infty} \frac{e^{-j\frac{2\pi n}{d_2}(y - y')}}{\left(\frac{2\pi n}{d_2}\right)^2} \right] \tag{2.244}$$

Taking out the denominators as common factor,  $\widetilde{G}_e(\bar{\rho}, \bar{\rho}')$  remains

$$\widetilde{G}_{e}(\bar{\rho}, \bar{\rho}') = \frac{e^{-j\bar{k}_{w0}\cdot(\bar{\rho}-\bar{\rho}')}}{A} \left[ \sum_{m=1}^{+\infty} \frac{e^{-j\frac{2\pi m}{d_{1}}(x-x')}}{\left(\frac{2\pi}{d_{2}}\right)^{2}} \sum_{n=1}^{+\infty} \frac{e^{-j\frac{2\pi n}{d_{2}}(y-y')} + e^{j\frac{2\pi n}{d_{2}}(y-y')}}{\left(\frac{md_{2}}{d_{1}}\right)^{2} + n^{2}} \right. \\
+ \sum_{m=1}^{+\infty} \frac{e^{j\frac{2\pi m}{d_{1}}(x-x')}}{\left(\frac{2\pi}{d_{2}}\right)^{2}} \sum_{n=1}^{+\infty} \frac{e^{-j\frac{2\pi n}{d_{2}}(y-y')} + e^{j\frac{2\pi n}{d_{2}}(y-y')}}{\left(\frac{md_{2}}{d_{1}}\right)^{2} + n^{2}} + \sum_{n=-\infty}^{+\infty} \frac{e^{-j\frac{2\pi n}{d_{2}}(y-y')}}{\left(\frac{2\pi n}{d_{2}}\right)^{2}} \\
+ \sum_{m=1}^{+\infty} \frac{e^{-j\frac{2\pi m}{d_{1}}(x-x')}}{\left(\frac{2\pi m}{d_{1}}\right)^{2}} + \sum_{m=1}^{+\infty} \frac{e^{j\frac{2\pi m}{d_{1}}(x-x')}}{\left(\frac{2\pi m}{d_{1}}\right)^{2}}\right] \tag{2.245}$$

that is,

$$\widetilde{G}_{e}(\bar{\rho}, \bar{\rho}') = \frac{e^{-jk_{w0}(\rho - \rho')}}{A} \left[ \sum_{m=1}^{+\infty} \frac{e^{-j\frac{2\pi m}{d_{1}}(x - x')}}{\left(\frac{2\pi}{d_{2}}\right)^{2}} \sum_{n=1}^{+\infty} \frac{2\cos\left(\frac{2\pi n}{d_{2}}(y - y')\right)}{\left(\frac{md_{2}}{d_{1}}\right)^{2} + n^{2}} + \sum_{m=1}^{+\infty} \frac{e^{j\frac{2\pi m}{d_{1}}(x - x')}}{\left(\frac{2\pi}{d_{2}}\right)^{2}} \right] \\
\sum_{n=1}^{+\infty} \frac{2\cos\left(\frac{2\pi n}{d_{2}}(y - y')\right)}{\left(\frac{md_{2}}{d_{1}}\right)^{2} + n^{2}} + \sum_{n=-\infty}^{+\infty} \frac{e^{-j\frac{2\pi n}{d_{1}}(y - y')}}{\left(\frac{2\pi n}{d_{2}}\right)^{2}} + \sum_{m=-\infty}^{+\infty} \frac{e^{-j\frac{2\pi m}{d_{1}}(x - x')}}{\left(\frac{2\pi m}{d_{1}}\right)^{2}} \right] \tag{2.246}$$

Now, we can rewrite  $\widetilde{G}_e(\bar{\rho}, \bar{\rho}')$  as the summation of three series

$$\widetilde{G}_{e}(\bar{\rho}, \bar{\rho}') = \frac{e^{-j\bar{k}_{w0}\cdot(\bar{\rho}-\bar{\rho}')}}{A} \left[ 4 \sum_{m=1}^{+\infty} \sum_{n=1}^{+\infty} \frac{\cos\left(\frac{2\pi m}{d_{1}}(x-x')\right) \cos\left(\frac{2\pi n}{d_{2}}(y-y')\right)}{\left(\frac{2\pi m}{d_{1}}\right)^{2} + \left(\frac{2\pi n}{d_{2}}\right)^{2}} + \sum_{\substack{n=-\infty\\n\neq 0}}^{+\infty} \frac{e^{-j\frac{2\pi n}{d_{2}}(y-y')}}{\left(\frac{2\pi n}{d_{2}}\right)^{2}} + \sum_{\substack{m=-\infty\\m\neq 0}}^{+\infty} \frac{e^{-j\frac{2\pi m}{d_{1}}(x-x')}}{\left(\frac{2\pi m}{d_{1}}\right)^{2}} \right] \tag{2.247}$$

$$\widetilde{G}_e(\bar{\rho}, \bar{\rho}') = \frac{e^{-j\bar{k}_{w0}\cdot(\bar{\rho}-\bar{\rho}')}}{A} [4S_1 + S_2 + S_3]$$
 (2.248)

It should be pointed out that the series  $S_2$  and  $S_3$  can be summed analytically as previously. However, we have to apply the theory of two dimensional summation by parts technique (see Appendix A.1) reported in [9] to the series  $S_1$ . This leads to the splitting of the series into two parts

$$S_{1} = \sum_{m=1}^{+\infty} \sum_{n=1}^{+\infty} \frac{\cos\left(\frac{2\pi m}{d_{1}}(x - x')\right) \cos\left(\frac{2\pi n}{d_{2}}(y - y')\right)}{\left(\frac{2\pi m}{d_{1}}\right)^{2} + \left(\frac{2\pi n}{d_{2}}\right)^{2}}$$

$$= \sum_{m=1}^{M-1} \sum_{n=1}^{N-1} \frac{\cos\left(\frac{2\pi m}{d_{1}}(x - x')\right) \cos\left(\frac{2\pi n}{d_{2}}(y - y')\right)}{\left(\frac{2\pi m}{d_{1}}\right)^{2} + \left(\frac{2\pi n}{d_{2}}\right)^{2}}$$

$$+ \sum_{m=M}^{+\infty} \sum_{n=N}^{+\infty} \frac{\cos\left(\frac{2\pi m}{d_{1}}(x - x')\right) \cos\left(\frac{2\pi n}{d_{2}}(y - y')\right)}{\left(\frac{2\pi m}{d_{1}}\right)^{2} + \left(\frac{2\pi n}{d_{2}}\right)^{2}}$$
(2.249)

Remembering that the transformation that can be applied in  $R_{M,N}$  is

$$R_{M,N} = \sum_{m=M}^{+\infty} \sum_{n=N}^{+\infty} \widetilde{G}_{m,n}^{(-1,-1)} f_m^{(+1)} h_n^{(+1)} = \sum_{i=1}^{+\infty} \sum_{k=1}^{+\infty} \widetilde{G}_{M,N}^{(-i,-k)} f_{M-1}^{(i+1)} h_{N-1}^{(k+1)}$$
(2.250)

we can identify terms as follows in order to apply the previous relation.

$$R_{M,N} = \sum_{m=M}^{+\infty} \sum_{n=N}^{+\infty} \frac{1}{\underbrace{\left(\frac{2\pi m}{d_1}\right)^2 + \left(\frac{2\pi n}{d_2}\right)^2}_{\widetilde{G}_{m,n}^{(-1,-1)}}} \underbrace{\cos\left(\frac{2\pi m}{d_1}(x-x')\right)}_{f_m^{(+1)}} \underbrace{\cos\left(\frac{2\pi n}{d_2}(y-y')\right)}_{h_n^{(+1)}}$$
(2.251)

Using the first order approximation of  $R_{M,N}$ ,

$$R_{M,N} = \widetilde{G}_{M,N}^{(-1,-1)} f_{M-1}^{(+2)} h_{N-1}^{(+2)}$$
(2.252)

where

$$\widetilde{G}_{M,N}^{(-1,1)} = \widetilde{G}_{m,n}^{(-1,1)} \Big|_{\substack{m=M\\n=N}} = \frac{1}{\left(\frac{2\pi m}{d_1}\right)^2 + \left(\frac{2\pi n}{d_2}\right)^2} \Big|_{\substack{m=M\\n=N}} = \frac{1}{\left(\frac{2\pi M}{d_1}\right)^2 + \left(\frac{2\pi N}{d_2}\right)^2}$$
(2.253)

$$f_{M-1}^{(+2)} = \sum_{k=m+1}^{+\infty} f_k^{(+1)} \Big|_{m=M-1} = \sum_{k=m+1}^{+\infty} \cos\left(\frac{2\pi k}{d_1}(x-x')\right) \Big|_{m=M-1}$$

$$= \frac{\cos\left[\left(m+1\right)\left(\frac{2\pi}{d_1}(x-x')\right)\right] - \cos\left[m\left(\frac{2\pi}{d_1}(x-x')\right)\right]}{2\left[1-\cos\left(\frac{2\pi}{d_1}(x-x')\right)\right]} \Big|_{m=M-1}$$

$$= \frac{\cos\left[M\left(\frac{2\pi}{d_1}(x-x')\right)\right] - \cos\left[\left(M-1\right)\left(\frac{2\pi}{d_1}(x-x')\right)\right]}{2\left[1-\cos\left(\frac{2\pi}{d_1}(x-x')\right)\right]}$$

$$h_{N-1}^{(+2)} = \sum_{k=n+1}^{+\infty} h_k^{(+1)} \Big|_{n=N-1} = \sum_{k=n+1}^{+\infty} \cos\left(\frac{2\pi k}{d_2}(y-y')\right) \Big|_{n=N-1}$$

$$= \frac{\cos\left[\left(n+1\right)\left(\frac{2\pi}{d_2}(y-y')\right)\right] - \cos\left[n\left(\frac{2\pi}{d_2}(y-y')\right)\right]}{2\left[1-\cos\left(\frac{2\pi}{d_2}(y-y')\right)\right]} \Big|_{n=N-1}$$

$$= \frac{\cos\left[N\left(\frac{2\pi}{d_2}(y-y')\right)\right] - \cos\left[\left(N-1\right)\left(\frac{2\pi}{d_2}(y-y')\right)\right]}{2\left[1-\cos\left(\frac{2\pi}{d_2}(y-y')\right)\right]}$$

$$= \frac{1}{2\left[1-\cos\left(\frac{2\pi}{d_2}(y-y')\right)\right]}$$

 $R_{M,N}$  can be summed as

$$R_{M,N} = \widetilde{G}_{M,N}^{(-1,-1)} f_{M-1}^{(+2)} h_{N-1}^{(+2)}$$

$$= \frac{\left(\cos\left(\frac{2\pi(x-x')M}{d_1}\right) - \cos\left(\frac{2\pi(M-1)(x-x')}{d_1}\right)\right) \cdot \left(\cos\left(\frac{2\pi(y-y')N}{d_2}\right) - \cos\left(\frac{2\pi(N-1)(y-y')}{d_2}\right)\right)}{4\left[\left(\frac{2\pi M}{d_1}\right)^2 + \left(\frac{2\pi N}{d_2}\right)^2\right] \left[1 - \cos\left(\frac{2\pi(x-x')}{d_1}\right)\right] \left[1 - \cos\left(\frac{2\pi(y-y')}{d_2}\right)\right]}$$
(2.256)

and therefore,  $S_1$  is given by the summation of the initial numerical part  $S_{M-1,N-1}$  and the obtained analytical part  $R_{M,N}$ .

So, we have accelerated the spectral Green's function by retaining the first term in Kummer's transformation. This asymptotic retained term can be summed using the combination of the analytical summation of cosine series and the summation by parts technique. Through this technique, we are able to transform the original series into a sum of an an-

alytical part and a numerical but finite part. On the other hand, the parameters M and N, which split the initial series, have to be optimally adjusted as required.

# 2.3.5 Option B.4. Approach of $\left(\frac{2\pi m}{d_1}, \frac{2\pi n}{d_2}\right)$ : Analytical Sum in One Index.

The last alternative that we propose to add the asymptotic part in Kummer's transformation is summing the remaining series in an analytical way at least in one dimension. This can reduce the dimensionality of the problem thanks to sum analytically the series in one index. This option is carried out with the extraction of the first and the second term. The series that appear when we extract more than two terms cannot be summed analytically.

#### • Extraction of one term.

For this procedure, we start from (2.247). As has been mentioned before, the series  $S_2$  and  $S_3$  can be written analytically. For this purpose, the series  $S_2$  can be transformed as

$$S_{2} = \sum_{\substack{n=-\infty\\n\neq 0}}^{+\infty} \frac{e^{-j\frac{2\pi n}{d_{2}}(y-y')}}{\left(\frac{2\pi n}{d_{2}}\right)^{2}} = \sum_{n=1}^{+\infty} \frac{e^{-j\frac{2\pi n}{d_{2}}(y-y')}}{\left(\frac{2\pi n}{d_{2}}\right)^{2}} + \sum_{n=-\infty}^{-1} \frac{e^{-j\frac{2\pi n}{d_{2}}(y-y')}}{\left(\frac{2\pi n}{d_{2}}\right)^{2}}$$

$$= \sum_{n=1}^{+\infty} \frac{e^{-j\frac{2\pi n}{d_{2}}(y-y')}}{\left(\frac{2\pi n}{d_{2}}\right)^{2}} + \sum_{n=1}^{+\infty} \frac{e^{j\frac{2\pi n}{d_{2}}(y-y')}}{\left(\frac{2\pi n}{d_{2}}\right)^{2}} = \sum_{n=1}^{+\infty} \frac{\cos\left(\frac{2\pi n}{d_{2}}(y-y')\right)}{\left(\frac{2\pi n}{d_{2}}\right)^{2}}$$

$$(2.257)$$

and using the relation given in (2.239),  $S_2$  is expressed analytically as

$$S_{2} = \frac{2}{\left(\frac{2\pi}{d_{2}}\right)^{2}} \sum_{n=1}^{+\infty} \frac{\cos\left(\frac{2\pi(y-y')}{d_{2}}n\right)}{n^{2}} = \frac{2}{\left(\frac{2\pi}{d_{2}}\right)^{2}} \left[ \frac{\left(\frac{2\pi(y-y')}{d_{2}}\right)^{2}}{4} - \frac{\pi\left(\frac{2\pi(y-y')}{d_{2}}\right)}{2} + \frac{\pi^{2}}{6} \right]$$

$$= \frac{(y-y')^{2}}{2} - \frac{(y-y')d_{2}}{2} + \frac{d_{2}^{2}}{12}$$

$$(2.258)$$

Likewise, the series  $S_3$  is rewritten as

$$S_{3} = \frac{2}{\left(\frac{2\pi}{d_{1}}\right)^{2}} \sum_{m=1}^{+\infty} \frac{\cos\left(\frac{2\pi(x-x')}{d_{1}}m\right)}{m^{2}} = \frac{2}{\left(\frac{2\pi}{d_{1}}\right)^{2}} \left[\frac{\left(\frac{2\pi(x-x')}{d_{1}}\right)^{2}}{4} - \frac{\pi\left(\frac{2\pi(x-x')}{d_{1}}\right)}{2} + \frac{\pi^{2}}{6}\right]$$

$$= \frac{(x-x')^{2}}{2} - \frac{(x-x')d_{1}}{2} + \frac{d_{1}^{2}}{12}$$

$$(2.259)$$

On the other hand, the series  $S_1$  can be solved analytically

$$S_1 = \sum_{n=1}^{+\infty} \frac{\cos\left(\frac{2\pi n}{d_2}(y - y')\right)}{\left(\frac{md_2}{d_1}\right)^2 + n^2}$$
 (2.260)

by using the follow relation

$$\sum_{n=1}^{+\infty} \frac{\cos(nx)}{a^2 + n^2} = \frac{\pi}{2a} \frac{\cosh((\pi - x)a)}{\sinh(\pi a)} - \frac{1}{2a^2}$$
 (2.261)

as

$$S_{1} = \frac{\pi}{2\frac{md_{2}}{d_{1}}} \frac{\cosh\left[\left(\pi - \left(\frac{2\pi}{d_{2}}(y - y')\right)\right)\frac{md_{2}}{d_{1}}\right]}{\sinh(\pi\frac{md_{2}}{d_{1}})} - \frac{1}{2\left(\frac{md_{2}}{d_{1}}\right)^{2}}$$

$$= \frac{\pi d_{1}}{2md_{2}} \frac{\cosh\left[\left(\pi - \left(\frac{2\pi}{d_{2}}(y - y')\right)\right)\frac{md_{2}}{d_{1}}\right]}{\sinh(\pi\frac{md_{2}}{d_{1}})} - \frac{d_{1}^{2}}{2\left(md_{2}\right)^{2}}$$
(2.262)

Finally, we can conclude that  $\widetilde{G}_e(\bar{\rho}, \bar{\rho}')$  can be expressed as

$$\widetilde{G}_{e}(\bar{\rho}, \bar{\rho}') = \frac{e^{-j\bar{k}_{w0}\cdot(\bar{\rho}-\bar{\rho}')}}{A} \left[ \sum_{m=1}^{+\infty} \frac{4S_{1}\cos\left(\frac{2\pi m}{d_{1}}(x-x')\right)}{\left(\frac{2\pi}{d_{2}}\right)^{2}} + S_{2} + S_{3} \right]$$
(2.263)

where the series  $S_1$ ,  $S_2$  and  $S_3$  have been analytically calculated.

## • Extraction of two terms.

In this alternative not only the first term but also the second term have an analytical expression. For this reason, we are interested in the extraction of the second asymptotic term and summing it by the same procedure as the previous one.

In this case, the  $\widetilde{G}_e(\bar{\rho}, \bar{\rho}')$  series that we have to efficiently sum is

$$\widetilde{G}_{e}(\bar{\rho}, \bar{\rho}') = \frac{1}{A} \sum_{\substack{m = -\infty \\ \forall m, n - \{m = n = 0\}}}^{+\infty} \sum_{\substack{n = -\infty \\ m = n = 0}}^{+\infty} \left[ \frac{1}{\left(\frac{2\pi m}{d_{1}}\right)^{2} + \left(\frac{2\pi n}{d_{2}}\right)^{2}} - \frac{z_{u} + z_{v}}{\left(\left(\frac{2\pi m}{d_{1}}\right)^{2} + \left(\frac{2\pi n}{d_{2}}\right)^{2}\right)^{2}} \right] e^{-j\bar{k}_{mn}\cdot(\bar{\rho}-\bar{\rho}')}$$
(2.264)

where

$$z_u = k_{x0}^2 - k^2/2 + \frac{4\pi m k_{x0}}{d_1}$$
 (2.265a)

$$z_v = k_{y0}^2 - k^2/2 + \frac{4\pi n k_{y0}}{d_2}$$
 (2.265b)

$$z_u + z_v = \underbrace{k_{x0}^2 + k_{y0}^2 - k^2}_{k_t} + \frac{4\pi m k_{x0}}{d_1} + \frac{4\pi n k_{y0}}{d_2}$$
 (2.265c)

Using this, we can rewrite the series  $\widetilde{G}_e(\bar{\rho}, \bar{\rho}')$  as

$$\widetilde{G}_{e}(\bar{\rho}, \bar{\rho}') = \underbrace{\frac{e^{-j\bar{k}_{w0} \cdot (\bar{\rho} - \bar{\rho}')}}{A} \sum_{\substack{m = -\infty \\ \forall m, n - \{m = n = 0\}}}^{+\infty} \sum_{\substack{n = -\infty \\ m = n = 0\}}}^{+\infty} \frac{e^{-j\frac{2\pi n}{d_{1}}(x - x')} e^{-j\frac{2\pi n}{d_{2}}(y - y')}}{\left(\frac{2\pi n}{d_{1}}\right)^{2} + \left(\frac{2\pi n}{d_{2}}\right)^{2}} - \underbrace{\frac{e^{-j\bar{k}_{w0} \cdot (\bar{\rho} - \bar{\rho}')}}{A} \sum_{\substack{m = -\infty \\ \forall m, n - \{m = n = 0\}}}^{+\infty} \sum_{\substack{n = -\infty \\ \forall m, n - \{m = n = 0\}}}^{+\infty} \frac{(z_{u} + z_{v})e^{-j\frac{2\pi n}{d_{1}}(x - x')} e^{-j\frac{2\pi n}{d_{2}}(y - y')}}{\left(\left(\frac{2\pi m}{d_{1}}\right)^{2} + \left(\frac{2\pi n}{d_{2}}\right)^{2}\right)^{2}}} \underbrace{S_{h}} \tag{2.266}$$

The first series  $S_a$  has been summed previously. Therefore, the new series that we have to sum is

$$S_{b} = \frac{e^{-j\bar{k}_{w0}\cdot(\bar{\rho}-\bar{\rho}')}}{A} \underbrace{\sum_{\substack{m=-\infty\\\forall m,n-\{m=n=0\}}}^{+\infty} \sum_{\substack{n=-\infty\\\forall m,n-\{m=n=0\}}}^{+\infty} \frac{(z_{u}+z_{v})e^{-j\frac{2\pi m}{d_{1}}(x-x')}e^{-j\frac{2\pi n}{d_{2}}(y-y')}}{\left(\left(\frac{2\pi m}{d_{1}}\right)^{2}+\left(\frac{2\pi n}{d_{2}}\right)^{2}\right)^{2}}$$
(2.267)

Specifically, we focus on summing the series S. This series can be split according to positive and negative m

$$S = \sum_{m=1}^{+\infty} \sum_{n=-\infty}^{+\infty} \frac{\left(k_t + \frac{4\pi m k_{x0}}{d_1} + \frac{4\pi n k_{y0}}{d_2}\right) e^{-j\frac{2\pi m}{d_1}(x-x')} e^{-j\frac{2\pi n}{d_2}(y-y')}}{\left(\left(\frac{2\pi m}{d_1}\right)^2 + \left(\frac{2\pi n}{d_2}\right)^2\right)^2}$$

$$+ \sum_{m=1}^{+\infty} \sum_{n=-\infty}^{+\infty} \frac{\left(k_t - \frac{4\pi m k_{x0}}{d_1} + \frac{4\pi n k_{y0}}{d_2}\right) e^{j\frac{2\pi m}{d_1}(x-x')} e^{-j\frac{2\pi n}{d_2}(y-y')}}{\left(\left(\frac{2\pi m}{d_1}\right)^2 + \left(\frac{2\pi n}{d_2}\right)^2\right)^2}$$

$$+ \sum_{n=-\infty}^{+\infty} \frac{\left(k_t + \frac{4\pi n k_{y0}}{d_2}\right) e^{-j\frac{2\pi n}{d_2}(y-y')}}{\left(\frac{2\pi n}{d_2}\right)^4}$$

$$(2.268)$$

and now we split the series according to positive and negative n

$$S = \sum_{m=1}^{+\infty} \sum_{n=1}^{+\infty} \frac{\left(k_t + \frac{4\pi m k_{x_0}}{d_1} + \frac{4\pi n k_{y_0}}{d_2}\right) e^{-j\frac{2\pi m}{d_1}(x-x')} e^{-j\frac{2\pi n}{d_2}(y-y')}}{\left(\left(\frac{2\pi m}{d_1}\right)^2 + \left(\frac{2\pi n}{d_2}\right)^2\right)^2}$$

$$+ \sum_{m=1}^{+\infty} \sum_{n=1}^{+\infty} \frac{\left(k_t + \frac{4\pi m k_{x_0}}{d_1} - \frac{4\pi n k_{y_0}}{d_2}\right) e^{-j\frac{2\pi m}{d_1}(x-x')} e^{j\frac{2\pi n}{d_2}(y-y')}}{\left(\left(\frac{2\pi m}{d_1}\right)^2 + \left(\frac{2\pi n}{d_2}\right)^2\right)^2}$$

$$+ \sum_{m=1}^{+\infty} \sum_{n=1}^{+\infty} \frac{\left(k_t - \frac{4\pi m k_{x_0}}{d_1} + \frac{4\pi n k_{y_0}}{d_2}\right) e^{j\frac{2\pi m}{d_1}(x-x')} e^{-j\frac{2\pi n}{d_2}(y-y')}}{\left(\left(\frac{2\pi m}{d_1}\right)^2 + \left(\frac{2\pi n}{d_2}\right)^2\right)^2}$$

$$+ \sum_{m=1}^{+\infty} \sum_{n=1}^{+\infty} \frac{\left(k_t - \frac{4\pi m k_{x_0}}{d_1} - \frac{4\pi n k_{y_0}}{d_2}\right) e^{j\frac{2\pi m}{d_1}(x-x')} e^{j\frac{2\pi n}{d_2}(y-y')}}{\left(\left(\frac{2\pi m}{d_1}\right)^2 + \left(\frac{2\pi n}{d_2}\right)^2\right)^2}$$

$$+ \sum_{m=1}^{+\infty} \frac{\left(k_t + \frac{4\pi m k_{x_0}}{d_1}\right) e^{-j\frac{2\pi n}{d_1}(x-x')}}{\left(\frac{2\pi m}{d_1}\right)^4} + \sum_{m=1}^{+\infty} \frac{\left(k_t - \frac{4\pi m k_{x_0}}{d_1}\right) e^{j\frac{2\pi m}{d_1}(x-x')}}{\left(\frac{2\pi m}{d_2}\right)^4}$$

$$+ \sum_{n=1}^{+\infty} \frac{\left(k_t + \frac{4\pi n k_{y_0}}{d_2}\right) e^{-j\frac{2\pi n}{d_2}(y-y')}}{\left(\frac{2\pi n}{d_2}\right)^4} + \sum_{n=1}^{+\infty} \frac{\left(k_t - \frac{4\pi n k_{y_0}}{d_2}\right) e^{j\frac{2\pi n}{d_2}(y-y')}}{\left(\frac{2\pi n}{d_2}\right)^4}$$

Regrouping terms, the series S can be expressed as follows

$$S = \sum_{m=1}^{+\infty} \sum_{n=1}^{+\infty} 4k_t \frac{\cos\left(\frac{2\pi m}{d_1}(x - x')\right) \cos\left(\frac{2\pi n}{d_2}(y - y')\right)}{\left(\left(\frac{2\pi m}{d_1}\right)^2 + \left(\frac{2\pi n}{d_2}\right)^2\right)^2} + \sum_{m=1}^{+\infty} \sum_{n=1}^{+\infty} \frac{-16j\pi m k_{x0}}{d_1} \frac{\sin\left(\frac{2\pi m}{d_1}(x - x')\right) \cos\left(\frac{2\pi n}{d_2}(y - y')\right)}{\left(\left(\frac{2\pi m}{d_1}\right)^2 + \left(\frac{2\pi n}{d_2}\right)^2\right)^2} + \sum_{m=1}^{+\infty} \sum_{n=1}^{+\infty} \frac{-16j\pi n k_{y0}}{d_2} \frac{\cos\left(\frac{2\pi m}{d_1}(x - x')\right) \sin\left(\frac{2\pi n}{d_2}(y - y')\right)}{\left(\left(\frac{2\pi m}{d_1}\right)^2 + \left(\frac{2\pi n}{d_2}\right)^2\right)^2} + \sum_{m=1}^{+\infty} 2k_t \frac{\cos\left(\frac{2\pi m}{d_1}(x - x')\right)}{\left(\frac{2\pi m}{d_1}\right)^4} + \sum_{m=1}^{+\infty} \frac{-8j\pi m k_{x0}}{d_1} \frac{\sin\left(\frac{2\pi m}{d_1}(x - x')\right)}{\left(\frac{2\pi m}{d_1}\right)^4} + \sum_{n=1}^{+\infty} 2k_t \frac{\cos\left(\frac{2\pi n}{d_2}(y - y')\right)}{\left(\frac{2\pi n}{d_2}\right)^4} + \sum_{n=1}^{+\infty} \frac{-8j\pi n k_{y0}}{d_2} \frac{\sin\left(\frac{2\pi n}{d_2}(y - y')\right)}{\left(\frac{2\pi n}{d_2}\right)^4}$$

Using the following notation, the series S can be obtained as the sum of these series

$$S = S_1 + S_2 + S_3 + S_4 + S_5 + S_6 + S_7 (2.271)$$

Now, we try to find a way to express analytically these series. For this purpose, we use the following relation

$$\sum_{n=0}^{+\infty} \frac{\cos(nx)}{(a^2 + n^2)^2} = \frac{1}{2a^4} + \frac{\pi}{4a^3} \operatorname{cosech}(\pi a) \left[ \cosh(a(\pi - x)) + ax \sinh(a(\pi - y)) \right] + \frac{\pi^2}{4a^2} \operatorname{cosech}^2(\pi a) \cosh(ax)$$
(2.272)

to obtain the summation of the next series

$$\sum_{n=1}^{+\infty} \frac{\cos(nx)}{(a^2 + n^2)^2} = \sum_{n=0}^{+\infty} \frac{\cos(nx)}{(a^2 + n^2)^2} - \frac{1}{a^4} = \frac{1}{2a^4} + \frac{\pi}{4a^3} \operatorname{cosech}(\pi a) \left[ \cosh(a(\pi - x)) + ax \sinh(a(\pi - y)) \right] + \frac{\pi^2}{4a^2} \operatorname{cosech}^2(\pi a) \cosh(ax) - \frac{1}{a^4} = \frac{-1}{2a^4} + \frac{\pi}{4a^3} \operatorname{cosech}(\pi a) \left[ \cosh(a(\pi - x)) + ax \sinh(a(\pi - y)) \right] + \frac{\pi^2}{4a^2} \operatorname{cosech}^2(\pi a) \cosh(ax)$$

$$(2.273)$$

With the previous identity, we can rewrite the series  $S_1$  as

$$S_{1} = \sum_{m=1}^{+\infty} 4k_{t} \frac{\cos\left(\frac{2\pi m}{d_{1}}(x - x')\right)}{\left(\frac{2\pi}{d_{2}}\right)^{4}} \sum_{n=1}^{+\infty} \frac{\cos\left(\frac{2\pi (y - y')}{d_{2}}n\right)}{\left(\left(\frac{md_{2}}{d_{1}}\right)^{2} + n^{2}\right)^{2}} = \sum_{m=1}^{+\infty} 4k_{t} \frac{\cos\left(\frac{2\pi m}{d_{1}}(x - x')\right)}{\left(\frac{2\pi}{d_{2}}\right)^{4}}$$

$$\left\{\frac{-1}{2a^{4}} + \frac{\pi}{4a^{3}}\operatorname{cosech}(\pi a)\left[\cosh(a(\pi - Y)) + aY\sinh(a(\pi - Y))\right] + \frac{\pi^{2}}{4a^{2}}\operatorname{cosech}^{2}(\pi a)\cosh(aY)\right\}$$

$$(2.274)$$

The second series  $S_2$  is transformed as

$$S_{2} = \sum_{m=1}^{+\infty} \sum_{n=1}^{+\infty} \frac{-16j\pi m k_{x0}}{d_{1}} \frac{\sin\left(\frac{2\pi m}{d_{1}}(x - x')\right) \cos\left(\frac{2\pi n}{d_{2}}(y - y')\right)}{\left(\left(\frac{2\pi m}{d_{1}}\right)^{2} + \left(\frac{2\pi n}{d_{2}}\right)^{2}\right)^{2}}$$

$$= \sum_{n=1}^{+\infty} \frac{-16j\pi k_{x0}}{d_{1}} \frac{\cos\left(\frac{2\pi n}{d_{2}}(y - y')\right)}{\left(\frac{2\pi}{d_{1}}\right)^{2}} \sum_{m=1}^{+\infty} \frac{m \sin\left(\frac{2\pi (x - x')}{d_{1}}m\right)}{\left(\left(\frac{nd_{1}}{d_{2}}\right)^{2} + m^{2}\right)^{2}}$$

$$(2.275)$$

and using the following relation

$$\sum_{n=1}^{+\infty} \frac{n \sin(nx)}{(a^2 + n^2)^2} = -\frac{\pi^2}{4a} \sinh(ax) \operatorname{cosech}^2(\pi a) + \frac{\pi x}{4a} \left[ \cosh(a(\pi - x)) \operatorname{cosech}(\pi a) \right]$$
(2.276)

 $S_2$  can be expressed as

$$S_{2} = \sum_{n=1}^{+\infty} \frac{-16j\pi k_{x0}}{d_{1}} \frac{\cos\left(\frac{2\pi n}{d_{2}}(y - y')\right)}{\left(\frac{2\pi}{d_{1}}\right)^{2}} \left\{ -\frac{\pi^{2}}{4b} \sinh(bX) \operatorname{cosech}^{2}(\pi b) + \frac{\pi X}{4b} \left[\cosh(b(\pi - X)) \operatorname{cosech}(\pi b)\right] \right\}$$
(2.277)

Similarly, the series  $S_3$  remains

$$S_{3} = \sum_{m=1}^{+\infty} \frac{-16j\pi k_{y0}}{d_{2}} \frac{\cos\left(\frac{2\pi m}{d_{1}}(x - x')\right)}{\left(\frac{2\pi}{d_{2}}\right)^{2}} \left\{ -\frac{\pi^{2}}{4a} \sinh(aY) \operatorname{cosech}^{2}(\pi a) + \frac{\pi Y}{4a} \left[ \cosh(a(\pi - Y)) \operatorname{cosech}(\pi a) \right] \right\}$$
(2.278)

Thus, we have reduced the dimensionality of the previous doubles series. The rest of the series are one-dimensional, and for that reason, they remains as they are

$$S_4 = \sum_{m=1}^{+\infty} 2k_t \frac{\cos\left(\frac{2\pi m}{d_1}(x - x')\right)}{\left(\frac{2\pi m}{d_1}\right)^4} = \frac{2k_t}{\left(\frac{2\pi}{d_1}\right)^4} \sum_{m=1}^{+\infty} \frac{\cos\left(\frac{2\pi m}{d_1}(x - x')\right)}{m^4}$$
(2.279)

$$S_5 = \sum_{m=1}^{+\infty} \frac{-8j\pi m k_{x0}}{d_1} \frac{\sin\left(\frac{2\pi m}{d_1}(x - x')\right)}{\left(\frac{2\pi m}{d_1}\right)^4} = \frac{-8j\pi k_{x0}}{d_1\left(\frac{2\pi}{d_1}\right)^4} \sum_{m=1}^{+\infty} \frac{\sin\left(\frac{2\pi m}{d_1}(x - x')\right)}{m^3}$$
(2.280)

$$S_6 = \frac{2k_t}{\left(\frac{2\pi}{d_2}\right)^4} \sum_{n=1}^{+\infty} \frac{\cos\left(\frac{2\pi n}{d_2}(y - y')\right)}{n^4}$$
 (2.281)

$$S_7 = \frac{-8j\pi k_{y0}}{d_2 \left(\frac{2\pi}{d_2}\right)^4} \sum_{n=1}^{+\infty} \frac{\sin\left(\frac{2\pi n}{d_2}(y - y')\right)}{n^3}$$
 (2.282)

As stated above, the series involved in the calculation of the remaining part in Kummer's transformation have been efficiently summed in one index. This results in a one-dimensional summation of the remaining part. This approach has not been generalized to Q terms because the following terms that appear in the extraction of Kummer's transformation do not have an analytical form. Nevertheless, the development done in this approach implies a significant improvement over the slow convergence of the original series, as will be shown in Chapter 3.

As in the previous chapter, a comparison between the different techniques reported in this section to sum the asymptotic series in this second form of applying Kummer's transformation will be reported in Chapter 3.

In addition, in Chapter 3 we compare the improvement that implies the use of each approach in the application of the spectral Kummer's transformation and we analyse the advantages of using one or the other strategy. In advance, we could suppose that, depending on the case that we are interested in, it would be better using one or the other approach.

As a general conclusion, we have proposed for each approach different methods of summing the remaining part.

#### 1. The first one is using Ewald's method.

As has been discussed before, this alternative allows us to use the acceleration resulted by applying Kummer's transformation and sum efficiently the retained terms through Ewald's method.

Thanks to the proposed Kummer-Ewald technique, we can take advantage of the rapidly convergence of Ewald's components without the need to calculate all the special functions involved in these series. This is because here we do not have to calculate all of them, we have to calculate only those needed. Thus, by using this

proposed Kummer-Ewald method we are able to choose the effort that we want to invest in each technique. This technique has been outlined for the extraction of Q terms in the first approach and two terms in the case of the second approach.

#### 2. The second one is using the Lerch transcendent.

This mathematical function gives us the possibility of expressing the remaining part in a semi-closed form. As can be noted, the Lerch transcendent is defined as an infinite summation. This alternative has been developed only for the second approach in Kummer's transformation because of the nature of the retained part. For this reason, although it is evaluated as an infinite sum, the remaining series is independent from the frequency.

#### 3. The third one is using the summation by parts technique.

As already explained, this transformation consists of accelerating the series basing on their oscillation behaviours [9]. It allows us to express the remaining part as a sum of an analytical part plus a numerical but finite part. This technique has been applied in the second approach for the extraction of the first term in Kummer's transformation.

#### 4. The last one is summing analytically in one index.

This alternative allows us to reduce the dimensionality of the series. This is because we use analytical results to sum the series in one index [23]. As the previous option, this alternative has been only outlined for the second approach in Kummer's transformation because of the nature of the remaining part. In addition, it is important to highlight that we have been able to sum analytically in one index the remaining series in the extraction of the first and the second term.

The above conclusions will be proved through programming the proposed techniques and the numerical results will be shown in Chapter 3.

# 2.4 Green's Functions of Rectangular Waveguides and 2-D Cavities

In rectangular waveguides and 2-D cavities, the Green's functions can be formulated using the classical theory of images with respect to four perfect electric conductors. This theory implies that the actual system can be replaced by an equivalent system formed by the combination of the real and the introduced virtual sources (images) [1]. In this section, we first obtain the different components of the outstanding Green's functions involved in these problems from the general 2-D Green's functions with 2-D periodicity. The components in this problem are the same than the ones reported in Section 1.2 for the case of 1-D periodicity. They are the Green's functions of the magnetic and electric scalar and vector potentials. Once these components are described, we apply Kummer's transformation to some of them (Subsection 2.4.1) in order to accelerate their convergences.

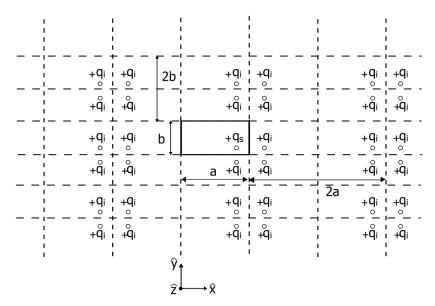
To describe the outstanding components of Green's functions it is advisable representing the possible scenarios in these problems. It should be pointed out that from now on, we use the particular case of phase-shifted array. This is because the sources here are aligned due to the geometry of the problem, as will be shown.

Thus, the Fig. 2.3(a) represents the combination of the actual source and its images when a magnetic charge is placed near the electric conductors. Being a magnetic charge, the images have the same sign as the actual source. This distribution is employed to evaluate the Green's function of the magnetic scalar potential  $G_W$ .

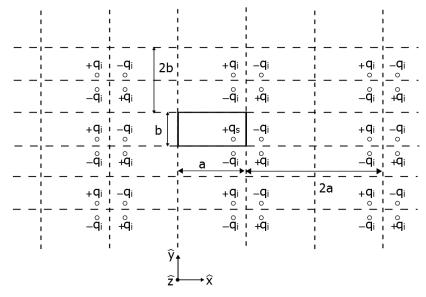
On the other hand, Fig. 2.3(b) represents the combination of the actual source and its images when an electric charge is placed near the electric conductors. Being an electric charge, the images alternate the positive and negative signs. This distribution is employed to evaluate the Green's function of the electric scalar potential  $G_V$ .

The Fig. 2.4 represents the combination of the actual source and its images when a magnetic current dipole  $\vec{m}_s$  is placed near the electric conductors in the x-direction (Fig. 2.4(a)), in the y-direction (Fig. 2.4(b)) and in the z-direction (Fig. 2.4(c)). Being a magnetic current dipole, the images change the sign or orientation when the actual source is perpendicular to the electric conductor. On the contrary, the images have the same sign as the actual source when the magnetic current dipole is parallel to the electric conductor. These distributions are employed to calculate the dyadic components of the Green's function of the electric vector potential  $G_F^{xx}$ ,  $G_F^{yy}$  and  $G_F^{zz}$ , respectively.

Finally, the Fig. 2.5 represents the combination of the actual source and its images when an electric current dipole  $\vec{j}_s$  is placed near the electric conductors in the x-direction (Fig. 2.5(a)), in the y-direction (Fig. 2.5(b)) and in the z-direction (Fig. 2.5(c)). Being an electric current dipole, the images change the sign or orientation when the actual source is parallel to the electric conductor. On the contrary, the images have the same sign as the actual source when the electric current dipole is perpendicular to the electric conductor. These distributions are employed to calculate the dyadic components of the Green's function of the magnetic vector potential  $G_A^{xx}$ ,  $G_A^{yy}$  and  $G_A^{zz}$ , respectively.

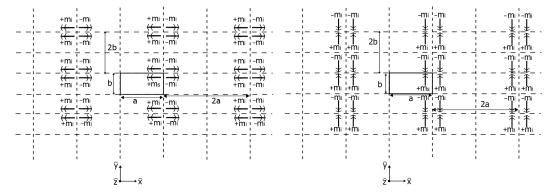


(a) Distribution of the actual magnetic charge  $q_s$  and its images  $q_i$  for a rectangular cavity.

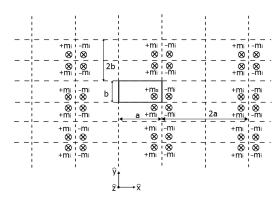


(b) Distribution of the actual electric charge  $q_s$  and its images  $q_i$  for a rectangular cavity.

Figure 2.3: Distribution of the actual and virtual sources. The width of the cavity in the x-direction is a and and in y-direction is b. Thus, the images are distributed in quadruples separated by a distance of 2a in x-direction and 2b in y-direction. It is satisfied that  $q_s = q_i$ .

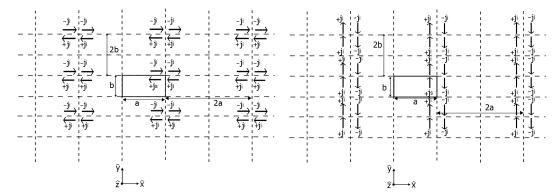


(a) Actual and virtual sources produced by a magnetic current dipole oriented in x-direction. (b) Actual and virtual sources produced by a magnetic current dipole oriented in y-direction.

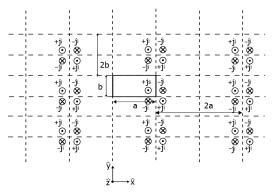


(c) Actual and virtual sources produced by a magnetic current dipole oriented in z-direction.

Figure 2.4: Distribution of the actual magnetic current dipole  $\vec{m}_s$  and its images  $\vec{m}_i$  for a rectangular waveguide or 2-D cavity. It is satisfied that  $m_s = m_i$ . The width of the cavity in the x-direction is a and and in y-direction is b. Thus, the images are distributed in quadruples separated by a distance of 2a in x-direction and 2b in y-direction.



(a) Actual and virtual sources produced by an (b) Actual and virtual sources produced by an electelectric current dipole oriented in x-direction.



(c) Actual and virtual sources produced by an electric current dipole oriented in z-direction.

Figure 2.5: Distribution of the actual electric current dipole  $\vec{j}_s$  and its images  $\vec{j}_i$  for a rectangular waveguide or 2-D cavity. It is satisfied that  $j_s = j_i$ . The width of the cavity in the x-direction is a and and in y-direction is b. Thus, the images are distributed in quadruples separated by a distance of 2a in x-direction and 2b in y-direction.

As stated above, the shown figures illustrate that we have to employ the formulation related to the particular case of phase-shifted array due to the geometry of the problem.

Once we have represented the possible scenarios to obtain the most relevant functions involved in these problems, we are going to define the series  $\tilde{G}_{+}(\bar{\rho}, \bar{\rho}')$  and  $\tilde{G}_{-}(\bar{\rho}, \bar{\rho}')$  as the basis of some of these Green's functions and they are going to be formulated using the spatial and spectral representations of the 2-D Green's function with 2-D periodicity. The spatial series  $G(\bar{\rho}, \bar{\rho}')$  is given by

$$G(\bar{\rho}, \bar{\rho}') = \frac{1}{4j} \sum_{m=-\infty}^{+\infty} \sum_{n=-\infty}^{+\infty} H_0^{(2)}(kS_{mn}) e^{-j\bar{k}_{w0}\cdot\bar{\rho}_{mn}}$$
(2.283)

where 
$$S_{mn} = \sqrt{(x - x' - md_1)^2 + (y - y' - nd_2)^2}$$

On the other hand, the spectral series  $\widetilde{G}(\bar{\rho}, \bar{\rho}')$  is given by

$$\widetilde{G}(\bar{\rho}, \bar{\rho}') = \frac{1}{A} \sum_{m=-\infty}^{+\infty} \sum_{n=-\infty}^{+\infty} \frac{e^{-j\bar{k}_{mn} \cdot (\bar{\rho} - \bar{\rho}')}}{|\bar{k}_{mn}|^2 - k^2}$$
(2.284)

where

$$\bar{k}_{mn} = \bar{k}_{w0} + \frac{2\pi}{A} \left[ m(\bar{a}_2 \times \hat{z}) + n(\hat{z} \times \bar{a}_1) \right] = \left( k_{x0} + \frac{2\pi m}{d_1} \right) \hat{x} + \left( k_{y0} + \frac{2\pi n}{d_2} \right) \hat{y} \quad (2.285)$$

The series  $\widetilde{G}_{+}(\bar{\rho}, \bar{\rho}')$  and  $\widetilde{G}_{-}(\bar{\rho}, \bar{\rho}')$  are composed by the combination of four general 2-D periodic Green's functions with different sources. In the first one, the source is (x', y'), in the second one is (x', -y'), in the third one is (-x', y') and in the fourth one is (-x', -y'). In all cases, the period is  $d_1 = 2a$  and  $d_2 = 2b$  and  $\theta = 0^{\circ}$  due to the direction of the wave incident on the array. We use the following notation for these four sources

$$S_{mn++} = \sqrt{(x - x' - 2am)^2 + (y - y' - 2bn)^2}$$
 (2.286a)

$$S_{mn+-} = \sqrt{(x - x' - 2am)^2 + (y + y' - 2bn)^2}$$
 (2.286b)

$$S_{mn+-} = \sqrt{(x+x'-2am)^2 + (y-y'-2bn)^2}$$
 (2.286c)

$$S_{mn--} = \sqrt{(x + x' - 2am)^2 + (y + y' - 2bn)^2}$$
 (2.286d)

According to this, the spatial Green's function  $G_+(\bar{\rho}, \bar{\rho}')$  can be expressed as the sum of four general periodic Green's functions as

$$G_{+}(\bar{\rho}, \bar{\rho}') = \frac{1}{4j} \sum_{m=-\infty}^{+\infty} \sum_{n=-\infty}^{+\infty} H_{0}^{(2)}(kS_{mn++}) + \frac{1}{4j} \sum_{m=-\infty}^{+\infty} \sum_{n=-\infty}^{+\infty} H_{0}^{(2)}(kS_{mn+-})$$

$$+ \frac{1}{4j} \sum_{m=-\infty}^{+\infty} \sum_{n=-\infty}^{+\infty} H_{0}^{(2)}(kS_{mn-+}) + \frac{1}{4j} \sum_{m=-\infty}^{+\infty} \sum_{n=-\infty}^{+\infty} H_{0}^{(2)}(kS_{mn--})$$

$$= \frac{1}{4j} \sum_{m=-\infty}^{+\infty} \sum_{n=-\infty}^{+\infty} \left[ H_{0}^{(2)}(k\sqrt{(x-x'-2am)^{2}+(y-y'-2bn)^{2}}) + H_{0}^{(2)}(k\sqrt{(x-x'-2am)^{2}+(y-y'-2bn)^{2}}) + H_{0}^{(2)}(k\sqrt{(x+x'-2am)^{2}+(y-y'-2bn)^{2}}) \right]$$

$$+ H_{0}^{(2)}(k\sqrt{(x+x'-2am)^{2}+(y-y'-2bn)^{2}})$$

$$+ H_{0}^{(2)}(k\sqrt{(x+x'-2am)^{2}+(y+y'-2bn)^{2}})$$

Using Poisson's formula, its alternative spectral  $\widetilde{G}_{+}(\bar{\rho}, \bar{\rho}')$  series is obtained. It is important to note that in this case  $k_{x0} = 0$  and  $k_{y0} = 0$  and  $\bar{k}_{mn}$  remains

$$\bar{k}_{mn} = \left(k_{x0} + \frac{2\pi m}{2a}\right)\hat{x} + \left(k_{y0} + \frac{2\pi n}{2b}\right)\hat{y} = \frac{\pi m}{a}\hat{x} + \frac{\pi n}{b}\hat{y}$$
(2.288)

Therefore, the spectral formulation can be written as

$$\widetilde{G}_{+}(\bar{\rho}, \bar{\rho}') = \frac{1}{4a} \sum_{m=-\infty}^{+\infty} \sum_{n=-\infty}^{+\infty} \frac{1}{\left(\frac{2\pi m}{2a}\right)^{2} + \left(\frac{2\pi n}{2b}\right)^{2} - k^{2}} \left[ e^{-j\frac{\pi m(x-x')}{a}} e^{-j\frac{\pi n(y-y')}{b}} + e^{-j\frac{\pi m(x-x')}{a}} e^{-j\frac{\pi m(x-x')}{b}} \right] \\
e^{-j\frac{\pi n(y+y')}{b}} + e^{-j\frac{\pi m(x+x')}{a}} e^{-j\frac{\pi n(y-y')}{b}} + e^{-j\frac{\pi m(x+x')}{a}} e^{-j\frac{\pi n(y+y')}{b}} \right] \\
= \frac{1}{4a} \sum_{m=-\infty}^{+\infty} \sum_{n=-\infty}^{+\infty} \frac{1}{\left(\frac{\pi m}{a}\right)^{2} + \left(\frac{\pi n}{b}\right)^{2} - k^{2}} \left[ e^{-j\frac{\pi mx}{a}} e^{+j\frac{\pi mx'}{a}} e^{-j\frac{\pi ny}{b}} e^{+j\frac{\pi ny'}{b}} + e^{-j\frac{\pi mx}{a}} e^{+j\frac{\pi mx'}{a}} e^{-j\frac{\pi ny}{b}} e^{+j\frac{\pi ny'}{b}} + e^{-j\frac{\pi ny}{a}} e^{-j\frac{\pi ny}{b}} e^{-j\frac{\pi ny}{b}} \right] \\
e^{-j\frac{\pi ny}{b}} e^{-j\frac{\pi ny'}{b}} + e^{-j\frac{\pi mx}{a}} e^{-j\frac{\pi mx'}{a}} e^{-j\frac{\pi ny}{b}} e^{+j\frac{\pi ny'}{b}} + e^{-j\frac{\pi nx}{a}} e^{-j\frac{\pi ny}{b}} e^{-j\frac{\pi ny}{b}} \right]$$
(2.289)

This series can be rewritten by grouping terms as

$$\widetilde{G}_{+}(\bar{\rho}, \bar{\rho}') = \frac{1}{4ab} \sum_{m=-\infty}^{+\infty} \sum_{n=-\infty}^{+\infty} \frac{1}{\left(\frac{\pi m}{a}\right)^{2} + \left(\frac{\pi n}{b}\right)^{2} - k^{2}} \left[ e^{-j\frac{\pi mx}{a}} e^{-j\frac{\pi ny'}{b}} e^{j\frac{\pi ny'}{b}} 2 \left( \frac{e^{+j\frac{\pi mx'}{a}} + e^{-j\frac{\pi mx'}{a}}}{2} \right) + e^{-j\frac{\pi mx}{a}} e^{-j\frac{\pi ny}{b}} e^{-j\frac{\pi ny'}{b}} 2 \left( \frac{e^{+j\frac{\pi mx'}{a}} + e^{-j\frac{\pi mx'}{a}}}{2} \right) \right] \\
= \frac{1}{4ab} \sum_{m=-\infty}^{+\infty} \sum_{n=-\infty}^{+\infty} \frac{1}{\left(\frac{\pi m}{a}\right)^{2} + \left(\frac{\pi n}{b}\right)^{2} - k^{2}} \left[ e^{-j\frac{\pi mx}{a}} e^{-j\frac{\pi ny}{b}} 2 \cos \left(\frac{\pi mx'}{a}\right) 2 \right] \\
\left( \frac{e^{+j\frac{\pi ny'}{b}} + e^{-j\frac{\pi ny'}{b}}}{2} \right) \right] \\
= \frac{1}{ab} \sum_{m=-\infty}^{+\infty} \sum_{n=-\infty}^{+\infty} \frac{1}{\left(\frac{\pi m}{a}\right)^{2} + \left(\frac{\pi n}{b}\right)^{2} - k^{2}} e^{-j\frac{\pi mx}{a}} e^{-j\frac{\pi ny}{b}} \cos \left(\frac{\pi mx'}{a}\right) \cos \left(\frac{\pi ny'}{b}\right) \\
= \frac{1}{ab} \sum_{m=-\infty}^{+\infty} \sum_{n=-\infty}^{+\infty} \frac{1}{\left(\frac{\pi m}{a}\right)^{2} + \left(\frac{\pi n}{b}\right)^{2} - k^{2}} e^{-j\frac{\pi mx}{a}} e^{-j\frac{\pi ny}{b}} \cos \left(\frac{\pi mx'}{a}\right) \cos \left(\frac{\pi ny'}{b}\right) \\
= \frac{1}{ab} \sum_{m=-\infty}^{+\infty} \sum_{n=-\infty}^{+\infty} \frac{1}{\left(\frac{\pi m}{a}\right)^{2} + \left(\frac{\pi n}{b}\right)^{2} - k^{2}} e^{-j\frac{\pi nx}{a}} e^{-j\frac{\pi ny}{b}} \cos \left(\frac{\pi mx'}{a}\right) \cos \left(\frac{\pi ny'}{b}\right) \\
= \frac{1}{ab} \sum_{m=-\infty}^{+\infty} \sum_{n=-\infty}^{+\infty} \frac{1}{\left(\frac{\pi m}{a}\right)^{2} + \left(\frac{\pi n}{b}\right)^{2} - k^{2}} e^{-j\frac{\pi nx}{a}} e^{-j\frac{\pi ny}{b}} \cos \left(\frac{\pi mx'}{a}\right) \cos \left(\frac{\pi ny'}{b}\right) \\
= \frac{1}{ab} \sum_{m=-\infty}^{+\infty} \sum_{n=-\infty}^{+\infty} \frac{1}{\left(\frac{\pi m}{a}\right)^{2} + \left(\frac{\pi n}{b}\right)^{2} - k^{2}} e^{-j\frac{\pi ny}{a}} e^{-j\frac{\pi ny}{b}} \cos \left(\frac{\pi ny'}{a}\right) \cos \left(\frac{\pi ny'}{b}\right) \\
= \frac{1}{ab} \sum_{m=-\infty}^{+\infty} \sum_{n=-\infty}^{+\infty} \frac{1}{\left(\frac{\pi ny}{a}\right)^{2} + \left(\frac{\pi ny}{b}\right)^{2} - k^{2}} e^{-j\frac{\pi ny}{a}} e^{-j\frac{\pi ny}{b}} \cos \left(\frac{\pi ny'}{a}\right) \cos \left(\frac{\pi ny'}{b}\right) \\
= \frac{1}{ab} \sum_{m=-\infty}^{+\infty} \sum_{n=-\infty}^{+\infty} \frac{1}{\left(\frac{\pi ny}{a}\right)^{2} + \left(\frac{\pi ny}{b}\right)^{2} - k^{2}} e^{-j\frac{\pi ny}{a}} e^{-j\frac{\pi ny}{b}} \cos \left(\frac{\pi ny'}{a}\right) \cos \left(\frac{\pi ny'}{b}\right) \cos \left(\frac{\pi ny'}{b}\right) \cos \left(\frac{\pi ny'}{a}\right) \cos \left(\frac{\pi ny'}{b}\right) \cos \left(\frac{\pi ny'}{b}$$

Due to the fact that this is an even function with respect to  $k_x = \frac{\pi m}{a}$ , the exponential  $e^{-jk_xx}$  evaluated in m between  $(-\infty, +\infty)$  can be written as  $2\epsilon_m \cos(k_xx)$  evaluated in m between  $(0, +\infty)$ . On the other hand,  $\widetilde{G}_+(\bar{\rho}, \bar{\rho}')$  is an even function with respect to  $k_y = \frac{\pi n}{b}$ , thus the exponential  $e^{-jk_yy}$  evaluated in n between  $(-\infty, +\infty)$  can be written as  $2\epsilon_n \cos(k_yy)$  between  $(0, +\infty)$ . This procedure is detailed in Appendix A.2.

According to this,  $\widetilde{G}_{+}(\bar{r}, \bar{r}')$  is given by

$$\widetilde{G}_{+}(\bar{\rho},\bar{\rho}') = \frac{2\epsilon_{m}}{ab} \sum_{m=0}^{+\infty} \sum_{n=-\infty}^{+\infty} \frac{1}{\left(\frac{\pi m}{a}\right)^{2} + \left(\frac{\pi n}{b}\right)^{2} - k^{2}} e^{-j\frac{\pi ny}{b}} \cos\left(\frac{\pi mx}{a}\right) \cos\left(\frac{\pi mx'}{a}\right) \cos\left(\frac{\pi ny'}{b}\right)$$

$$= \frac{4\epsilon_{mn}}{ab} \sum_{m=0}^{+\infty} \sum_{n=0}^{+\infty} \frac{\cos\left(\frac{\pi mx}{a}\right) \cos\left(\frac{\pi mx'}{a}\right) \cos\left(\frac{\pi ny}{b}\right) \cos\left(\frac{\pi ny'}{b}\right)}{\left(\frac{\pi m}{a}\right)^{2} + \left(\frac{\pi n}{b}\right)^{2} - k^{2}}$$
(2.291)

where  $\epsilon_{m0} = \epsilon_{0n} = 1/2$  and  $\epsilon_{mn} = 1$  for m > 0 and n > 0 (see Appendix A.2).

On the other hand, in the case of the function composed by the subtraction of the images, we have the sum of four periodic Green's functions with different sources and additionally, two of them are inverted. Thus, the spatial series  $G_{-}(\bar{\rho}, \bar{\rho}')$  in this case is the subtraction of these periodic Green's functions

$$G_{-}(\bar{\rho}, \bar{\rho}') = \frac{1}{4j} \sum_{m=-\infty}^{+\infty} \sum_{n=-\infty}^{+\infty} H_{0}^{(2)}(kS_{mn++}) - \frac{1}{4j} \sum_{m=-\infty}^{+\infty} \sum_{n=-\infty}^{+\infty} H_{0}^{(2)}(kS_{mn+-})$$

$$- \frac{1}{4j} \sum_{m=-\infty}^{+\infty} \sum_{n=-\infty}^{+\infty} H_{0}^{(2)}(kS_{mn-+}) + \frac{1}{4j} \sum_{m=-\infty}^{+\infty} \sum_{n=-\infty}^{+\infty} H_{0}^{(2)}(kS_{mn--})$$

$$= \frac{1}{4j} \sum_{m=-\infty}^{+\infty} \sum_{n=-\infty}^{+\infty} \left[ H_{0}^{(2)}(k\sqrt{(x-x'-2am)^{2}+(y-y'-2bn)^{2}}) - H_{0}^{(2)}(k\sqrt{(x-x'-2am)^{2}+(y-y'-2bn)^{2}}) - H_{0}^{(2)}(k\sqrt{(x+x'-2am)^{2}+(y-y'-2bn)^{2}}) + H_{0}^{(2)}(k\sqrt{(x+x'-2am)^{2}+(y+y'-2bn)^{2}}) \right]$$

$$+ H_{0}^{(2)}(k\sqrt{(x+x'-2am)^{2}+(y+y'-2bn)^{2}})$$

The alternative spectral series  $\widetilde{G}_{-}(\bar{\rho},\bar{\rho}')$  given by the application of Poisson's formula is

$$\widetilde{G}_{-}(\bar{\rho}, \bar{\rho}') = \frac{1}{4a} \sum_{m=-\infty}^{+\infty} \sum_{n=-\infty}^{+\infty} \frac{1}{\left(\frac{2\pi m}{2a}\right)^{2} + \left(\frac{2\pi n}{2b}\right)^{2} - k^{2}} \left[ e^{-j\frac{\pi m(x-x')}{a}} e^{-j\frac{\pi n(y-y')}{b}} - e^{-j\frac{\pi m(x-x')}{a}} \right] \\
e^{-j\frac{\pi n(y+y')}{b}} - e^{-j\frac{\pi m(x+x')}{a}} e^{-j\frac{\pi n(y-y')}{b}} + e^{-j\frac{\pi m(x+x')}{a}} e^{-j\frac{\pi n(y+y')}{b}} \right] \\
= \frac{1}{4a} \sum_{m=-\infty}^{+\infty} \sum_{n=-\infty}^{+\infty} \frac{1}{\left(\frac{\pi m}{a}\right)^{2} + \left(\frac{\pi n}{b}\right)^{2} - k^{2}} \left[ e^{-j\frac{\pi mx}{a}} e^{+j\frac{\pi mx'}{a}} e^{-j\frac{\pi ny}{b}} e^{+j\frac{\pi ny'}{b}} - e^{-j\frac{\pi mx}{a}} e^{+j\frac{\pi mx'}{a}} e^{-j\frac{\pi ny}{b}} \right] \tag{2.293}$$

This series can be rewritten by grouping terms as

$$\widetilde{G}_{-}(\bar{\rho}, \bar{\rho}') = \frac{1}{4ab} \sum_{m=-\infty}^{+\infty} \sum_{n=-\infty}^{+\infty} \frac{1}{\left(\frac{\pi m}{a}\right)^{2} + \left(\frac{\pi n}{b}\right)^{2} - k^{2}} \left[ e^{-j\frac{\pi mx}{a}} e^{-j\frac{\pi ny}{b}} e^{j\frac{\pi ny'}{b}} 2j \right] \\
\left( \frac{e^{+j\frac{\pi mx'}{a}} - e^{-j\frac{\pi mx'}{a}}}{2j} \right) - e^{-j\frac{\pi mx}{a}} e^{-j\frac{\pi ny}{b}} e^{-j\frac{\pi ny'}{b}} 2j \left( \frac{e^{+j\frac{\pi mx'}{a}} - e^{-j\frac{\pi mx'}{a}}}{2j} \right) \right] \\
= \frac{1}{4ab} \sum_{m=-\infty}^{+\infty} \sum_{n=-\infty}^{+\infty} \frac{1}{\left(\frac{\pi m}{a}\right)^{2} + \left(\frac{\pi n}{b}\right)^{2} - k^{2}} \left[ e^{-j\frac{\pi mx}{a}} e^{-j\frac{\pi ny}{b}} 2j \sin\left(\frac{\pi mx'}{a}\right) 2j \right] \\
\left( \frac{e^{+j\frac{\pi ny'}{b}} - e^{-j\frac{\pi ny'}{b}}}{2j} \right) \right] \\
= \frac{-1}{ab} \sum_{m=-\infty}^{+\infty} \sum_{n=-\infty}^{+\infty} \frac{1}{\left(\frac{\pi m}{a}\right)^{2} + \left(\frac{\pi n}{b}\right)^{2} - k^{2}} e^{-j\frac{\pi mx}{a}} e^{-j\frac{\pi ny}{b}} \sin\left(\frac{\pi mx'}{a}\right) \sin\left(\frac{\pi ny'}{b}\right) \\
= \frac{-1}{ab} \sum_{m=-\infty}^{+\infty} \sum_{n=-\infty}^{+\infty} \frac{1}{\left(\frac{\pi m}{a}\right)^{2} + \left(\frac{\pi n}{b}\right)^{2} - k^{2}} e^{-j\frac{\pi mx}{a}} e^{-j\frac{\pi ny}{b}} \sin\left(\frac{\pi mx'}{a}\right) \sin\left(\frac{\pi ny'}{b}\right) \\
= \frac{-1}{ab} \sum_{m=-\infty}^{+\infty} \sum_{n=-\infty}^{+\infty} \frac{1}{\left(\frac{\pi m}{a}\right)^{2} + \left(\frac{\pi n}{b}\right)^{2} - k^{2}} e^{-j\frac{\pi mx}{a}} e^{-j\frac{\pi ny}{b}} \sin\left(\frac{\pi mx'}{a}\right) \sin\left(\frac{\pi ny'}{b}\right) \\
= \frac{-1}{ab} \sum_{m=-\infty}^{+\infty} \sum_{n=-\infty}^{+\infty} \frac{1}{\left(\frac{\pi m}{a}\right)^{2} + \left(\frac{\pi n}{b}\right)^{2} - k^{2}} e^{-j\frac{\pi ny}{a}} e^{-j\frac{\pi ny}{b}} \sin\left(\frac{\pi mx'}{a}\right) \sin\left(\frac{\pi ny'}{b}\right) \\
= \frac{-1}{ab} \sum_{m=-\infty}^{+\infty} \sum_{n=-\infty}^{+\infty} \frac{1}{\left(\frac{\pi ny}{a}\right)^{2} + \left(\frac{\pi ny}{b}\right)^{2} - k^{2}} e^{-j\frac{\pi ny}{a}} e^{-j\frac{\pi ny}{b}} \sin\left(\frac{\pi ny'}{a}\right) \sin\left(\frac{\pi ny'}{b}\right) \\
= \frac{-1}{ab} \sum_{m=-\infty}^{+\infty} \sum_{n=-\infty}^{+\infty} \frac{1}{\left(\frac{\pi ny}{a}\right)^{2} + \left(\frac{\pi ny}{b}\right)^{2} - k^{2}} e^{-j\frac{\pi ny}{a}} e^{-j\frac{\pi ny}{b}} \sin\left(\frac{\pi ny'}{a}\right) \sin\left(\frac{\pi ny'}{b}\right) \\
= \frac{-1}{ab} \sum_{m=-\infty}^{+\infty} \sum_{n=-\infty}^{+\infty} \frac{1}{\left(\frac{\pi ny}{a}\right)^{2} + \left(\frac{\pi ny}{b}\right)^{2} - k^{2}} e^{-j\frac{\pi ny}{a}} e^{-j\frac{\pi ny}{b}} \sin\left(\frac{\pi ny'}{a}\right) \sin\left(\frac{\pi ny'}{b}\right) e^{-j\frac{\pi ny}{b}} e^{-j\frac{\pi ny}{a}} e^{-j\frac{\pi ny}{b}} e^{-j\frac{\pi ny}$$

Due to the fact that this is an odd function with respect to  $k_x = \frac{\pi m}{a}$ , the exponential  $e^{-jk_xx}$  evaluated in m between  $(-\infty, +\infty)$  can be written as  $-2j\sin(k_xx)$  evaluated in m between  $(1, +\infty)$ . On the other hand,  $\widetilde{G}_{-}(\bar{\rho}, \bar{\rho}')$  is an odd function with respect to  $k_y = \frac{\pi n}{b}$ , thus the exponential  $e^{-jk_yy}$  evaluated in n between  $(-\infty, +\infty)$  can be written as  $-2j\sin(k_yy)$  between  $(1, +\infty)$ . This procedure is detailed in Appendix A.2.

$$\widetilde{G}_{-}(\bar{\rho}, \bar{\rho}') = \frac{-(-2j)}{ab} \sum_{m=1}^{+\infty} \sum_{n=-\infty}^{+\infty} \frac{1}{\left(\frac{\pi m}{a}\right)^{2} + \left(\frac{\pi n}{b}\right)^{2} - k^{2}} e^{-j\frac{\pi ny}{b}} \sin\left(\frac{\pi mx}{a}\right) \sin\left(\frac{\pi mx'}{a}\right) \sin\left(\frac{\pi mx'}{a}\right) \sin\left(\frac{\pi mx'}{a}\right) \sin\left(\frac{\pi mx'}{a}\right) \sin\left(\frac{\pi ny}{b}\right) \sin\left(\frac{\pi ny'}{b}\right) \sin\left(\frac{\pi ny'}{b}\right) \sin\left(\frac{\pi ny'}{b}\right) = \frac{4}{ab} \sum_{m=1}^{+\infty} \sum_{n=1}^{+\infty} \frac{\sin\left(\frac{\pi mx}{a}\right) \sin\left(\frac{\pi ny}{b}\right) \sin\left(\frac{\pi ny}{b}\right) \sin\left(\frac{\pi ny'}{b}\right)}{\left(\frac{\pi m}{a}\right)^{2} + \left(\frac{\pi n}{b}\right)^{2} - k^{2}}$$

$$(2.295)$$

These two series  $\widetilde{G}_{+}(\bar{\rho}, \bar{\rho}')$  and  $\widetilde{G}_{-}(\bar{\rho}, \bar{\rho}')$  are the basis of some of the Green's functions involved in rectangular waveguide and cavity problems. We are going to take them for future studies but it is important to note that other combinations of these Green's functions are also possible. These series could be formulated in a similar way. Due to the fact that all of them are slowly convergent, it is important to apply some acceleration techniques to improve their convergence. For this reason, the series  $\widetilde{G}_{+}(\bar{\rho}, \bar{\rho}')$  and  $\widetilde{G}_{-}(\bar{\rho}, \bar{\rho}')$  are our

starting point in the following developments but the outlined techniques could be easily extended for the rest of possible combinations.

### 2.4.1 Application of Kummer's Transformation

As in the general case of 2-D periodic Green's functions, it is also necessary to accelerate the convergence of the series involved in rectangular waveguide and cavity problems. For this reason, once we have obtained some of the basis functions involved in the evaluation of the magnetic and electric scalar and vector potentials, the transformations applied to the general Green's functions will be also applied in this particular case.

The same techniques can be used in these problems and, for instance, Ewald's method was proposed in [19]. The other strategy consists of accelerating the rectangular waveguide and cavity Green's functions by using Kummer's transformation [21].

The difference in this case with respect to the general Green's function is that  $k_{x0} = 0$  and  $k_{y0} = 0$  due to  $\theta = 0^{\circ}$ . As we have mentioned before, if  $k_{x0} = 0$  and  $k_{y0} = 0$ , the two different approaches considered in Kummer's transformation become the same and therefore we can take the advantages of each approach. Thus, all the proposed methods in the previous section can be also particularized when  $k_{x0} = 0$  and  $k_{y0} = 0$  to sum the remaining part.

Specifically, in this section we will apply the spectral Kummer's transformation by means of extracting one and two terms and we focus on summing the asymptotic terms through reducing the dimensionality of the series thanks to the analytical summation in one index. It should be pointed out that the other combinations of these Green's functions can be accelerated in a similar way. The procedure would be the same as the presented below.

#### • Extraction of one term.

The procedure to be followed is the same that in the previous sections. Firstly, we start with the series  $\widetilde{G}_{+}(\bar{\rho}, \bar{\rho}')$ .

$$\widetilde{G}_{+}(\bar{\rho},\bar{\rho}') = \frac{4\epsilon_{mn}}{ab} \sum_{m=0}^{+\infty} \sum_{n=0}^{+\infty} \frac{\cos\left(\frac{\pi mx}{a}\right)\cos\left(\frac{\pi mx'}{a}\right)\cos\left(\frac{\pi ny}{b}\right)\cos\left(\frac{\pi ny'}{b}\right)}{\left(\frac{\pi m}{a}\right)^{2} + \left(\frac{\pi n}{b}\right)^{2} - k^{2}}$$
(2.296)

Applying Kummer's transformation,  $\widetilde{G}_{+}(\bar{\rho}, \bar{\rho}')$  can be written as

$$\widetilde{G}_{+}(\bar{\rho}, \bar{\rho}') = \frac{4\epsilon_{mn}}{ab} \sum_{\substack{m=0\\\forall m, n-\{m=n=0\}}}^{+\infty} \sum_{\substack{n=0\\\forall m, n-\{m=n=0\}}}^{+\infty} \left[ \frac{1}{\left(\frac{\pi m}{a}\right)^{2} + \left(\frac{\pi n}{b}\right)^{2} - k^{2}} - \frac{1}{\left(\frac{\pi m}{a}\right)^{2} + \left(\frac{\pi n}{b}\right)^{2}} \right] \\
\cos\left(\frac{\pi mx}{a}\right) \cos\left(\frac{\pi mx'}{a}\right) \cos\left(\frac{\pi ny}{b}\right) \cos\left(\frac{\pi ny'}{b}\right) + \widetilde{G}_{00} \\
+ \underbrace{\frac{4\epsilon_{mn}}{ab}}_{\forall m, n-\{m=n=0\}}^{+\infty} \sum_{\substack{n=0\\\forall m, n-\{m=n=0\}}}^{+\infty} \frac{\cos\left(\frac{\pi mx}{a}\right) \cos\left(\frac{\pi mx'}{a}\right) \cos\left(\frac{\pi ny}{b}\right) \cos\left(\frac{\pi ny'}{b}\right)}{\left(\frac{\pi m}{a}\right)^{2} + \left(\frac{\pi n}{b}\right)^{2}}$$

$$\widetilde{G}_{e+}$$
(2.297)

 $\widetilde{G}_{00}$  is the value of the series in m=n=0 where we do not apply the extraction. The series  $\widetilde{G}_{e+}$  has to be efficiently summed

$$\widetilde{G}_{e+} = \frac{4\epsilon_{mn}}{ab} \sum_{\substack{m=0\\ \forall m,n-\{m=n=0\}}}^{+\infty} \sum_{\substack{n=0\\ \forall m,n-\{m=n=0\}}}^{+\infty} \frac{\cos\left(\frac{\pi mx}{a}\right)\cos\left(\frac{\pi mx'}{a}\right)\cos\left(\frac{\pi ny}{b}\right)\cos\left(\frac{\pi ny'}{b}\right)}{\left(\frac{\pi m}{a}\right)^2 + \left(\frac{\pi n}{b}\right)^2}$$

$$= \underbrace{\frac{4}{ab} \sum_{m=1}^{+\infty} \sum_{n=1}^{+\infty} \frac{\cos\left(\frac{\pi mx}{a}\right)\cos\left(\frac{\pi mx'}{a}\right)\cos\left(\frac{\pi ny}{b}\right)\cos\left(\frac{\pi ny'}{b}\right)}{\left(\frac{\pi m}{a}\right)^2 + \left(\frac{\pi n}{b}\right)^2}}_{S_1}$$

$$+ \underbrace{\frac{2}{ab} \sum_{m=1}^{+\infty} \frac{\cos\left(\frac{\pi mx}{a}\right)\cos\left(\frac{\pi mx'}{a}\right)}{\left(\frac{\pi m}{a}\right)^2}}_{S_2} + \underbrace{\frac{2}{ab} \sum_{n=1}^{+\infty} \frac{\cos\left(\frac{\pi ny}{b}\right)\cos\left(\frac{\pi ny'}{b}\right)}{\left(\frac{\pi b}{b}\right)^2}}_{S_2}$$

$$(2.298)$$

The strategy followed to sum these series is trying to find an analytical expression for the summation in one index to reduce the dimensionality of the series. We first start with the series  $S_1$ 

$$S_1 = \frac{4}{ab} \sum_{m=1}^{+\infty} \cos\left(\frac{\pi mx}{a}\right) \cos\left(\frac{\pi mx'}{a}\right) \sum_{n=1}^{+\infty} \frac{\cos\left(\frac{\pi ny}{b}\right) \cos\left(\frac{\pi ny'}{b}\right)}{\left(\frac{\pi m}{a}\right)^2 + \left(\frac{\pi n}{b}\right)^2}$$
(2.299)

Applying the following trigonometric identity

$$\cos(A)\cos(B) = \frac{\cos(A-B) + \cos(A+B)}{2}$$
 (2.300)

 $S_1$  can be expressed as follows

$$S_{1} = \frac{4}{ab} \sum_{m=1}^{+\infty} \cos\left(\frac{\pi mx}{a}\right) \cos\left(\frac{\pi mx'}{a}\right) \frac{1}{2} \sum_{n=1}^{+\infty} \frac{\cos\left(\frac{\pi n(y-y')}{b}\right) + \cos\left(\frac{\pi n(y+y')}{b}\right)}{\left(\frac{\pi m}{a}\right)^{2} + \left(\frac{\pi n}{b}\right)^{2}}$$

$$= \frac{2}{ab} \sum_{m=1}^{+\infty} \cos\left(\frac{\pi mx}{a}\right) \cos\left(\frac{\pi mx'}{a}\right) \left[\sum_{n=1}^{+\infty} \frac{\cos\left(\frac{\pi n(y-y')}{b}\right)}{\left(\frac{\pi}{b}\right)^{2} \left[\left(\frac{mb}{a}\right)^{2} + n^{2}\right]} + \sum_{n=1}^{+\infty} \frac{\cos\left(\frac{\pi n(y+y')}{b}\right)}{\left(\frac{\pi}{b}\right)^{2} \left[\left(\frac{mb}{a}\right)^{2} + n^{2}\right]}\right]$$

$$(2.301)$$

In the knowledge that the summations in n that appear in (2.301) can be analytically expressed as follows

$$\sum_{n=1}^{+\infty} \frac{\cos(xn)}{w^2 + n^2} = \frac{\pi}{2w} \frac{\cosh[(\pi - x)w]}{\sinh(\pi w)} - \frac{1}{2w^2}$$
 (2.302)

 $S_1$  can be written as

$$S_{1} = \frac{2}{ab} \sum_{m=1}^{+\infty} \cos\left(\frac{\pi mx}{a}\right) \cos\left(\frac{\pi mx'}{a}\right) \left(\frac{b}{\pi}\right)^{2} \left[\frac{\pi}{2\left(\frac{mb}{a}\right)} \frac{\cosh\left[\left(\pi - \left(\frac{\pi(y-y')}{b}\right)\right) \frac{mb}{a}\right]}{\sinh(\pi\left(\frac{mb}{a}\right))} - \frac{1}{2\left(\frac{mb}{a}\right)^{2}} + \frac{\pi}{2\left(\frac{mb}{a}\right)} \frac{\cosh\left[\left(\pi - \left(\frac{\pi(y+y')}{b}\right)\right) \frac{mb}{a}\right]}{\sinh(\pi\left(\frac{mb}{a}\right))} - \frac{1}{2\left(\frac{mb}{a}\right)^{2}}\right]$$

$$= \frac{2}{ab} \sum_{m=1}^{+\infty} \cos\left(\frac{\pi mx}{a}\right) \cos\left(\frac{\pi mx'}{a}\right) \left(\frac{b}{\pi}\right)^{2} \left[\frac{\pi a}{2mb} \frac{\cosh\left[\left(\pi - \left(\frac{\pi(y-y')}{b}\right)\right) \frac{mb}{a}\right]}{\sinh(\pi\left(\frac{mb}{a}\right))} + \frac{\pi a}{2mb} \frac{\cosh\left[\left(\pi - \left(\frac{\pi(y+y')}{b}\right)\right) \frac{mb}{a}\right]}{\sinh(\pi\left(\frac{mb}{a}\right))} - \frac{a^{2}}{(mb)^{2}}\right]$$

$$(2.303)$$

Now, we continue with series  $S_2$ .

$$S_{2} = \frac{2}{ab} \sum_{m=1}^{+\infty} \frac{\cos\left(\frac{\pi mx}{a}\right) \cos\left(\frac{\pi mx'}{a}\right)}{\left(\frac{\pi m}{a}\right)^{2}} = \frac{2}{ab} \sum_{m=1}^{+\infty} \frac{\cos\left(\frac{\pi m(x-x')}{a}\right) + \cos\left(\frac{\pi m(x+x')}{a}\right)}{2\left(\frac{\pi}{a}\right)^{2} m^{2}}$$
$$= \frac{a^{2}}{ab\pi^{2}} \sum_{m=1}^{+\infty} \left[ \frac{\cos\left(\frac{\pi m(x-x')}{a}\right)}{m^{2}} + \frac{\cos\left(\frac{\pi m(x+x')}{a}\right)}{m^{2}} \right]$$
(2.304)

In the knowledge that the summations in n that appear in (2.304) can be analytically expressed as follows

$$\sum_{n=1}^{+\infty} \frac{\cos(xn)}{n^2} = \frac{x^2}{4} - \frac{x\pi}{2} + \frac{\pi^2}{6}$$
 (2.305)

 $S_2$  can be written as

$$S_{2} = \frac{a}{b\pi^{2}} \left[ \frac{\left(\frac{\pi(x-x')}{a}\right)^{2}}{4} - \frac{\left(\frac{\pi(x-x')}{a}\right)\pi}{2} + \frac{\pi^{2}}{6} + \frac{\left(\frac{\pi(x+x')}{a}\right)^{2}}{4} - \frac{\left(\frac{\pi(x+x')}{a}\right)\pi}{2} + \frac{\pi^{2}}{6} \right]$$

$$= \frac{a}{2b\pi^{2}} \left[ \frac{1}{2} \left(\frac{\pi(x-x')}{a}\right)^{2} - \frac{\pi^{2}(x-x')}{a} + \frac{2\pi^{2}}{3} + \frac{1}{2} \left(\frac{\pi(x+x')}{a}\right)^{2} - \frac{\pi^{2}(x+x')}{a} \right]$$
(2.306)

and similarly  $S_3$  can be written as

$$S_3 = \frac{b}{2a\pi^2} \left[ \frac{1}{2} \left( \frac{\pi(y - y')}{b} \right)^2 - \frac{\pi^2(y - y')}{b} + \frac{2\pi^2}{3} + \frac{1}{2} \left( \frac{\pi(y + y')}{b} \right)^2 - \frac{\pi^2(y + y')}{b} \right]$$
(2.307)

Therefore,  $\widetilde{G}_{e+}$  can be defined as

$$\widetilde{G}_{e+} = \frac{2}{ab} \sum_{m=1}^{+\infty} \cos\left(\frac{\pi m x}{a}\right) \cos\left(\frac{\pi m x'}{a}\right) \left(\frac{b}{\pi}\right)^{2} \left[\frac{\pi a}{2mb} \frac{\cosh\left[\left(\pi - \left(\frac{\pi(y-y')}{b}\right)\right) \frac{mb}{a}\right]}{\sinh(\pi\left(\frac{mb}{a}\right))} + \frac{\pi a}{2mb} \frac{\cosh\left[\left(\pi - \left(\frac{\pi(y+y')}{b}\right)\right) \frac{mb}{a}\right]}{\sinh(\pi\left(\frac{mb}{a}\right))} - \frac{a^{2}}{(mb)^{2}}\right] + \frac{a}{2b\pi^{2}} \left[\frac{1}{2} \left(\frac{\pi(x-x')}{a}\right)^{2} - \frac{\pi^{2}(x-x')}{a} + \frac{2\pi^{2}}{3} + \frac{1}{2} \left(\frac{\pi(x+x')}{a}\right)^{2} - \frac{\pi^{2}(x+x')}{a}\right] + \frac{b}{2a\pi^{2}} \left[\frac{1}{2} \left(\frac{\pi(y-y')}{b}\right)^{2} - \frac{\pi^{2}(y-y')}{b} + \frac{2\pi^{2}}{3} + \frac{1}{2} \left(\frac{\pi(y+y')}{b}\right)^{2} - \frac{\pi^{2}(y+y')}{b}\right] \right] \tag{2.308}$$

An alternative option to sum  $\widetilde{G}_{e+}$  is reported in [23,25], where the following relation is proposed to sum efficiently the asymptotic part

$$\widetilde{G}_{e+} = \frac{a}{3b} + \frac{x^2 + x'^2}{2ab} - \frac{x}{b} - \frac{1}{4\pi} \sum_{m=-\infty}^{+\infty} \ln\left(4T_m^+ T_m^- e^{-2|X_m|}\right)$$
(2.309)

where

$$T_m^{\pm} = \cosh(X_m) - \cos(Y^{\pm}) \tag{2.310a}$$

$$X_m = \frac{\pi}{b} \left[ x - \left( m + \frac{1}{2} \right) a - (-1)^m \left( x' - \frac{a}{2} \right) \right]$$
 (2.310b)

$$Y^{\pm} = \frac{\pi}{b}(y \pm y') \tag{2.310c}$$

The summation by using this last option is more efficient than the previous one due to the transformation into a logarithmic series. Now, we continue applying Kummer's transformation to the series  $\widetilde{G}_{-}(\bar{\rho}, \bar{\rho}')$ 

$$\widetilde{G}_{-}(\overline{\rho}, \overline{\rho}') = \frac{4}{ab} \sum_{m=1}^{+\infty} \sum_{n=1}^{+\infty} \left[ \frac{1}{\left(\frac{\pi m}{a}\right)^{2} + \left(\frac{\pi n}{b}\right)^{2} - k^{2}} - \frac{1}{\left(\frac{\pi m}{a}\right)^{2} + \left(\frac{\pi n}{b}\right)^{2}} \right] \\
\sin\left(\frac{\pi mx}{a}\right) \sin\left(\frac{\pi mx'}{a}\right) \sin\left(\frac{\pi ny}{b}\right) \sin\left(\frac{\pi ny'}{b}\right) \\
+ \underbrace{\frac{4}{ab} \sum_{m=1}^{+\infty} \sum_{n=1}^{+\infty} \frac{\sin\left(\frac{\pi mx}{a}\right) \sin\left(\frac{\pi mx'}{a}\right) \sin\left(\frac{\pi ny}{b}\right) \sin\left(\frac{\pi ny'}{b}\right)}_{\widetilde{G}_{c}}}_{\widetilde{G}_{c}} \tag{2.311}$$

The series  $\widetilde{G}_{e-}$  has to be efficiently summed

$$\widetilde{G}_{e-} = \frac{4}{ab} \sum_{m=1}^{+\infty} \sum_{n=1}^{+\infty} \frac{\sin\left(\frac{\pi mx}{a}\right) \sin\left(\frac{\pi mx'}{a}\right) \sin\left(\frac{\pi ny}{b}\right) \sin\left(\frac{\pi ny'}{b}\right)}{\left(\frac{\pi m}{a}\right)^2 + \left(\frac{\pi n}{b}\right)^2}$$
(2.312)

As stated before, the strategy to sum this series is trying to find an analytical expression for the summation in one index to reduce the dimensionality of the series.

$$\widetilde{G}_{e-} = \frac{4}{ab} \sum_{m=1}^{+\infty} \sin\left(\frac{\pi mx}{a}\right) \sin\left(\frac{\pi mx'}{a}\right) \sum_{n=1}^{+\infty} \frac{\sin\left(\frac{\pi ny}{b}\right) \sin\left(\frac{\pi ny'}{b}\right)}{\left(\frac{\pi m}{a}\right)^2 + \left(\frac{\pi n}{b}\right)^2}$$
(2.313)

Applying the following trigonometric identity

$$\sin(A)\sin(B) = \frac{\cos(A-B) - \cos(A+B)}{2}$$
 (2.314)

 $\widetilde{G}_{e-}$  remains

$$\widetilde{G}_{e-} = \frac{4}{ab} \sum_{m=1}^{+\infty} \sin\left(\frac{\pi mx}{a}\right) \sin\left(\frac{\pi mx'}{a}\right) \frac{1}{2} \sum_{n=1}^{+\infty} \frac{\cos\left(\frac{\pi n(y-y')}{b}\right) - \cos\left(\frac{\pi n(y+y')}{b}\right)}{\left(\frac{\pi m}{a}\right)^2 + \left(\frac{\pi n}{b}\right)^2}$$

$$= \frac{2}{ab} \sum_{m=1}^{+\infty} \sin\left(\frac{\pi mx}{a}\right) \sin\left(\frac{\pi mx'}{a}\right) \left[\sum_{n=1}^{+\infty} \frac{\cos\left(\frac{\pi n(y-y')}{b}\right)}{\left(\frac{\pi}{b}\right)^2 \left[\left(\frac{mb}{a}\right)^2 + n^2\right]} - \sum_{n=1}^{+\infty} \frac{\cos\left(\frac{\pi n(y+y')}{b}\right)}{\left(\frac{\pi}{b}\right)^2 \left[\left(\frac{mb}{a}\right)^2 + n^2\right]}\right]$$

$$(2.315)$$

In the knowledge that the summations in n that appear in (2.301) can be analytically expressed as follows

$$\sum_{n=1}^{+\infty} \frac{\cos(xn)}{w^2 + n^2} = \frac{\pi}{2w} \frac{\cosh[(\pi - x)w]}{\sinh(\pi w)} - \frac{1}{2w^2}$$
 (2.316)

We can sum  $\widetilde{G}_{e-}$  as

$$\widetilde{G}_{e-} = \frac{2}{ab} \sum_{m=1}^{+\infty} \sin\left(\frac{\pi mx}{a}\right) \sin\left(\frac{\pi mx'}{a}\right) \left(\frac{b}{\pi}\right)^2 \left[\frac{\pi}{2\left(\frac{mb}{a}\right)} \frac{\cosh\left[\left(\pi - \left(\frac{\pi(y-y')}{b}\right)\right) \frac{mb}{a}\right]}{\sinh(\pi\left(\frac{mb}{a}\right))} - \frac{1}{2\left(\frac{mb}{a}\right)^2} - \frac{\pi}{2\left(\frac{mb}{a}\right)} \frac{\cosh\left[\left(\pi - \left(\frac{\pi(y+y')}{b}\right)\right) \frac{mb}{a}\right]}{\sinh(\pi\left(\frac{mb}{a}\right))} + \frac{1}{2\left(\frac{mb}{a}\right)^2}\right]$$

$$= \frac{2}{ab} \sum_{m=1}^{+\infty} \sin\left(\frac{\pi mx}{a}\right) \sin\left(\frac{\pi mx'}{a}\right) \left(\frac{b}{\pi}\right)^2 \frac{\pi}{2\left(\frac{mb}{a}\right) \sinh(\pi\left(\frac{mb}{a}\right))}$$

$$\left\{\cosh\left[\left(\pi - \left(\frac{\pi(y-y')}{b}\right)\right) \frac{mb}{a}\right] - \cosh\left[\left(\pi - \left(\frac{\pi(y+y')}{b}\right)\right) \frac{mb}{a}\right]\right\}$$

$$(2.317)$$

Regrouping terms,  $\widetilde{G}_{e-}$  is finally written as

$$\widetilde{G}_{e-} = \frac{1}{\pi} \sum_{m=1}^{+\infty} \frac{\sin\left(\frac{\pi mx}{a}\right) \sin\left(\frac{\pi mx'}{a}\right)}{m \sinh\left(\pi \frac{mb}{a}\right)}$$

$$\left\{ \cosh\left[\frac{mb}{a} \left(\pi - \frac{\pi(y - y')}{b}\right)\right] - \cosh\left[\frac{mb}{a} \left(\pi - \frac{\pi(y + y')}{b}\right)\right] \right\}$$
(2.318)

An alternative option to sum  $\widetilde{G}_{e-}$  is reported in [23,25], where the following relation is proposed to sum efficiently the asymptotic part

$$\widetilde{G}_{e-} = \frac{1}{4\pi} \sum_{m=-\infty}^{+\infty} (-1)^m \ln \frac{T_m^+}{T_m^-}$$
(2.319)

where  $T_m$ ,  $X_m$  and Y are defined in (2.310a), (2.310b) and (2.310c), respectively.

Thus, through Kummer's transformation we have been able to accelerate the convergence of the spectral series involved in rectangular waveguide and cavity problems by the extraction of one term and the analytical sum of this in one index.

#### • Extraction of two terms.

In this part we are interested in the extraction of one more term in order to accelerate even more the convergence of these functions. The advantage is that the following retained term can also be summed analytically in one index.

Thus, we can apply Kummer's transformation through the extraction of the first two terms by particularizing the expression (2.117) in the Option A and (2.122) in the Option B for  $k_{x0} = k_{y0} = 0$ .

$$\widetilde{G}_{+}(\overline{\rho}, \overline{\rho}') = \frac{4\epsilon_{mn}}{ab} \sum_{\substack{m=0\\\forall m,n-\{m=n=0\}}}^{+\infty} \sum_{n=0}^{+\infty} \left[ \frac{1}{\left(\frac{\pi m}{a}\right)^{2} + \left(\frac{\pi n}{b}\right)^{2} - k^{2}} - \left(\frac{1}{\left(\frac{\pi m}{a}\right)^{2} + \left(\frac{\pi n}{b}\right)^{2}} + \frac{k^{2}}{\left(\left(\frac{\pi m}{a}\right)^{2} + \left(\frac{\pi n}{b}\right)^{2}\right)^{2}} \right) \right] \cos\left(\frac{\pi mx}{a}\right) \cos\left(\frac{\pi mx'}{a}\right) \cos\left(\frac{\pi my'}{b}\right) \cos\left(\frac{\pi ny'}{b}\right) + \widetilde{G}_{00}$$

$$+ \underbrace{\frac{4\epsilon_{mn}}{ab} \sum_{m=0}^{+\infty} \sum_{n=0}^{+\infty} \sum_{n=0}^{+\infty} \frac{\cos\left(\frac{\pi mx}{a}\right) \cos\left(\frac{\pi mx'}{a}\right) \cos\left(\frac{\pi ny}{b}\right) \cos\left(\frac{\pi ny'}{b}\right)}{\left(\frac{\pi m}{a}\right)^{2} + \left(\frac{\pi n}{b}\right)^{2}}$$

$$+ \underbrace{\frac{4\epsilon_{mn}}{ab} \sum_{m=0}^{+\infty} \sum_{n=0}^{+\infty} \sum_{n=0}^{+\infty} \frac{k^{2} \cos\left(\frac{\pi mx}{a}\right) \cos\left(\frac{\pi mx'}{a}\right) \cos\left(\frac{\pi ny}{b}\right) \cos\left(\frac{\pi ny'}{b}\right)}{\left(\left(\frac{\pi m}{a}\right)^{2} + \left(\frac{\pi n}{b}\right)^{2}\right)^{2}}$$

$$\widetilde{G}_{e2+}$$

$$(2.320)$$

The first series  $\widetilde{G}_{e1+}$  has already been summed in the extraction of one term by two different procedures. The second series  $\widetilde{G}_{e2+}$  is the subject of study in this part and can be separate into

$$\widetilde{G}_{e2+} = \frac{4\epsilon_{mn}k^{2}}{ab} \sum_{\substack{m=0\\ \forall m,n-\{m=n=0\}}}^{+\infty} \sum_{\substack{n=0\\ \forall m,n-\{m=n=0\}}}^{+\infty} \frac{\cos\left(\frac{\pi mx}{a}\right)\cos\left(\frac{\pi mx'}{a}\right)\cos\left(\frac{\pi ny}{b}\right)\cos\left(\frac{\pi ny'}{b}\right)}{\left(\left(\frac{\pi m}{a}\right)^{2} + \left(\frac{\pi n}{b}\right)^{2}\right)^{2}}$$

$$= \underbrace{\frac{4k^{2}}{ab}}_{m=1}^{+\infty} \sum_{n=1}^{+\infty} \frac{\cos\left(\frac{\pi mx}{a}\right)\cos\left(\frac{\pi mx'}{a}\right)\cos\left(\frac{\pi ny}{b}\right)\cos\left(\frac{\pi ny'}{b}\right)}{\left(\left(\frac{\pi m}{a}\right)^{2} + \left(\frac{\pi n}{b}\right)^{2}\right)^{2}}$$

$$+ \underbrace{\frac{2k^{2}}{ab}}_{m=1}^{+\infty} \frac{\cos\left(\frac{\pi mx}{a}\right)\cos\left(\frac{\pi mx'}{a}\right)}{\left(\frac{\pi m}{a}\right)^{4}} + \underbrace{\frac{2k^{2}}{ab}}_{S_{2}}^{+\infty} \frac{\cos\left(\frac{\pi ny}{b}\right)\cos\left(\frac{\pi ny'}{b}\right)}{\left(\frac{\pi n}{b}\right)^{4}}$$

$$(2.321)$$

where the series  $S_2$  and  $S_3$  cannot be reduced because they are one dimensional summations and they cannot be expressed analytically. Thus, we have to sum the series  $S_1$ 

$$S_{1} = \frac{4k^{2}}{ab} \sum_{m=1}^{+\infty} \sum_{n=1}^{+\infty} \frac{\cos\left(\frac{\pi mx}{a}\right)\cos\left(\frac{\pi mx'}{a}\right)\cos\left(\frac{\pi ny}{b}\right)\cos\left(\frac{\pi ny'}{b}\right)}{\left(\left(\frac{\pi m}{a}\right)^{2} + \left(\frac{\pi n}{b}\right)^{2}\right)^{2}}$$

$$= \frac{4k^{2}}{ab} \sum_{m=1}^{+\infty} \frac{\cos\left(\frac{\pi mx}{a}\right)\cos\left(\frac{\pi mx'}{a}\right)}{\left(\frac{\pi}{b}\right)^{4}} \sum_{n=1}^{+\infty} \frac{\cos\left(\frac{\pi ny}{b}\right)\cos\left(\frac{\pi ny'}{b}\right)}{\left(\left(\frac{bm}{a}\right)^{2} + n^{2}\right)^{2}}$$

$$(2.322)$$

Using the trigonometric identity written in (2.300),  $S_1$  can be summed as follows

$$S_{1} = \frac{4k^{2}}{ab} \sum_{m=1}^{+\infty} \frac{\cos\left(\frac{\pi mx}{a}\right)\cos\left(\frac{\pi mx'}{a}\right)}{2\left(\frac{\pi}{b}\right)^{4}} \underbrace{\sum_{n=1}^{+\infty} \frac{\cos\left(\frac{\pi n(y-y')}{b}\right) + \cos\left(\frac{\pi n(y+y')}{b}\right)}{\left(\left(\frac{bm}{a}\right)^{2} + n^{2}\right)^{2}}}_{S}$$

$$= \frac{4k^{2}}{ab} \sum_{m=1}^{+\infty} \frac{\cos\left(\frac{\pi mx}{a}\right)\cos\left(\frac{\pi mx'}{a}\right)}{2\left(\frac{\pi}{b}\right)^{4}} \cdot S$$

$$(2.323)$$

where S can be expressed as

$$S = \sum_{n=1}^{+\infty} \frac{\cos\left(\frac{\pi n(y-y')}{b}\right) + \cos\left(\frac{\pi n(y+y')}{b}\right)}{\left(\left(\frac{bm}{a}\right)^2 + n^2\right)^2} = \sum_{n=1}^{+\infty} \frac{\cos\left(\frac{\pi n(y-y')}{b}\right)}{\left(\left(\frac{bm}{a}\right)^2 + n^2\right)^2} + \sum_{n=1}^{+\infty} \frac{\cos\left(\frac{\pi n(y+y')}{b}\right)}{\left(\left(\frac{bm}{a}\right)^2 + n^2\right)^2}$$
(2.324)

If we name  $w = \frac{bm}{a}$  and  $y_1 = \frac{\pi(y-y')}{b}$  and  $y_2 = \frac{\pi(y+y')}{b}$  and we use the following relation,

$$\sum_{n=1}^{+\infty} \frac{\cos(nx)}{(a^2 + n^2)^2} = \sum_{n=0}^{+\infty} \frac{\cos(nx)}{(a^2 + n^2)^2} - \frac{1}{a^4} = \frac{1}{2a^4} + \frac{\pi}{4a^3} \operatorname{cosech}(\pi a) \left[ \cosh(a(\pi - x)) + ax \sinh(a(\pi - y)) \right] + \frac{\pi^2}{4a^2} \operatorname{cosech}^2(\pi a) \cosh(ax) - \frac{1}{a^4} = \frac{-1}{2a^4} + \frac{\pi}{4a^3} \operatorname{cosech}(\pi a) \left[ \cosh(a(\pi - x)) + ax \sinh(a(\pi - y)) \right] + \frac{\pi^2}{4a^2} \operatorname{cosech}^2(\pi a) \cosh(ax)$$

$$(2.325)$$

the series S can be summed as

$$S = \frac{-1}{2w^4} + \frac{\pi}{4w^3} \operatorname{cosech}(\pi w) \left[ \cosh(w(\pi - y_1)) + wy_1 \sinh(w(\pi - y_1)) \right] + \frac{\pi^2}{4w^2}$$

$$\operatorname{cosech}^2(\pi w) \operatorname{cosh}(wy_1) - \frac{1}{2w^4} + \frac{\pi}{4w^3} \operatorname{cosech}(\pi w) \left[ \cosh(w(\pi - y_2)) + wy_2 \sinh(w(\pi - y_2)) \right] + \frac{\pi^2}{4w^2} \operatorname{cosech}^2(\pi w) \operatorname{cosh}(wy_2)$$

$$(2.326)$$

That is

$$S = \frac{-1}{2w^4} + \frac{\pi}{4w^3} \left[ \left( \frac{\cosh(wy_1)}{\tanh(w\pi)} - \sinh(wy_1) \right) + wy_1 \left( \cosh(wy_1) - \frac{\sinh(wy_1)}{\tanh(\pi w)} \right) \right]$$

$$+ \frac{\pi^2}{4w^2} \operatorname{cosech}^2(\pi w) \cosh(wy_1) - \frac{1}{2w^4} + \frac{\pi}{4w^3} \left[ \left( \frac{\cosh(wy_2)}{\tanh(w\pi)} - \sinh(wy_2) \right) \right]$$

$$+ wy_2 \left( \cosh(wy_2) - \frac{\sinh(wy_2)}{\tanh(\pi w)} \right) \right] + \frac{\pi^2}{4w^2} \operatorname{cosech}^2(\pi w) \cosh(wy_2)$$
(2.327)

Next, we continue applying the same procedure to the series  $\widetilde{G}_{-}(\bar{\rho}, \bar{\rho}')$ .

$$\widetilde{G}_{-}(\overline{\rho}, \overline{\rho}') = \frac{4}{ab} \sum_{m=1}^{+\infty} \sum_{n=1}^{+\infty} \left[ \frac{1}{\left(\frac{\pi m}{a}\right)^{2} + \left(\frac{\pi n}{b}\right)^{2} - k^{2}} - \left(\frac{1}{\left(\frac{\pi m}{a}\right)^{2} + \left(\frac{\pi n}{b}\right)^{2}} + \frac{k^{2}}{\left(\left(\frac{\pi m}{a}\right)^{2} + \left(\frac{\pi n}{b}\right)^{2}\right)^{2}} \right) \right] \sin\left(\frac{\pi mx}{a}\right) \sin\left(\frac{\pi mx'}{a}\right) \sin\left(\frac{\pi mx'}{a}\right) \sin\left(\frac{\pi ny}{b}\right) \sin\left(\frac{\pi ny'}{b}\right) \\
+ \underbrace{\frac{4}{ab} \sum_{m=1}^{+\infty} \sum_{n=1}^{+\infty} \frac{\sin\left(\frac{\pi mx}{a}\right) \sin\left(\frac{\pi mx'}{a}\right) \sin\left(\frac{\pi ny}{b}\right) \sin\left(\frac{\pi ny'}{b}\right)}_{\widetilde{G}_{e1-}}}_{\widetilde{G}_{e2-}} \\
+ \underbrace{\frac{4}{ab} \sum_{m=1}^{+\infty} \sum_{n=1}^{+\infty} \frac{k^{2} \sin\left(\frac{\pi mx}{a}\right) \sin\left(\frac{\pi mx'}{a}\right) \sin\left(\frac{\pi ny}{b}\right) \sin\left(\frac{\pi ny'}{b}\right)}_{\widetilde{G}_{e2-}}}_{\widetilde{G}_{e2-}} \\$$
(2.328)

The first series  $\widetilde{G}_{e1-}$  has already been summed in the extraction of one term by two different procedures. The second series  $\widetilde{G}_{e2-}$  is the subject of study in this part and can be separate into

$$\widetilde{G}_{e2-} = \frac{4k^2}{ab} \sum_{m=1}^{+\infty} \sum_{n=1}^{+\infty} \frac{\sin\left(\frac{\pi mx}{a}\right) \sin\left(\frac{\pi mx'}{a}\right) \sin\left(\frac{\pi ny}{b}\right) \sin\left(\frac{\pi ny'}{b}\right)}{\left(\left(\frac{\pi m}{a}\right)^2 + \left(\frac{\pi n}{b}\right)^2\right)^2}$$

$$= \frac{4k^2}{ab} \sum_{m=1}^{+\infty} \frac{\sin\left(\frac{\pi mx}{a}\right) \sin\left(\frac{\pi mx'}{a}\right)}{\left(\frac{\pi}{b}\right)^4} \sum_{n=1}^{+\infty} \frac{\sin\left(\frac{\pi ny}{b}\right) \sin\left(\frac{\pi ny'}{b}\right)}{\left(\left(\frac{bm}{a}\right)^2 + n^2\right)^2}$$
(2.329)

Using the trigonometric identity written in (2.314),  $\widetilde{G}_{e2-}$  can be summed as follows

$$\widetilde{G}_{e2-} = \frac{4k^2}{ab} \sum_{m=1}^{+\infty} \frac{\sin\left(\frac{\pi mx}{a}\right) \sin\left(\frac{\pi mx'}{a}\right)}{2\left(\frac{\pi}{b}\right)^4} \underbrace{\sum_{n=1}^{+\infty} \frac{\cos\left(\frac{\pi n(y-y')}{b}\right) - \cos\left(\frac{\pi n(y+y')}{b}\right)}{\left(\left(\frac{bm}{a}\right)^2 + n^2\right)^2}}_{S}$$

$$= \frac{4k^2}{ab} \sum_{m=1}^{+\infty} \frac{\sin\left(\frac{\pi mx}{a}\right) \sin\left(\frac{\pi mx'}{a}\right)}{2\left(\frac{\pi}{b}\right)^4} \cdot S$$
(2.330)

where S can be expressed as

$$S = \sum_{n=1}^{+\infty} \frac{\cos\left(\frac{\pi n(y-y')}{b}\right) - \cos\left(\frac{\pi n(y+y')}{b}\right)}{\left(\left(\frac{bm}{a}\right)^2 + n^2\right)^2} = \sum_{n=1}^{+\infty} \frac{\cos\left(\frac{\pi n(y-y')}{b}\right)}{\left(\left(\frac{bm}{a}\right)^2 + n^2\right)^2} - \sum_{n=1}^{+\infty} \frac{\cos\left(\frac{\pi n(y+y')}{b}\right)}{\left(\left(\frac{bm}{a}\right)^2 + n^2\right)^2}$$
(2.331)

If we employ the previous notation  $w = \frac{bm}{a}$ ,  $y_1 = \frac{\pi(y-y')}{b}$  and  $y_2 = \frac{\pi(y+y')}{b}$  and we use the following relation,

$$\sum_{n=1}^{+\infty} \frac{\cos(nx)}{(a^2 + n^2)^2} = \sum_{n=0}^{+\infty} \frac{\cos(nx)}{(a^2 + n^2)^2} - \frac{1}{a^4} = \frac{1}{2a^4} + \frac{\pi}{4a^3} \operatorname{cosech}(\pi a) \left[ \cosh(a(\pi - x)) + ax \sinh(a(\pi - y)) \right] + \frac{\pi^2}{4a^2} \operatorname{cosech}^2(\pi a) \cosh(ax) - \frac{1}{a^4} = \frac{-1}{2a^4} + \frac{\pi}{4a^3} \operatorname{cosech}(\pi a) \left[ \cosh(a(\pi - x)) + ax \sinh(a(\pi - y)) \right] + \frac{\pi^2}{4a^2} \operatorname{cosech}^2(\pi a) \cosh(ax)$$

$$(2.332)$$

the series S can be summed as

$$S = \frac{-1}{2w^4} + \frac{\pi}{4w^3} \operatorname{cosech}(\pi w) \left[ \cosh(w(\pi - y_1)) + wy_1 \sinh(w(\pi - y_1)) \right]$$

$$+ \frac{\pi^2}{4w^2} \operatorname{cosech}^2(\pi w) \cosh(wy_1) + \frac{1}{2w^4} - \frac{\pi}{4w^3} \operatorname{cosech}(\pi w) \left[ \cosh(w(\pi - y_2)) + wy_2 \sinh(w(\pi - y_2)) \right] - \frac{\pi^2}{4w^2} \operatorname{cosech}^2(\pi w) \cosh(wy_2) = \frac{\pi}{4w^3} \operatorname{cosech}(\pi w)$$

$$\left[ \cosh(w(\pi - y_1)) + wy_1 \sinh(w(\pi - y_1)) \right] + \frac{\pi^2}{4w^2} \operatorname{cosech}^2(\pi w) \cosh(wy_1) - \frac{\pi}{4w^3}$$

$$\operatorname{cosech}(\pi w) \left[ \cosh(w(\pi - y_2)) + wy_2 \sinh(w(\pi - y_2)) \right] - \frac{\pi^2}{4w^2} \operatorname{cosech}^2(\pi w) \cosh(wy_2)$$

$$(2.333)$$

That is

$$S = \frac{\pi}{4w^3} \left[ \left( \frac{\cosh(wy_1)}{\tanh(w\pi)} - \sinh(wy_1) \right) + wy_1 \left( \cosh(wy_1) - \frac{\sinh(wy_1)}{\tanh(\pi w)} \right) \right]$$

$$+ \frac{\pi^2}{4w^2} \operatorname{cosech}^2(\pi w) \cosh(wy_1) - \frac{\pi^2}{4w^2} \operatorname{cosech}^2(\pi w) \cosh(wy_2)$$

$$- \frac{\pi}{4w^3} \left[ \left( \frac{\cosh(wy_2)}{\tanh(w\pi)} - \sinh(wy_2) \right) + wy_2 \left( \cosh(wy_2) - \frac{\sinh(wy_2)}{\tanh(\pi w)} \right) \right]$$
(2.334)

This can be an alternative to improve the convergence of Green's functions involved in rectangular waveguide and cavity problems using only the second order approximation of Kummer's transformation.

To summarize, in this section we have accelerated the functions involved in the evaluation of the Green's functions in rectangular waveguide and 2-D cavity problems. The acceleration technique that has been used for this purpose is the spectral Kummer's transformation. It is important to note that this technique has been reported to the extraction of one and two terms.

Thus, the asymptotic retained terms have been summed efficiently through reducing the dimensionality of the series by means of summing analytically the remaining series in one index. This implies a significant improvement as will be shown in Chapter 3. This formulation can be easily extended to the other possible basis functions in rectangular waveguide and cavity problems.

As a general conclusion of this chapter, we have attempted to improve the convergence of the 2-D Green's functions with 2-D periodicity as an extension of our work developed in [11] and apply the acquired knowledge to accelerate the series involved in the practical case of rectangular waveguide and 2-D cavity problems.

# Chapter 3

# **Numerical Results**

In this chapter, we show the numerical results that have been obtained through the software tool developed to verify the reported methods. Thus, the convergence rate of each technique could be compared to each other. This allow us to discuss about the efficiency of the outlined methods and reach important conclusions.

This chapter is organized as follows. Section 3.1 show all the results derived from applying the transformations done in Chapter 1 for the 2-D Green's functions with 1-D periodicity. In this section, we first review both the direct convergence of the spectral and the spatial formulation of the 2-D Green's function with 1-D periodicity and the alternative convergence through the application of Ewald's method. This results are based on the formulation developed in [5, 11].

Once we have them as a starting point, we could compare these with the new strategies outlined in this work about the application of Kummer's transformation. Thus, we could compare the improvement that implies the use of each proposed approach and we could analyse the advantages of using one or the other strategy. In addition, a comparison between the different techniques reported to sum the asymptotic series when we use both approaches of applying Kummer's transformation will be carried out.

Finally, in this section we show the improvement in the computation of the parallel-plate waveguide Green's functions thanks to the use of the spectral Kummer's transformation. The results obtained from the extraction of one, two, three and Q terms will be compared.

On the other hand, in Section 3.2 we deal with the acceleration of the slowly convergent series involved in the computation of the 2-D Green's functions with 2-D periodicity and their gradients. First, we focus on the convergence obtained directly from the spatial and spectral formulation. Due to their slowly convergences, we show the results of applying both Ewald's method to the 2-D periodic Green's function and its gradient and Kummer's

transformation only to the spectral Green's function. In addition, we study the differences between the application of each approach in the spectral Kummer's transformation in order to deduce in which cases it is advisable to use one or the other. For each approach, we compare the different techniques presented in Chapter 2 to sum the retained part of the Kummer's transformation.

Lastly in this section, we show the improvement in the computation of the rectangular waveguide and 2-D cavity Green's functions thanks to the use of the spectral Kummer's transformation. The results obtained from the extraction of one and two terms will be compared.

It is important to note that the results obtained in this chapter verify the theoretical development carried out previously and represent the basis of the general conclusions obtained from this project.

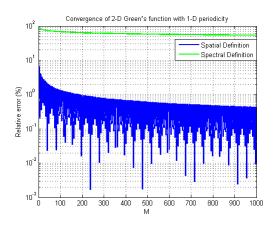
## 3.1 The 2-D Green's Functions With 1-D Periodicity

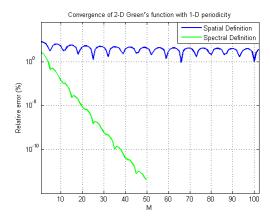
In this section, we show the relative error (%) of the 2-D Green's functions with 1-D periodicity evaluated by using their direct formulations and the employed methods to improve their convergences. Furthermore, we show the improvement obtained by applying Kummer's transformation to the practical Green's functions necessary in parallel-plate waveguide problems.

#### 3.1.1 Revisited of the Spectral Kummer's Transformation

In this part, we show the results of applying the spectral Kummer's transformation. It should be pointed out that the starting point to compare the techniques reported in Section 1.1 is the direct formulation of the spatial and the spectral Green's function. This formulation was developed in our previous work [11]. In [11], we also detailed the application of Ewald's method. This formulation will be used to show the improvement that this technique implies through programming it. Regarding Kummer's transformation, we compare the convergence rate provided by each approach and, for each approach, the different techniques proposed to sum the remaining part.

For the purposes described, in Fig. 3.1 we plot the relative error (%) of the 2-D Green's function with 1-D periodicity versus the number of terms used M. Fig. 3.1(a) shows the convergence rate for an observation point near the source  $(x,z)=(10^{-8}\lambda,10^{-8}\lambda)$  and Fig. 3.1(b) shows the convergence rate for an observation point far from the source  $(x,z)=(0.1\lambda,0.1\lambda)$ .





(a) The observation point is near the source (x, z) = (b) The observation point is far from the source  $(10^{-8}\lambda, 10^{-8}\lambda)$ .  $(x, z) = (0.1\lambda, 0.1\lambda)$ .

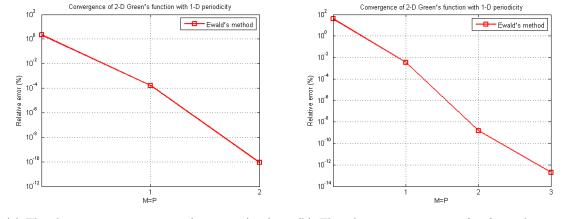
Figure 3.1: Relative error (%) of 2-D Green's function with 1-D periodicity for different observation points and for  $\theta = 45^{\circ}$  and  $d = 0.5\lambda$ .

As can be seen, when the observation point is far from the source, the spectral definition of the Green's function is rapidly convergent due to the exponential decay according to the distance between the source and the observation point. On the contrary, when the observation point is near the source, neither of the two definitions exhibit a rapid convergence. It can be noted that in this case the spatial definition ensures a smaller global relative error. Even so, we can conclude that the closer the observation point is to the source, the slower the convergence of the Green's functions is. For this reason, the real purpose is to accelerate the Green's function at this particular case.

Thus, the relative error (%) of the 2-D Green's function with 1-D periodicity evaluated through Ewald's method is shown in Fig. 3.2(a) for an observation point near the source  $(x,z)=(10^{-8}\lambda,10^{-8}\lambda)$  and in Fig. 3.2(b) for an observation point far from the source  $(x,z)=(0.1\lambda,0.1\lambda)$ . In both cases,  $\theta=45^{\circ}$  and  $d=0.5\lambda$ .

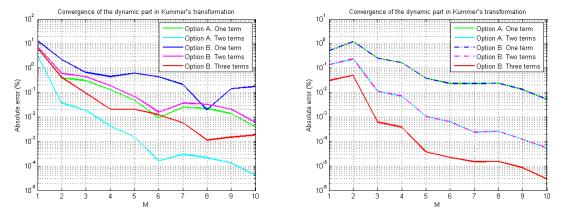
As can be noted, using Ewald's method we are able to compute the Green's function both near and far from the source with few terms. Only with the use of two Ewald's terms, a relative error (%) in the range of  $10^{-8}$  can be achieved.

Taking this as a starting point, the other method employed to accelerate the convergence of these Green's functions is Kummer's transformation. Some numerical results about the work previously done are reported in [11]. As a novelty, we study here two different approaches in the extraction of the asymptotic part. The formulation concerning these options is described in Section 1.1. To understand the importance of the improvement caused by each approach on the evaluation of the Green's function, Fig. 3.3 shows the absolute error (%) of the dynamic part, understood as the original series minus the



(a) The observation point is near the source (x,z)= (b) The observation point is far from the source  $(10^{-8}\lambda,10^{-8}\lambda)$ .  $(x,z)=(0.1\lambda,0.1\lambda)$ .

Figure 3.2: Relative error (%) of 2-D Green's function with 1-D periodicity evaluated through Ewald's method for different observation points and for  $\theta = 45^{\circ}$  and  $d = 0.5\lambda$ .



(a) The angle of incidence of the exitation plane wave is  $\theta=45^{\circ}$ . (b) The angle of incidence of the exitation plane wave is  $\theta=0^{\circ}$ .

Figure 3.3: Absolute error (%) of the dynamic part of the 2-D Green's function with 1-D periodicity when we apply Kummer's transformation by the two different appoaches proposed. The observation point is  $(x, z) = (0.1\lambda, 10^{-5}\lambda)$  and  $d = 0.5\lambda$ .

asymptotic series, when we extract several terms with both approaches for an arbitrary value of  $\theta = 45^{\circ}$  (see Fig. 3.3(a)) and for  $\theta = 0^{\circ}$  (see Fig. 3.3(b)).

There are two conclusions that could be derived from these figures. The first one is that the Option A, that is, the extraction through the approach of  $k_{xm}$ , is more accurate than the other one  $\left(\frac{2\pi m}{d}\right)$ . For this reason, to obtain a certain error we need less terms. This seems to indicate that when we use the Option A, we are taking a better approximation of the spectral series and therefore, the extraction of a certain number of terms results in a better improvement in comparison to the Option B for the same number of retained terms.

The disadvantage of the Option A is that the retained terms contain the working frequency because they contain the factor  $k_{x0}$ . This can be a drawback when we are interested in carrying out a frequency sweep due to the fact that the asymptotic part has to be recalculated in all steps.

The second conclusion that could be obtained is that the two different approaches become the same when  $\theta = 0^{\circ}$ . As mentioned before, the only term that distinguish these two options is  $k_{x0}$ . Thus, when  $\theta = 0^{\circ} \to k_{x0} = 0$ , they become the same. This conclusion has been obtained previously when we explain the formulation but, thanks to program these alternative dynamic parts, it has been proved.

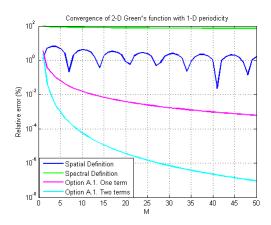
Once we have understood the difference of using each approach in the extraction of the asymptotic terms in Kummer's transformation, we go into detail about the simulation of the studied methods proposed in Chapter 1 to sum the remaining part.

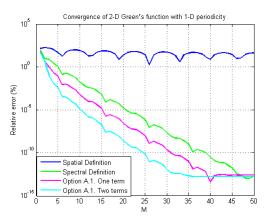
If we choose the Option A  $(k_{xm})$  to extract the asymptotic terms, we propose to sum it by the following options:

#### • Option A.1: Sum by Ewald's method.

This first alternative gives us the possibility of extracting one or two terms in Kummer's transformation and summing these by using Ewald's method. The formulation is detailed in Subsection 1.1.1. The results from the application of this technique are shown in Fig. 3.4 for different observation points.

As can be seen in this figure, through this formulation we are able to extract one or two terms, depending on the relative error that we need, and sum them efficiently thanks to the correspondence established between these terms in the spectral domain and these terms in Ewald's method.





(a) The observation point is near the source (x, z) = (b) The observation point is far from the source  $(10^{-8}\lambda, 10^{-8}\lambda)$ .  $(x, z) = (0.1\lambda, 0.1\lambda)$ .

Figure 3.4: Relative error (%) of 2-D Green's function with 1-D periodicity evaluated through Kummer's transformation for different observation points and for  $\theta = 45^{\circ}$ . The remaining part is summed by using Ewald's method.

#### • Option A.2: Lerch transcendent.

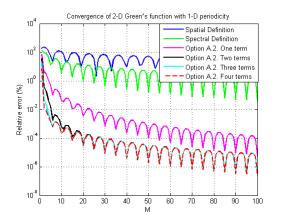
This second alternative gives us the possibility of extracting Q terms in Kummer's transformation and summing these by using the Lerch transcendent. The formulation is detailed in Subsection 1.1.2. The results from the application of this technique are shown in Fig. 3.5 for different observation points.

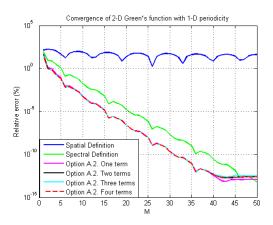
As can be seen in this figure, through this formulation we are able to extract the number of terms that we need, depending on the relative error, and sum them in a semi-closed form thanks to the use of the Lerch transcendent. It is important to note that the more terms we extract, the smaller value we obtain from them. Moreover, we should pointed out that the Lerch transcendent is implemented by a summation. So, the closer the observation point is to the source, the more terms in this summation are needed.

#### • Option A.3: Summation by parts technique.

The last alternative gives us the possibility of extracting Q terms in Kummer's transformation and summing these by using the summation by parts technique. The formulation is detailed in Subsection 1.1.3. The results from the application of this technique are shown in Fig. 3.6 for different observation points.

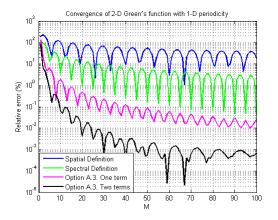
As can be seen in this figure, through this formulation we are able to extract the number of terms that we need, depending on the relative error, and sum one part numerically and the other analytically thanks to the use of the summation by parts technique. As in the previous case, the more terms we extract, the smaller value

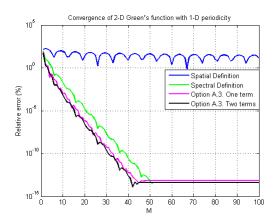




(a) The observation point is near the source (x, z) = (b) The observation point is far from the source  $(0.01\lambda, 10^{-5}\lambda)$ .  $(x, z) = (0.1\lambda, 0.1\lambda)$ .

Figure 3.5: Relative error (%) of 2-D Green's function with 1-D periodicity evaluated through Kummer's transformation for different observation points and for  $\theta = 45^{\circ}$ . The remaining part is summed by using the Lerch transcendent.





(a) The observation point is near the source (x,z)=(b) The observation point is far from the source  $(0.1\lambda,10^{-5}\lambda)$ .  $(x,z)=(0.1\lambda,0.1\lambda)$ .

Figure 3.6: Relative error (%) of 2-D Green's function with 1-D periodicity evaluated through Kummer's transformation for different observation points and for  $\theta = 45^{\circ}$ . The remaining part is summed using the summation by parts technique.

we obtain from them. Moreover, we should point out that if the observation point is getting closer to the source, the oscillating behaviour decreases. Therefore, the advantage of this method disappears, that is, more and more terms in the numerical summation are needed.

To summarize, we have shown the results of implementing the proposed methods to sum the remaining part when we use the first approach in the application of Kummer's transformation.

If we choose the Option B  $(\frac{2\pi m}{d})$  to extract the asymptotic terms, we propose to sum it by the following options:

#### • Option B.1: Sum by Ewald's method.

This first alternative gives us the possibility of extracting one term in Kummer's transformation and summing it by using Ewald's method. The formulation is detailed in Subsection 1.1.4. The result from the application of this technique is shown in Fig. 3.7 for different observation points.

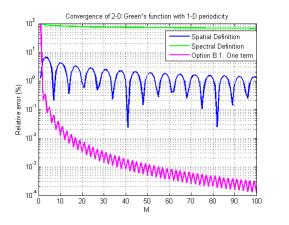
As can be seen in this figure, through this formulation we are able to extract the first asymptotic term and sum it efficiently thanks to the correspondence established between this term in the spectral domain and this term in Ewald's method.

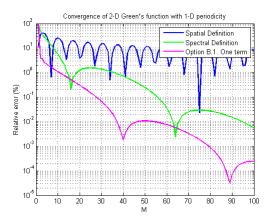
If we compare the Fig. 3.4 and the Fig. 3.7, we could observe the different improvement achieved by each approach that we have mentioned before. When one term is retained, the relative error obtained when we sum a certain number of terms M is smaller in the Option A than in the Option B.

#### • Option B.2: Polylogarithmic function.

This second alternative gives us the possibility of extracting Q terms in Kummer's transformation and summing these by using the polylogarithmic function. The formulation is detailed in Subsection 1.1.5. The results from the application of this technique are shown in Fig. 3.8 for different observation points.

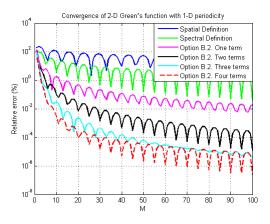
As can be seen in this figure, through this formulation we are able to extract the number of terms that we need, depending on the relative error, and sum them in a semi-closed form thanks to the use of the polylogarithmic function. It is important to note that the more terms we extract, the smaller value we obtain from them. Moreover, we should pointed out that the polylogarithmic function is implemented by a summation. So, the closer the observation point is to the source, the more terms in this summation are needed.

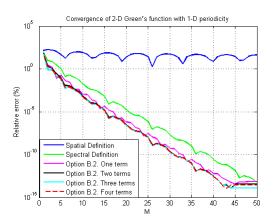




(a) The observation point is near the source (x, z) = (b) The observation point is far from the source  $(10^{-8}\lambda, 10^{-8}\lambda)$ .  $(x, z) = (0.1\lambda, 0.1\lambda)$ .

Figure 3.7: Relative error (%) of 2-D Green's function with 1-D periodicity evaluated through Kummer's transformation for different observation points and for  $\theta = 45^{\circ}$ . The remaining part is summed by using Ewald's method.





(a) The observation point is near the source (x,z)=(b) The observation point is far from the source  $(0.01\lambda,10^{-5}\lambda)$ .  $(x,z)=(0.1\lambda,0.1\lambda)$ .

Figure 3.8: Relative error (%) of 2-D Green's function with 1-D periodicity evaluated through Kummer's transformation for different observation points and for  $\theta = 45^{\circ}$ . The remaining part is summed by using polylogarithms.

The main advantage of this formulation is that the remaining part is quasi-static, so that, it is not necessary to recalculate the polylogarithms at each frequency step.

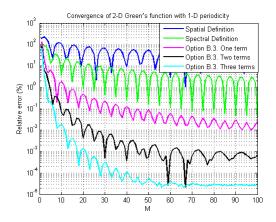
#### • Option B.3: Summation by parts technique.

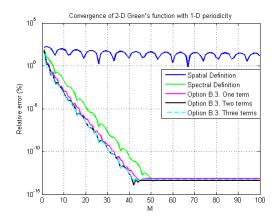
The last alternative gives us the possibility of extracting Q terms in Kummer's transformation and summing these by using the summation by parts technique. The formulation is detailed in Subsection 1.1.6. The results from the application of this technique are shown in Fig. 3.9 for different observation points.

As can be seen in this figure, through this formulation we are able to extract the number of terms that we need, depending on the relative error, and sum one part numerically and the other analytically thanks to the use of the summation by parts technique. As in the previous case, the more terms we extract, the smaller value we obtain from them. Moreover, we should pointed out that if the observation point is getting closer to the source, the oscillating behaviour decreases. Therefore, the advantage of this method disappears, that is, more and more terms in the numerical summation are needed.

To summarize, we have shown the results of implementing the proposed methods to sum the remaining part when we use the second approach in the application of Kummer's transformation.

As a general conclusion of this section, we have shown the convergence rate of the 2-D Green's functions with 1-D periodicity and the acceleration of these convergences achieved through the application of both Ewald's method and Kummer's transformation. We have compared the improvement and understood the differences of each approach and their advantages and disadvantages. Lastly, we have shown the implementation of the strategies reported to sum the remaining part to verify the formulations detailed in the theoretical sections.





(a) The observation point is near the source (x,z)= (b) The observation point is far from the source  $(0.1\lambda,10^{-5}\lambda)$ .  $(x,z)=(0.1\lambda,0.1\lambda)$ .

Figure 3.9: Relative error (%) of 2-D Green's function with 1-D periodicity evaluated through Kummer's transformation for different observation points and for  $\theta = 45^{\circ}$ . The remaining part is summed using the summation by parts technique.

#### 3.1.2 Green's Functions of Parallel-Plate Waveguides

In this subsection, we focus on the Green's functions involved in parallel-plate waveguide problems. Specifically, we study the convergence of the basis Green's functions  $G_+$  and  $G_-$  that we have outlined in Section 1.2.

In this practical case, we need to evaluate special Green's functions which are also slowly convergent. For this reason, it is necessary to apply some transformations to accelerate their computations. Thus, in this part we show the results obtained from the application of Kummer's transformation to these Green's functions. Specifically, we could see the improvement achieved from the extraction of one, two, three and Q terms.

For this purpose, Fig. 3.10 shows the relative error (%) of the Green's functions involved in parallel-plate waveguide problems for an observation point near the source  $(x, z) = (a/5 + a10^{-6}, a10^{-6})$  and Fig. 3.11 shows the relative error (%) of the Green's functions involved in parallel-plate waveguide problems for an observation point far from the source (x, z) = (4a/5, 4a/5). In these simulations  $a = 0.125\lambda$  and the source is located at  $(x', z') = (a/5\lambda, 0\lambda)$ .

As can be seen, these functions are slowly convergent both in the spatial and in the spectral domain. As in the general 2-D Green's function, when the observation point is far from the source, the spectral definition of the Green's function ensures a less global relative error and when the observation point is near the source, the spatial definition

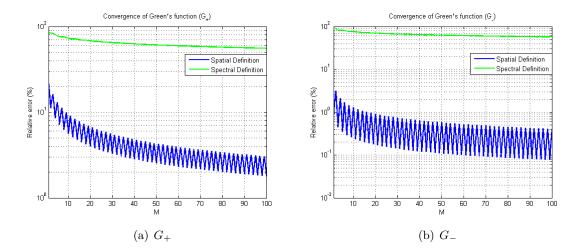


Figure 3.10: Relative error (%) of Green's functions in parallel-plate waveguides for an observation point near the source  $(x,z)=(a/5+a10^{-6},a10^{-6})$ . The source is located at  $(x',z')=(a/5\lambda,0\lambda)$ .

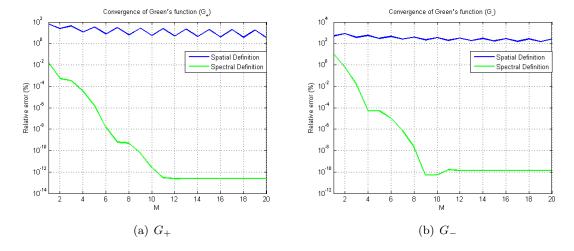


Figure 3.11: Relative error (%) of Green's functions in parallel-plate waveguides for an observation point far from the source (x, z) = (4a/5, 4a/5). The source is located at  $(x', z') = (a/5\lambda, 0\lambda)$ .

ensures a smaller global relative error. Even so, we can conclude that neither of the two definitions exhibit a good convergence for none of these cases.

For this reason and due to the importance of the efficiency in the computation of these functions in real problems, we need to apply some acceleration techniques to improve this slow convergence, particularly near the source.

To verify the formulation of Kummer's transformation applied to these Green's functions, we show the relative error (%) of  $G_+$  and  $G_-$  in Fig. 3.12 for an observation point near the source  $(x,z) = (a/5 + a10^{-6}, a10^{-6})$ , in Fig. 3.13 for an intermediate distance between the observation point and the source  $(x,z) = (2a/5, a10^{-5})$  and in Fig. 3.14 for an observation point far from the source (x,z) = (4a/5, 4a/5).

In these figures, we compare the convergence rate of this technique when different numbers of terms are extracted. As can be seen, in Fig. 3.14 the additional term proposed in [16,17] and used in the extraction of two terms helps when the observation point is far from the source because it is proportional to |z-z'|. However, in this case the convergence of the spectral definition without any transformation is fast enough. On the contrary, when the observation point is near the source, which is the interesting case due to its slow convergence, this additional term do not add any improvement over the extraction of only one term (see Fig. 3.12).

As can be see in this figure, when we extract three terms, a relative error (%) about  $10^{-6}$  can be achieved with less than 20 terms in the worst case scenario, that is, near the source.

As a general conclusion of this section, we have shown the convergence rate of the series involved in the computation of the Green's functions needed in parallel-plate waveguide problems. We have also shown the acceleration of this convergence achieved through the application of Kummer's transformation. The convergence rates that provide the extraction of one, two and three terms have been compared each other. This implies a considerable improvement on the evaluation of these Green's functions because a smaller relative error can be achieved with the summation of few terms in comparison to the original functions.

This can be used in different software tools which need to compute these Green's functions many times in the electromagnetic analysis of microwave devices inside parallel-plate waveguides and periodic structures.

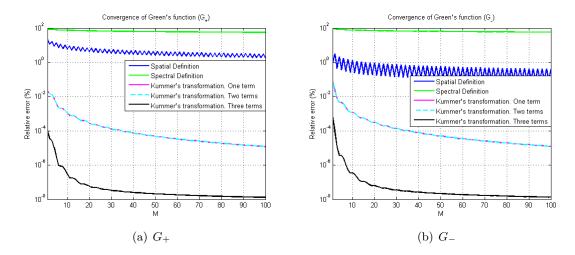


Figure 3.12: Relative error (%) of Green's functions in parallel-plate waveguides  $G_+$  and  $G_-$  for an observation point near the source  $(x,z)=(a/5+a10^{-6},a10^{-6})$ . The source is located at  $(x',z')=(a/5\lambda,0\lambda)$ . Comparison between different numbers of extracted terms in Kummer's technique.

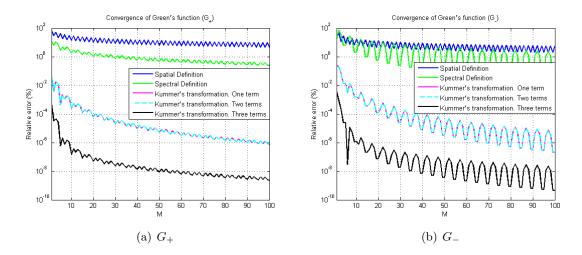


Figure 3.13: Relative error (%) of Green's functions in parallel-plate waveguides  $G_+$  and  $G_-$  for an intermediate distance between the observation point and the source  $(x,z)=(2a/5,a10^{-5})$ . The source is located at  $(x',z')=(a/5\lambda,0\lambda)$ . Comparison between different numbers of extracted terms in Kummer's technique.

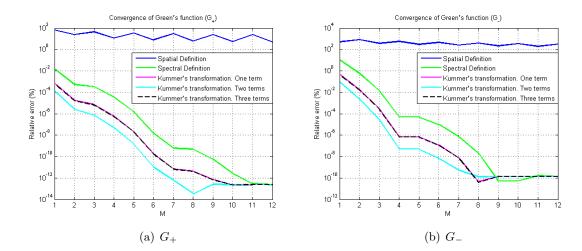


Figure 3.14: Relative error (%) of Green's functions in parallel-plate waveguides  $G_+$  and  $G_-$  for an observation point far from the source (x,z)=(4a/5,4a/5). The source is located at  $(x',z')=(a/5\lambda,0\lambda)$ . Comparison between different numbers of extracted terms in Kummer's technique.

## 3.2 The 2-D Green's Functions With 2-D Periodicity

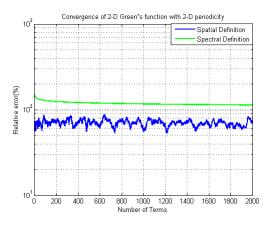
In this section, we show the relative error (%) of the 2-D Green's functions with 2-D periodicity achieved not only by the direct formulations but also by the applied methods to improve their convergences. Furthermore, we show the improvement obtained through applying Kummer's transformation to the practical Green's functions needed in the rectangular waveguide and 2-D cavity problems.

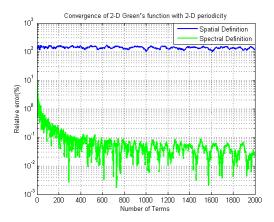
It is important to note that for the 2-D simulations, we sort the pairs (m, n) (which are the indexes of the summation) by order of importance in the convergence of the series. For this reason, the figures shown in this section plot the convergence versus de 'Number of terms' which are the number of the pairs (m, n) by order taken into account.

#### 3.2.1 Green's Functions and the Gradient of Green's Functions

Firstly, we focus on the convergence of the 2-D Green's function with 2-D periodicity and its gradient in both the spectral and the spatial domain. Thus, without any transformation we could analyse the convergence problems that these series exhibit. This leads us to apply any transformation on them in order to obtain a faster convergence rate. The same applies to the components of the gradient.

Specifically, Fig. 3.15 shows the relative error (%) of 2-D Green's function with 2-D periodicity in the spectral and spatial domains for an observation point near the source





(a) The observation point is near the source (x,y)= (b) The observation point is far from the source  $(10^{-8}\lambda, 10^{-8}\lambda)$ .  $(x,y)=(0.1\lambda, 0.1\lambda)$ .

Figure 3.15: Relative error (%) of spectral and spatial 2-D Green's functions with 2-D periodicity evaluated through the direct formulations for  $\theta = 45^{\circ}$  and  $\phi = 45^{\circ}$ . In both cases,  $d_1 = d_2 = 0.25\lambda$ .

 $(x,y)=(10^{-8}\lambda,10^{-8}\lambda)$  (see Fig. 3.15(a)) and for an observation point far from the source  $(x,y)=(0.1\lambda,0.1\lambda)$  (see Fig. 3.15(b)). In both cases,  $\theta=45^\circ$  and  $\phi=45^\circ$  and  $d_1=d_2=0.25\lambda$ .

As can be seen, these functions are slowly convergent in both domains. This slow convergence is independent of the location of the observation point. This is an important difference with respect to 2-D Green's function with 1-D periodicity because neither near or far from the source the 2-D periodic Green's function exhibits a good convergence. Also, it can be seen in the spectral definition, where the exponential decay factor has disappeared. Thus, we can conclude that neither of the two definitions exhibit a good convergence for none of these cases. Even so, when the observation point is far from the source, the spectral definition of the Green's function ensures a less global relative error. On the contrary, when the observation point is near the source, the spatial definition ensures a smaller global relative error.

Once we have seen the convergence rate of the direct formulations, we focus on their gradients. For this aim, Fig. 3.16 plots the x and y components of the gradient of the 2-D Green's functions with 2-D periodicity for an observation point near the source. On the other hand, Fig. 3.17 plots the x and y components for an observation point far from the source. The formulation of these components is detailed in Subsection 2.1.2.

These figures show that the components of the gradients are also slowly convergent in both domains. This convergence problem happens not only near the source but also far from the source.

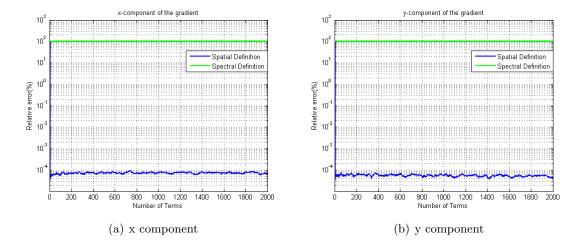


Figure 3.16: Relative error (%) of the gradient of spectral and spatial 2-D Green's functions with 2-D periodicity for an observation point near the source  $(x, y) = (10^{-8}\lambda, 10^{-8}\lambda)$ , with  $\theta = 45^{\circ}$  and  $\phi = 45^{\circ}$ . In both cases,  $d_1 = d_2 = 0.25\lambda$ .

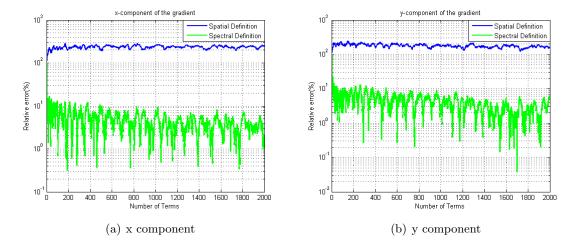


Figure 3.17: Relative error (%) of the gradient of spectral and spatial 2-D Green's functions with 2-D periodicity for an observation point far from the source(x, y) = (0.1 $\lambda$ , 0.1 $\lambda$ ), with  $\theta = 45^{\circ}$  and  $\phi = 45^{\circ}$ . In both cases,  $d_1 = d_2 = 0.25\lambda$ .

Thus, as a general conclusion of this section, the extremely slow convergences of the 2-D Green's functions with 2-D periodicity and their gradients seem to indicate that it is especially important to apply any of the acceleration methods proposed in the following section.

#### 3.2.2 Ewald's Method

As stated above, the 2-D periodic Green's functions and the components of their gradients are extremely slowly convergent. For this reason, in Chapter 2 we have explained some acceleration techniques to apply on them.

One of the employed transformation is Ewald's method. This technique provides an alternative series to evaluate the Green's function with a faster convergence rate. As the formulation of Ewald's components is detail in Section 2.2, we now show the convergence rate of the 2-D periodic Green's function and its gradient evaluated through this technique.

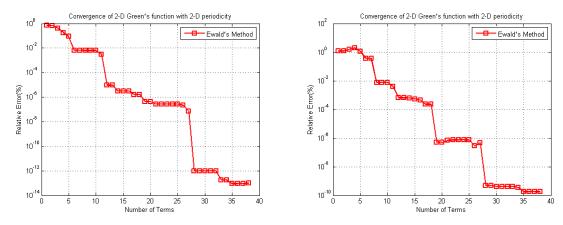
Thus, Fig. 3.18 shows the relative error (%) of the 2-D periodic Green's function using Ewald's method for an observation point near the source  $(x, y) = (10^{-8}\lambda, 10^{-8}\lambda)$  (see Fig. 3.18(a)) and for an observation point far from the source  $(x, y) = (0.1\lambda, 0.1\lambda)$  (see Fig. 3.18(b)).

As we can see in these figure, Ewald's method provides a rapidly convergence both near and far from the source. Through the application of this technique, we could obtain a relative error (%) in the range of  $10^{-8}$  in less that 30 terms in the one-dimensional summation. This confirms that Ewald's method is one of the best in most scenarios because of its versatility and good compromise between accuracy and efficiency.

Now, we apply this technique to the components of the gradient of the Green's function. The results of this procedure, explained in Subsection 2.2.1, are shown in Fig. 3.19(a) for an observation point near the source  $(x, y) = (10^{-8}\lambda, 10^{-8}\lambda)$  and in Fig. 3.19(b) for an observation point far from the source  $(x, y) = (0.1\lambda, 0.1\lambda)$ .

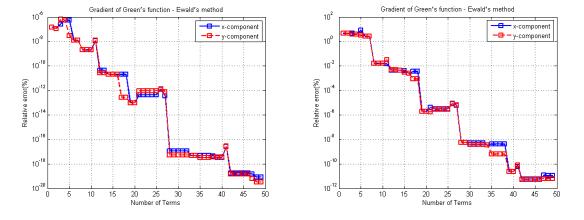
These figures show a great improvement of the convergence rate in the evaluation of the gradient obtaining a relative error (%) about  $10^{-10}$  using less than 15 terms. Remember that if we use the direct definition of the gradient, we need a lot of terms to obtain a relative error much larger than this.

As a general conclusion of this section, we have verified that, through Ewald's method, a small number of terms is needed to obtain the 2-D Green's function and its gradient with high accuracy. Although this technique might imply a very good improvement over the direct formulations, we will show the numerical results obtained from the application



(a) The observation point is near the source (x,y)= (b) The observation point is far from the source  $(10^{-8}\lambda,10^{-8}\lambda)$ .  $(x,y)=(0.1\lambda,0.1\lambda)$ .

Figure 3.18: Relative error (%) of the 2-D Green's function with 2-D periodicity evaluated by using Ewald's method for different observation points with  $\theta = 45^{\circ}$  and  $\phi = 45^{\circ}$ . In both cases,  $d_1 = d_2 = 0.25\lambda$ .



(a) The observation point is near the source (x,y)=(b) The observation point is far from the source  $(10^{-8}\lambda,10^{-8}\lambda)$ .  $(x,y)=(0.1\lambda,0.1\lambda)$ .

Figure 3.19: Relative error (%) of the gradient of the 2-D Green's function with 2-D periodicity evaluated by using Ewald's method for different observation points with  $\theta=45^{\circ}$  and  $\phi=45^{\circ}$ . In both cases,  $d_1=d_2=0.25\lambda$ .

of other techniques in order to offer the readers the advantages and disadvantages of each method by comparison.

#### 3.2.3 Spectral Kummer's Transformation

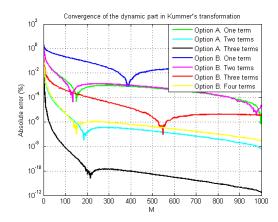
The other acceleration technique explained in Chapter 2 is Kummer's transformation. This technique achieves an improvement of the convergence through the extraction of the asymptotic term and its efficient summation. This leads to a faster evaluation rate in comparison to the computation of the 2-D periodic Green's functions without applying any transformation. As the formulation of Kummer's method is detailed in Section 2.3, we now show the relative error (%) of the 2-D Green's function with 2-D periodicity evaluated through this technique. In addition, we compare the convergence rate achieved by each approach and, for each approach, the different techniques proposed to sum the remaining part.

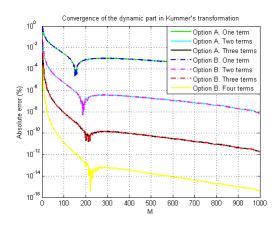
Firstly, in Fig. 3.20 we plot the convergence rate of the dynamic part when we apply Kummer's transformation by using either approach. Fig. 3.20(a) shows the result when we use an arbitrary angle of incidence  $\theta = 45^{\circ}$  and Fig. 3.20(a) shows the result when we use the particular angle of incidence  $\theta = 0^{\circ}$ .

This figure is important to understand the difference between the two approaches in the application of Kummer's technique. As we summarized in Section 3.1.1 for the case of 2-D Green's function with 1-D periodicity, there are two conclusions. The first is that the Option A  $(\bar{k}_{mn})$  is more accurate than the other one so, we are taking a better approximation of the spectral series. Therefore, the extraction of a certain number of terms results in a better improvement in comparison to the Option B  $\left(\frac{2\pi m}{d_1}, \frac{2\pi n}{d_2}\right)$  for the same number of retained terms.

The advantage of the Option B compared to the other one is that the retained terms do not contain the working frequency. This is the perfect situation when we are interested in carrying out a frequency sweep due to the fact that the asymptotic part is no longer necessary to be recalculated in all steps. This results in a computational time saving.

The second conclusion that could be obtained is that the two different approaches become the same when  $\theta = 0^{\circ}$ . As mentioned before, the only terms that distinguish these two options in the case of 2-D Green's function with 2-D periodicity is  $\bar{k}_{w0}$ . Thus, when  $\theta = 0^{\circ} \to \bar{k}_{w0} = 0$ , they become the same. This conclusion has been previously obtained when we explain the formulation but, thanks to program these alternative dynamic parts, it has been proved.





(a) The angle of incidence of the exitation plane wave is  $\theta=45^{\circ}.$ 

(b) The angle of incidence of the exitation plane wave is  $\theta=0^{\circ}$ .

Figure 3.20: Absolute error (%) of the dynamic part of the 2-D Green's function with 2-D periodicity when we apply Kummer's transformation by the two different appoaches proposed. The observation point is  $(x,y) = (0.01\lambda, 0.001\lambda)$ . In both cases,  $d_1 = d_2 = 0.25\lambda$ .

It is important to note that the dynamic part is the component responsible to ensure the convergence rate, that is, the convergence rate is imposed by the dynamic part. Hence, the importance of choosing optimally the strategy in the extraction of the asymptotic terms in Kummer's technique. Another issue will be how to sum the remaining part.

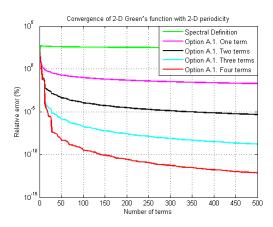
So, once we have understood the difference of using one or the other approach in the extraction of the asymptotic terms in Kummer's transformation, we go into detail about the simulation of the studied methods proposed in Chapter 2 to sum the remaining part.

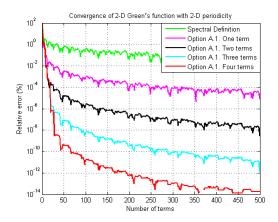
If we choose the Option A  $(\bar{k}_{mn})$  to extract the asymptotic terms, we propose to sum it by the following option:

#### • Option A.1: Sum by Ewald's method.

This first alternative gives us the possibility of extracting one, two and Q terms in Kummer's transformation and summing these by using Ewald's method. The formulation is detailed in Subsection 2.3.1. The results from the application of this technique are shown in Fig. 3.21 for different observation points.

As can be seen in this figure, through this formulation we are able to extract one, two, three and four terms, particularising the general formulation according to the relative error that we need, and sum them efficiently thanks to the the correspondence established between these terms in the spectral domain and these terms in Ewald's method.





(a) The observation point is near the source (x,y)=(b) The observation point is far from the source  $(0.0001\lambda,0.0001\lambda)$ .  $(x,y)=(0.1\lambda,0.1\lambda)$ .

Figure 3.21: Relative error (%) of 2-D Green's function with 2-D periodicity evaluated through Kummer's transformation for different observation points. The remaining part is summed by using Ewald's method. In both cases,  $d_1 = d_2 = 0.25\lambda$ ,  $\theta = 45^{\circ}$  and  $\phi = 45^{\circ}$ .

If we choose the Option B  $\left(\frac{2\pi m}{d_1}, \frac{2\pi n}{d_2}\right)$  to extract the asymptotic terms, we propose to sum it by the following options:

#### • Option B.1: Sum by Ewald's method.

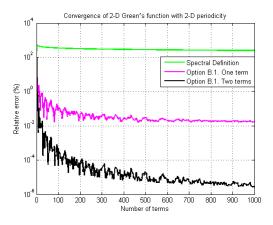
This first alternative gives us the possibility of extracting one or two terms in Kummer's transformation and summing these by using Ewald's method. The formulation is detailed in Subsection 2.3.2. The result from the application of this technique is shown in Fig. 3.22 for different observation points.

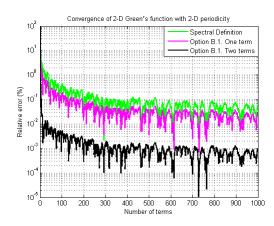
As can be seen in this figure, through this formulation we are able to extract the first and the second asymptotic terms and sum them efficiently thanks to the the correspondence established between this term in the spectral domain and this term in Ewald's method.

If we compare the Fig. 3.21 and the Fig. 3.22, we could observe the different improvement achieved by each approach that we have mentioned before. When one term is retained, the relative error obtained when we sum a certain number of terms is smaller in the Option A than in the Option B.

#### • Option B.2: Lerch transcendent.

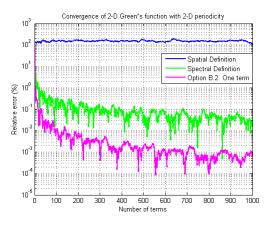
This second alternative gives us the possibility of extracting the first term in Kummer's transformation and summing it by using the Lerch transcendent. The formulation is detailed in Subsection 2.3.3. The results from the application of this technique are shown in Fig. 3.23 for different observation points.

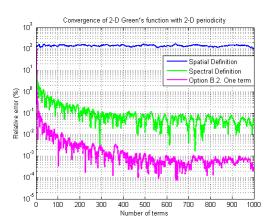




(a) The observation point is near the source (x,y)=(b) The observation point is far from the source  $(0.0001\lambda,0.0001\lambda)$ .  $(x,y)=(0.1\lambda,0.1\lambda)$ .

Figure 3.22: Relative error (%) of 2-D Green's function with 2-D periodicity evaluated through Kummer's transformation for different observation points. The remaining part is summed by using Ewald's method. In both cases,  $d_1 = d_2 = 0.25\lambda$ ,  $\theta = 45^{\circ}$  and  $\phi = 45^{\circ}$ .





(a) The observation point is near the source (x,y)=(b) The observation point is far from the source  $(0.1\lambda,0.0001\lambda)$ .  $(x,y)=(0.1\lambda,0.1\lambda)$ .

Figure 3.23: Relative error (%) of 2-D Green's function with 2-D periodicity evaluated through Kummer's transformation for different observation points. The remaining part is summed by using the Lerch transcendent. In both cases,  $d_1 = d_2 = 0.25\lambda$ ,  $\theta = 45^{\circ}$  and  $\phi = 0^{\circ}$ .

As can be seen in this figure, through this formulation we are able to extract the first asymptotic term and sum it in a semi-closed form thanks to the use of the Lerch transcendent.

It is important to note that the closer the observation point is to the source, the more terms are needed to obtain an accurate sum in the Lerch transcendent, that is, more and more computational time is invested.

#### • Option B.3: Summation by parts technique.

The third alternative gives us the possibility of extracting the first term in Kummer's transformation and summing it by using the summation by parts technique. The formulation is detailed in Subsection 2.3.4. The results from the application of this technique are shown in Fig. 3.24 for different observation points.

As can be seen in this figure, through this formulation we are able to extract the first asymptotic term and sum one part numerically and the other analytically thanks to the use of the summation by parts technique. As in the previous case, the closer the observation point is to the source, the more terms are needed to obtain an accurate sum in the numerical part, that is, more and more computational time is invested.

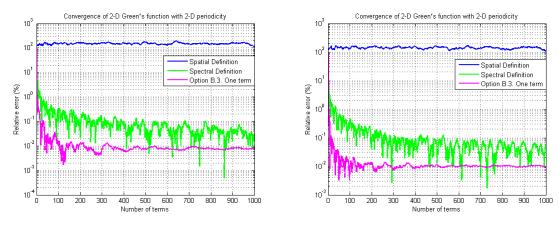
#### • Option B.4: Analytical sum in one index.

The last alternative gives us the possibility of extracting the first and the second terms in Kummer's transformation and summing these analytically in one index. The formulation is detailed in Subsection 2.3.5. The results from the application of this technique are shown in Fig. 3.25 for different observation points.

As can be seen in Fig. 3.25, through this formulation we are able to extract the first and the second asymptotic term and sum them analytically in one index, thus reducing the dimensionality of the series that has to be summed. As mentioned before, the closer the observation point is to the source, the more terms are needed to obtain an accurate sum in the remaining index, that is, more and more computational time is invested.

These proposed methods are interesting from a theoretical point of view but they spend more time than using Ewald's method to sum the remaining part when we use Kummer's transformation to evaluate the Green's function. This is because they are numerically convergent and therefore, it is advisable to use other possible alternatives when we need to compute the 2-D periodic Green's function in a practical case.

As a general conclusion of this section, we have shown the convergence rate of the 2-D Green's functions with 2-D periodicity and the acceleration of this convergence achieved



(a) The observation point is near the source (x,y)=(b) The observation point is far from the source  $(0.1\lambda,0.0001\lambda)$ .  $(x,y)=(0.1\lambda,0.1\lambda)$ .

Figure 3.24: Relative error (%) of 2-D Green's function with 2-D periodicity evaluated through Kummer's transformation for different observation points. The remaining part is summed using the summation by parts technique. In both cases,  $d_1 = d_2 = 0.25\lambda$ ,  $\theta = 45^{\circ}$  and  $\phi = 0^{\circ}$ .

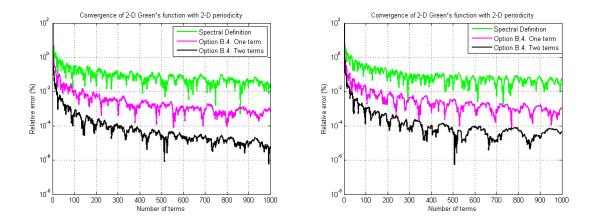


Figure 3.25: Relative error (%) of 2-D Green's function with 2-D periodicity evaluated through Kummer's transformation for different observation points. The remaining part is summed by using the analytical sum in one index. In both cases,  $d_1 = d_2 = 0.25\lambda$ ,  $\theta = 45^{\circ}$  and  $\phi = 0^{\circ}$ .

 $(x,y) = (0.1\lambda, 0.1\lambda).$ 

(b) The observation point is far from the source

(a) The observation point is near the source (x, y) =

 $(0.1\lambda, 0.0001\lambda).$ 

through the application of Kummer's transformation. We have compared the improvement and understood the differences of each approach and their advantages and disadvantages. Lastly, we have shown the implementation of the strategies reported to sum the remaining part to verify the formulations detailed in the theoretical sections.

#### 3.2.4 Green's Functions of Rectangular Waveguides and 2-D Cavities

In this subsection, we focus on the 2-D periodic Green's functions involved in rectangular waveguide and cavity problems. Specifically, we study the convergence of the basis Green's functions  $G_+$  and  $G_-$  that we have outlined in Section 2.4. These are interesting cases due to their practical use. In real problems, the Green's functions involved in these cases are needed and, in most cases, it is necessary to compute these functions many times. So, we need to evaluate these special Green's functions which are also slowly convergent and we need to evaluate them many times. For this reason, it is important to apply some transformation to accelerate their convergences.

Thus, in this part we show the results obtained from the evaluation of theses Green's functions through their spectral formulations and then the application of Kummer's transformation to improve their convergences. Specifically, we could see the improvement achieved from the extraction of one and two terms.

For this purpose, Fig. 3.26 shows the relative error (%) of the Green's functions involved in rectangular waveguide and cavity problems for an observation point near the source  $(x,y) = (a/5 + 10^{-6}a, b/5 + 10^{-6}b)$  and Fig. 3.27 for an observation point far from the source (x,y) = (4a/5, 4b/5). In these simulations  $a = b = 0.125\lambda$  and the real source is located at (x',y') = (a/5,b/5).

As we can see, these functions computed by their direct spectral formulations are slowly convergent. For this reason and due to the importance of the efficiency in the computation of them in real problems, we have applied Kummer's technique to improve these extremely slow convergences. To verify the formulation of Kummer's transformation applied to these Green's functions, we show the relative error obtained by using the first and the second asymptotic term.

As can be noted, when we extract two terms using the formulation reported in the theoretical section, a relative error (%) about  $10^{-4}$  can be achieved with less than 40 terms in the worst case scenario, that is, near the source.

The first term has been summed by using the rapidly logarithmic summation in one index revised in 2.4.1. However, it is important to highlight that the additional second term improves the convergence but requires the evaluation of the second series using the

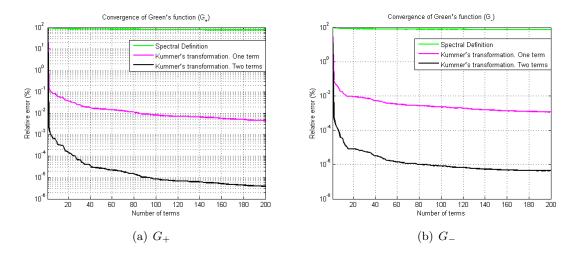


Figure 3.26: Relative error (%) of the 2-D periodic Green's functions  $G_+$  and  $G_-$  evaluated by using the spectral and Kummer's formulations for an observation point near the source  $(x,y)=(a/5+10^{-6}a,b/5+10^{-6}b)$  and  $\phi=0^{\circ}$ . In both cases,  $a=b=0.125\lambda$  and the source is located at (x',y')=(a/5,b/5).

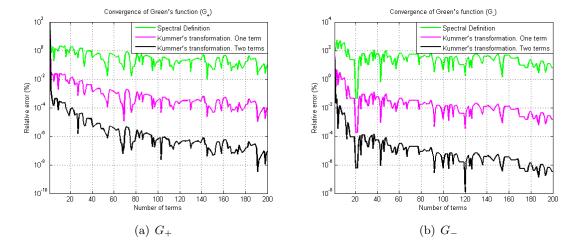


Figure 3.27: Relative error (%) of the 2-D periodic Green's functions  $G_+$  and  $G_-$  evaluated by using the spectral and Kummer's formulations for an observation point far from the source (x,y)=(4a/5,4b/5) and  $\phi=0^{\circ}$ . In both cases,  $a=b=0.125\lambda$  and the source is located at (x',y')=(a/5,b/5).

one index summation. This sum is analytical in one index but the series resulted in the other index has not been efficiently modified. Thus, it needs more terms and can produce computational errors due the use of hyperbolic functions. For this reason, the number of terms used to sum this series has to be careful adjusted.

As a general conclusion of this section, we have shown the convergence rate of the series involved in the computation of the Green's functions needed in rectangular waveguide and cavity problems. We have also shown the acceleration of their convergences achieved through the application of Kummer's transformation. We have compared the convergence rate of this technique when different numbers of terms are extracted. This implies a considerable improvement on the evaluation of these Green's functions because a smaller relative error can be achieved with the summation of few terms in comparison to the original functions.

Other techniques proposed in Section 2.3 can be particularized to this case and can be used to sum the remaining part when we apply Kummer's transformation in rectangular waveguide and cavity problems. This can be used in software which need to compute these Green's functions many times in the electromagnetic analysis of rectangular waveguides, 2-D cavities and periodic structures.

# Chapter 4

# Using FEST3D to Analyse Microstrip Structures

In this chapter, we carry out a study about the analysis of microstrip structures using the software tool FEST3D in collaboration with our external partners at Universidad Politécnica de Valencia. FEST3D (Fullwave Electromagnetic Simulation Tool) [26] is an efficient software tool for the accurate analysis and design of complex passive microwave components based on waveguide technology by means of advanced modal techniques. Specifically, FEST3D is based on an integral equation technique efficiently solved by the Method of Moments. In addition, it employs the Boundary Integral-Resonant Mode Expansion (BI-RME) method, which is a very efficient electromagnetic model of microwave propagation physics, to extract the modal chart of complex waveguides and cavities with arbitrary cross-section. The advantage of FEST3D is the possibility of combining these methods to ensure a high degree of accuracy, as well as reduced computational resources (in terms of CPU time and memory). The final objective of this software tool is to help the microwave components designing and manufacturing industries to decrease both the time to market and the development costs for the next generation of communication systems.

In this context, we will examine how FEST3D responds to the analysis of different structures based on coaxial to microstrip transitions. First, we study some intermediate cases using microstrip lines and coaxial excitations and then, we analyse the structure under study, this is, a coaxial to microstrip transition, for different microstrip thickness and different dielectric permittivity in the pin transition. In addition, in this chapter we will determine the dimensions and the parameters which most influence FEST3D convergence in the analysis of this type of structures.

To this end, a discussion about the parameters and the computational time needed to achieve accurate results will be carried out. These simulated performances will be compared to the ones obtained using the software tool, HFSS. HFSS (High Frequency Electromagnetic Field Simulation) [27] is another commercial tool for simulating 3-D, full-wave, electromagnetic fields.

## 4.1 Introduction to the Original Structure Under Study

The structure under study is the coaxial to microstrip transition shown in Fig. 4.1. This design consists of two coaxial ports that excite, across two pins, the microstrip line with an original thickness of 17 micrometers. The physical parameters and dimensions of this circuit are reported in Table 4.1, 4.1, 4.2, 4.3 and 4.4.

Dimensions of the coaxial cables	
$r_{in}$	0.64 mm
$r_{out}$	2.03 mm
$\Delta r$	10 mm
$L_{coax}$	10 mm
$\epsilon_r$	2.1

Table 4.1: Dimensions of the coaxial cables.

Dimensions of the pin waveguide	
$r_{in}$	$0.64~\mathrm{mm}$
h	1.524 mm
$a \times b$	$20 \text{ mm} \times 20 \text{ mm}$
$\epsilon_r$	3.55

Table 4.2: Dimensions of the pin waveguide.

Dimensions of the metallic microstrip waveguide	
t	$0.017~\mathrm{mm}$
w	3.41 mm
$L_{microstrip}$	12 mm

Table 4.3: Dimensions of the metallic microstrip waveguide.

The two coaxial ports have been implemented in FEST3D using two coaxial waveguides. On the other hand, the top part of the circuit has been implemented using a short-circuited rectangular waveguide. Finally, the layers that contain the two pins of excitation and

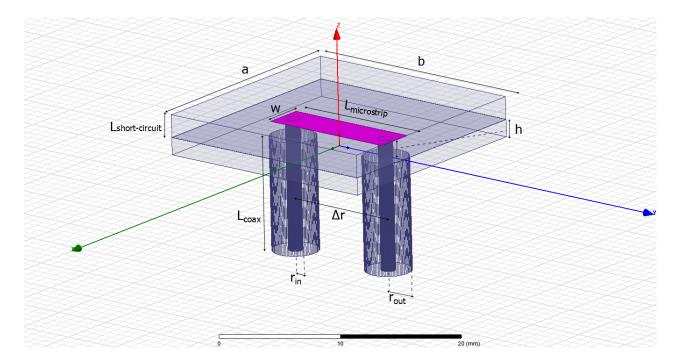


Figure 4.1: The original structure under study. A two coaxial ports to microstrip transition.

Dimensions of the short-circuited waveguide	
$L_{short-circuit}$	2 mm
$a \times b$	$20~\mathrm{mm} \times 20~\mathrm{mm}$

Table 4.4: Dimensions of the short-circuited waveguide.

the microstrip line have been implemented using two Arbitrary Rectangular Waveguides (ARW). Due to this, the computation of the electromagnetic fields inside these waveguides will be based on BI-RME method. It is important to note that the original thickness of the microstrip line is 17 micrometers.

Once we have defined the design that interests us, the main strategy will be the efficient analysis of some structures by means of adjusting the following parameters:

- Number of accessible modes. This parameter controls the number of accessible modes
  of the waveguide. Only the accessible modes of a waveguide are assumed to transmit
  electromagnetic fields (and energy) across the whole waveguide length.
- Number of MoM basis functions. This is the number of modes as basis functions used in the internal Method of Moments (MoM) to calculate the discontinuities attached to the waveguide.
- Number of Green's function terms. This parameter indicates the number of terms in the frequency-independent (static) part of the Green's function, which describes the discontinuities attached to the waveguide.
- Number of reference box modes. This parameter is adjusted when we use ARWs and controls the number of modes in the reference box used to generate the modes of the arbitrary cross-section.

In general, we adjust separately the parameters of the general specifications, the coaxial waveguides, the BI-RME pin waveguide and the BI-RME microstrip line waveguide.

#### 4.2 Intermediate Cases of Study

In this section, we first analyse some intermediate structures before the original in order to understand how FEST3D works when the different elements involved in the original structure are used. Then, we will be able to understand its behaviour in the case of the original circuit.

The first structure that has been analysed by our external partners is shown in Fig. 4.2. This circuit is very similar to the original one but the two pins in the intermediate BI-RME waveguide does not exist, so that, there is not any electric contact between the microstrip line and the coaxial excitations.

This one pole resonator with capacitive coaxial excitation has been computed using FEST3D and has been compared with the simulation result from HFSS in Fig. 4.3.

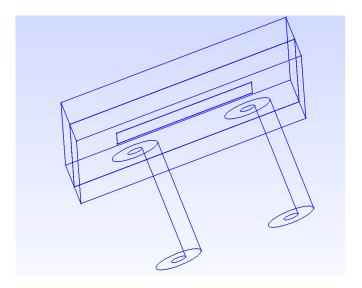


Figure 4.2: First intermediate case of study. One pole resonator with capacitive coaxial excitation.

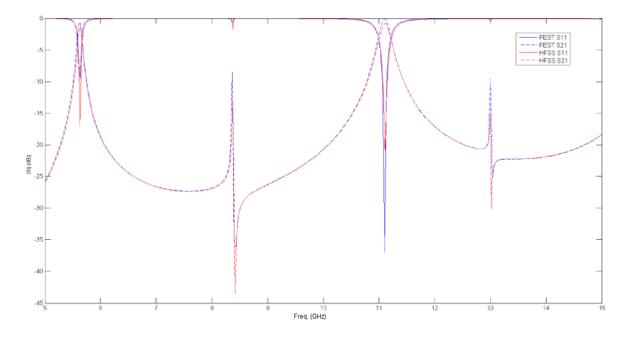


Figure 4.3: Results of comparing the simulation of the one pole resonator with capacitive coaxial excitation using FEST3D and HFSS.

This figure shows that FEST3D has reached convergence and, in this case, the agreement between FEST3D and HFSS is excellent.

Different parameters have been used in these simulations to reach convergence. Depending on the manufacturing accuracy and the computational time requested, the designer can choose the appropriate model. If we choose low modal parameters, the simulated response could exhibit a higher shift in frequency. On the contrary, if a large number of modes is used, the computational time increases but the frequency shift would be lower. In general, it is advisable to achieve a good compromise between accuracy and efficiency. In the case that we need to obtained very accurate results, the modal parameters would need to be increased, which results in investing more computational time.

The second intermediate structure is shown in Fig. 4.4. This is an inter-digital two pole filter where the resonators are connected to ground on one side, and the coaxial input/output are connected directly to the resonators. In this case, the dielectric permittivity of the two pin BI-RME waveguides is one (vaccum permittivity).

This structure has been analysed by our external partners using BI-RME 2D and BI-RME 3D. Fig. 4.5 shows that the agreement between the two simulators is generally quite good.

Based on these results, we can verify the good agreement between the solutions obtained using FEST3D and HFSS when we analyse a microstrip line with very small thickness implemented using a BI-RME waveguide (see Fig. 4.3). Moreover, excellent results have been obtained for the case of a microstrip line excited by a coaxial cables using an intermediate pin waverguide between the coaxials and the microstrip, as we can see in Fig. 4.5. This intermediate waveguide has been also implemented by a BI-RME waveguide with dielectric permittivity equal to one (vacuum permittivity).

As a conclusion of this section, we can be sure that if the dielectric permittivity in the ARWs is one, the thickness of the microstrip line does not affect so much the FEST3D convergence as well as the transition between the coaxial excitation and the microstrip line. Even though high parameters might be needed to reach convergence, the results are valid.

Once we have confirmed this, the following step will be to determine the influence of both the dielectric permittivity of the pin BI-RME waveguide and the thickness of the microstrip line on FEST3D accuracy.

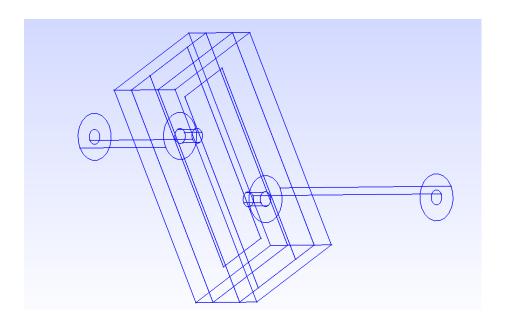


Figure 4.4: Second intermediate case of study. An inter-digital two pole filter.

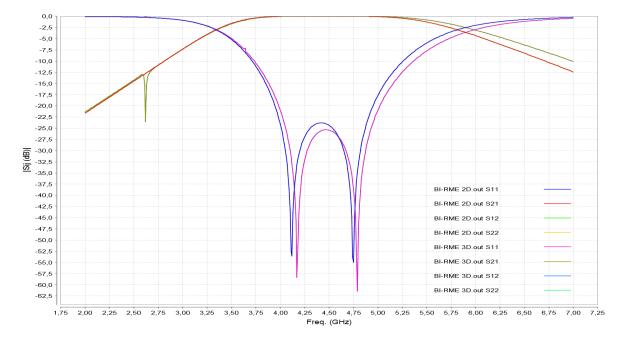


Figure 4.5: Results of comparing the simulation of the inter-digital two pole filter using BI-RME 2D and BI-RME 3D in FEST3D.

#### 4.3 Convergence Study of the Original Structure

For the general aim of this chapter, in this section we carry out a convergence analysis of the original case under study by following the steps provided in [26]. This convergence study has been performed for different microstrip thickness and different dielectric permittivity in order to determine how these parameters influence FEST3D convergence.

In addition, we try to identify the optimum parameters that provide a solution similar to the one obtained by using HFSS and that require the less computational time. In other words, we seek to ensure the smaller parameters needed to achieve accurate simulated output data. For this purpose, we carry out, for all the results reported in this section, a convergence analysis until we reach convergence.

The fist simulation result of the structure under study shown in Fig. 4.1 has been obtained with the parameters that appear in Table 4.5 and it is reported and compared to the one provided by HFSS in Fig. 4.6.

Parameters	Generals	Coaxials	Pin ARW	Microstrip ARW
Number of accessible modes	70	70	80	90
Number of MoM basis functions	200	200	200	300
Number of Green function terms	2179	2179	2845	3700
Number of reference box modes			5000	5000

Table 4.5: First parameters used in FEST3D simulations.

As can be seen, these results do not match entirely but they are very similar. To determine the effect of increasing the parameters adjusted in the microwaves components, we set higher parameters in BI-RME waveguides. Therefore, we use the modal parameters in Table 4.6 to simulate the same structure. The S-parameters that have been obtained are shown and compared to the simulated performance from HFSS in Fig 4.7.

Parameters	Generals	Coaxials	Pin ARW	Microstrip ARW
Number of accessible modes	70	70	150	150
Number of MoM basis functions	200	200	500	500
Number of Green function terms	2179	2179	9000	9000
Number of reference box modes			15000	15000

Table 4.6: Second parameters used in FEST3D simulations.

This seems to indicate that if higher parameters are used in BI-RME 2D, more accurate S-parameters can be achieved. It should be pointed out that if we increase even more the parameters, more coinciding results cannot be achieved. In fact, some parameters, as

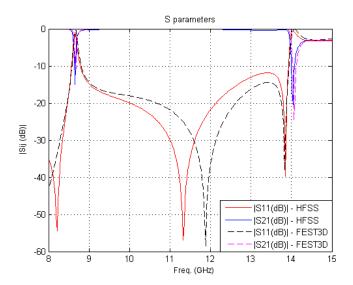


Figure 4.6: Comparison between the S-parameters obtained using FEST3D and HFSS. The thickness of the microstrip line is t = 0.017 mm and the dielectric permittivity of the pin waveguide is  $\epsilon_r = 3.55$ .

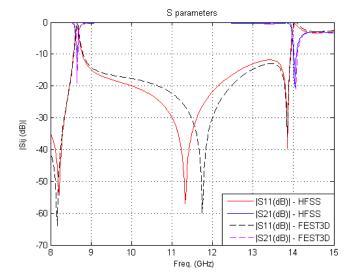


Figure 4.7: Comparison between the S-parameters obtained using FEST3D and HFSS. The thickness of the microstrip line is t = 0.017 mm and the dielectric permittivity of the pin waveguide is  $\epsilon_r = 3.55$ .

the number of MoM basis functions in the coaxial ports and in the microstrip ARW, can produce some numerical errors which can lead to computational errors or incorrect results.

This may be due to the thickness of the components that we have employed since we are analysing a very thin microstrip line using modal techniques focused on computing electromagnetic fields in microwave components based on waveguide technology. In addition, we have to remember that the important difference with the previous intermediate cases of study is the dielectric permittivity of the pin waveguide. For these reasons, the next step will be confirmed if the low accuracy of these simulations is produced by the use of dielectrics in BI-RME or it is due to the thickness of the microstrip line when we use dielectrics in BI-RME.

To determine if the thickness of the microstrip line has any influence on the achieved convergence, we carry out the same convergence study for a similar structure but with the thickness of the microstrip line fixed in 0.17 mm, that is, increased in an order of magnitude.

Using the parameters reported in Table 4.6, the S-parameters that we obtain are shown and compared to the result achieved by HFSS in Fig. 4.8. As can be noted, in this case the response is more coincident between both software tools than the case of 17 micrometers but they are not completely equals.

If we increase again in an order of magnitude the thickness of the microstrip line, that is, 1.7mm and we use the parameters reported in Table 4.6, the result is shown and compared to the simulated performance obtained from HFSS in Fig. 4.9.

In this case, the S-parameters are exactly the same, so we can conclude that, in this original structure, when the thickness is too small, FEST3D cannot achieve a simulated response as accurate as when the thickness is higher.

In addition, to verify if the dielectric contained in the pin BI-RME waveguide influences on the accuracy, the original structure with 17 micrometers of thickness and  $\epsilon_r = 1$  has been simulated using the parameters of Table 4.6. The performance from FEST3D is shown and compared to the simulation result from HFSS in Fig. 4.10.

As can be seen, the results in this case are more coincident than in the case of using  $\epsilon_r \neq$  1. Thus, we can state that if the microstrip line is thin and the dielectric permittivity in BI-RME is different to one, the simulated performance in FEST3D may not be completely equal to the obtained with HFSS. On the contrary, if we use vacuum or air inside this type of waveguides or if we use a higher thickness in the microstrip line, the accuracy achieved with FEST3D is better.

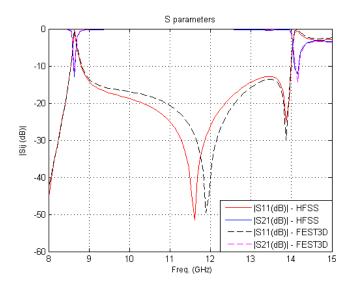


Figure 4.8: Comparison between the S-parameters obtained using FEST3D and HFSS. The thickness of the microstrip line is t = 0.17 mm and the dielectric permittivity of the pin waveguide is  $\epsilon_r = 3.55$ .

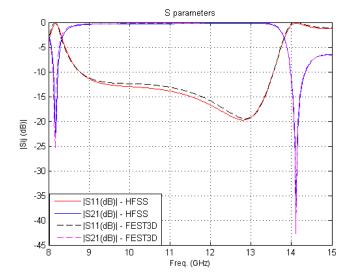


Figure 4.9: Comparison between the S-parameters obtained using FEST3D and HFSS. The thickness of the microstrip line is t = 1.7 mm and the dielectric permittivity of the pin waveguide is  $\epsilon_r = 3.55$ .

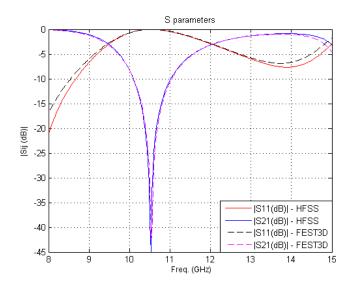


Figure 4.10: Comparison between the S-parameters obtained using FEST3D and HFSS. The thickness of the microstrip line is t = 0.017 mm and the dielectric permittivity of the pin waveguide is  $\epsilon_r = 1$ .

As a general conclusion of this chapter, we have determined that the thickness of the microstrip line is important to the convergence in FEST3D especially when the dielectric permittivity in BI-RME 2D is different from one. In the case of a very thin microstrip line and  $\epsilon_r = 1$ , the results have been quite good and the agreement between HFSS and FEST3D is excellent, as can be seen in the intermediate cases and in the original case under study.

Moreover, we can conclude that, taking into account these constraints and despite the fact that FEST3D has been optimized for the analysis and design of passive microwave components based on closed structures as waveguides and cavities, it behaves as expected and successfully when it is used to analyse this type of microstrip structures.

## Chapter 5

# General Conclusions and Future Lines of Research

#### 5.1 General Conclusions of the Project

This master's thesis has intended to be useful in the analysis and the comparison between the existing methods to the efficient computation of the periodic 2-D Green's functions. Specifically, the evaluation of the 2-D Green's functions with 1-D periodicity and 2-D periodicity has been addressed in this project with the aim of accelerating their convergences.

As final conclusions, we can highlight the following:

About the 2-D Green's functions with 1-D periodicity, we have continued the work developed in [11] by the review of Kummer's transformation. Another alternative in the extraction of the asymptotic terms has been reported. Consequently, we have proposed three different methods to sum the retained part for each approach.

The first one is using Ewald's method. This alternative give us the acceleration resulted by applying Kummer's transformation and sum efficiently the retained terms through Ewald's method. Thanks to the proposed Kummer-Ewald technique, we can take advantage of both the rapidly convergence of Ewald's components without the need to calculate all the special functions and the acceleration arisen from applying Kummer's technique.

The second one is using the Lerch transcendent and the polylogarithm. These functions allow us to express the remaining part in a semi-closed form. These two functions are analogous, one for the first approach and the other one for the second approach in the extraction of terms in Kummer's transformation.

The last one is using the summation by parts technique, which is based on the oscillating behaviour of the series to accelerate their convergences. Through this technique, the remaining series can be summed as a numerical part plus an analytical part.

In [11] we proposed as a future research to apply the obtained results to specific problems of structures with one-dimensional periodicity and extend the developed formulation to problems with two-dimensional periodicity.

For this reason, we have applied the acquired knowledge to accelerate the series involved in the practical case of parallel-plate waveguide problems. Thus, the functions involved in the evaluation of these Green's functions have been accelerated by using the spectral Kummer's transformation. The Q asymptotic retained terms have been expressed in a general form as the summation of polylogarithmic functions which have numerical solutions but are rapidly convergent and independent from the frequency.

About the 2-D Green's functions with 2-D periodicity, we have extended the acquired knowledge to the efficient computation of the double series involved in these particular Green's functions. The spectral and the spatial definition have been formulated and Ewald's method has been applied to accelerate their convergences. For this purpose, we have also applied the spectral Kummer's transformation. The two approaches proposed to compute the 2-D Green's functions with 1-D periodicity have been also studied for the two-dimensional periodicity. Consequently, we have reported different methods to sum the retained part for each approach.

The first one is using Ewald's method. As has been mentioned, through this alternative we take advantage of using simultaneously the acceleration resulted by applying Kummer's transformation and Ewald's method. This technique has been reported for the extraction of Q general terms in the first approach and for the extraction of the first term in the second approach.

Additionally, we have proposed that the first asymptotic term can be summed using the Lerch transcendent. This implies the possibility to write the asymptotic series, when we use the second approach, in a semi-closed form.

The third one is using the summation by parts technique. As in the case of onedimensional series, this method has been efficiently employed to accelerate the convergence of two-dimensional sequences. As stated, this technique is based on the oscillating behaviour of the series and adds the alternative to sum it as the summation of a numerical and an analytical part.

The last one consists of summing analytically the asymptotic series in one index. This implies a significant improvement thanks to reduce the dimensionality of the series. This

strategy has been developed in the case of extracting one and two terms. The following retained term in the application of Kummer's transformation do not allow us to sum it analytically.

As has been done with the 2-D Green's functions with 1-D periodicity, in the case of 2-D periodicity we have also applied the theoretical results to real and interesting practical problems such as the electromagnetic analysis of periodic structures. Specifically, we have formulated the Green's functions involved in rectangular waveguide and 2-D cavity problems. In addition, these slowly convergent functions have been accelerated through the application of Kummer's transformation. The retained terms have been efficiently summed by using the analytical summation in one index.

The theoretical formulations developed for the efficient computation of the 2-D Green's functions with 1-D and 2-D periodicities have been simulated and the numerical results have been shown. All this has given us the possibility of analysing the convergence rate achieved by each technique. Through comparing these numerical results, conclusions about the efficiency and the advantages of the reported methods have been drawn.

On the other hand and according to the second line of research dealt in this work, some microstrip to coaxial transitions have been analysed using the software tool FEST3D in order to study the compromise between accuracy and efficiency in the electromagnetic analysis of the studied structures. Simulation results have been shown to evaluate the capacity of this software to analyse this type of structures and have been compared with the results obtained by using another software tool HFSS.

Some interesting conclusions about the influence of the dielectric permittivity and the thickness of the microstrip line on the FEST3D convergence have been reached through the simulation of these structures with the collaboration of our external partners at Universidad Politécnica de Valencia.

To conclude, this work has intended to be useful in the investigation of the periodic Green's functions and to be a starting point in the analysis of zero-thickness microstrip structures. At personal level, this master's thesis can be seen as a continuation of my academic training in this field of research that started with my Final Degree Project [11] and could continue with a PhD.

#### 5.2 Future Lines of Research

The results obtained in this project will be useful to implement the Green's functions in software tools that required the evaluation of these series.

As already mentioned in the beginning, once we could evaluate the Green's functions efficiently and accurately, we would be able to apply the integral equation technique for the electromagnetic analysis of periodic structures such as parallel-plate and rectangular waveguides and cavities. Thus, the application and the study of the integral equation technique will be one of the future works.

Another important challenge will be the study of other kinds of Green's functions such as 3-D Green's functions with 1-D and 2-D periodicity and the Green's functions resulted by an array of point sources.

On the other hand, we will continue with the work focused on the analysis of microstrip structures through the mathematical development of a zero-thickness formulation based on Multimode Equivalent Networks (MENs) in collaboration with our external partners at Universidad Politécnica de Valencia.

Finally, we will design passive microwave components for satellite communication systems in Ka-band and Ku-band. This will imply the review and implementation of techniques about the synthesis and design of radiofrequency filters and multiplexors for space applications.

## Appendix A

## **Details of Formulations**

#### A.1 Theory of Summation by Parts Technique

In this appendix we revise the details of the formulation about the summation by parts technique reported in [9]. The summation by parts technique is used to accelerate the evaluation of slowly convergent series. The acceleration in this method arises from the oscillating behaviour of the series.

We first review the theory of this technique for summations in one dimension. Then, we revise this formulation for the case of two-dimensional series. The procedures presented in this appendix are used in Chapter 1 and Chapter 2 to sum efficiently the remaining part when we apply Kummer's transformation to the 2-D Green's functions with 1-D and 2-D periodicities.

#### A.1.1 Application to One-dimensional Sequences

The summation by parts technique consists of splitting the original infinite series  $S_{\infty}$  into to different series  $S_{N-1}$  and  $R_N$ .

$$\sum_{n=0}^{+\infty} = \sum_{N=1}^{N-1} + \sum_{n=N}^{+\infty}$$
(A.1)

Thus,

$$S_{\infty} = \sum_{n=0}^{+\infty} \widetilde{G}_n f_n = \underbrace{\sum_{n=0}^{N-1} \widetilde{G}_n f_n}_{S_{N-1}} + \underbrace{\sum_{n=N}^{+\infty} \widetilde{G}_n f_n}_{R_N}$$
(A.2)

The series  $S_{N-1}$  is no longer modified. However, we have to transform the series  $R_N$  in order to express it analytically. For this aim, we proceed as follows

$$R_N = \sum_{n=N}^{+\infty} \widetilde{G}_n^{(-1)} f_n^{(+1)} = \sum_{i=1}^{+\infty} \widetilde{G}_N^{(-i)} f_{N-1}^{(i+1)}$$
(A.3)

where the terms that appear in the previous summation are reported in [9] as

$$\widetilde{G}_n^{(-i)} = \widetilde{G}_{n+1}^{(-i+1)} - \widetilde{G}_n^{(-i+1)}$$
 for  $i = 2, 3, 4, ...$  (A.4a)

$$\widetilde{G}_n^{(-1)} = \widetilde{G}_n \tag{A.4b}$$

$$f_n^{(+i)} = \sum_{k=n+1}^{+\infty} f_k^{(i-1)}$$
 for  $i = 2, 3, 4, \dots$  (A.4c)

$$f_n^{(+1)} = f_n \tag{A.4d}$$

If we decide to use the first order approximation of  $R_N$ , we conclude that  $R_N$  could be written as

$$R_N = \widetilde{G}_N^{(-1)} f_{N-1}^{(+2)} \tag{A.5}$$

where

$$\widetilde{G}_N^{(-1)} = \widetilde{G}_n \Big|_{n=N} \tag{A.6a}$$

$$f_{N-1}^{(+2)} = \sum_{k=n+1}^{+\infty} f_k^{(+1)} \bigg|_{n=N-1}$$
(A.6b)

It should be pointed out that the term N, which divides the two series, has to be optimally adjusted according to the specific case.

The transformation presented in this subappendix has been used when we apply the summation by parts technique to accelerate the 2-D Green's function with 1-D periodicity in Subsection 1.1.3 and Subsection 1.1.6.

#### A.1.2 Application to Two-dimensional Sequences

Once we have gone into detail about the application of the summation by parts technique in one-dimensional series, we can extend it to the case of two-dimensional series. Following the summation by parts theory reported in [9], we split the original infinite series  $S_{\infty}$  into to different series  $S_{M-1,N-1}$  and  $R_{M,N}$  as follows

$$\sum_{m=0}^{+\infty} \sum_{n=0}^{+\infty} = \sum_{m=0}^{M-1} \sum_{n=0}^{N-1} + \sum_{m=M}^{+\infty} \sum_{n=N}^{+\infty}$$

$$= \sum_{M=1,N-1}^{+\infty} \sum_{n=0}^{+\infty} \sum_{n=N}^{+\infty} (A.7)$$

Thus,

$$S_{\infty} = \sum_{m=0}^{+\infty} \sum_{n=0}^{+\infty} \widetilde{G}_{m,n} f_m h_n = \underbrace{\sum_{m=0}^{M-1} \sum_{n=0}^{N-1} \widetilde{G}_{m,n} f_m h_n}_{S_{M-1,N-1}} + \underbrace{\sum_{m=M}^{+\infty} \sum_{n=N}^{+\infty} \widetilde{G}_{m,n} f_m h_n}_{R_{M,N}}$$
(A.8)

The series  $S_{M-1,N-1}$  is no longer modified. However, we have to transform the series  $R_{M,N}$  in order to express it analytically. For this aim, we proceed as follows

$$R_{M,N} = \sum_{m=M}^{+\infty} \sum_{n=N}^{+\infty} \widetilde{G}_{m,n}^{(-1,-1)} f_m^{(+1)} h_n^{(+1)} = \sum_{i=1}^{+\infty} \sum_{k=1}^{+\infty} \widetilde{G}_{M,N}^{(-i,-k)} f_{M-1}^{(i+1)} h_{N-1}^{(k+1)}$$
(A.9)

where the terms that appear in the previous summation are reported in [9] as

$$\widetilde{G}_{m,n}^{(-i,-k)} = \widetilde{G}_{m+1,n}^{(-i+1,k)} - \widetilde{G}_{m,n}^{(-i+1,-k)} \qquad \text{for } i = 1, 2, 3, 4, \dots \text{ and } k = 1, 2, 3, 4, \dots i = k \neq 1$$
(A.10a)

$$f_m^{(+i)} = \sum_{k=m+1}^{+\infty} f_k^{(i-1)}$$
 for  $i = 1, 2, 3, 4, \dots$  and  $k = 1, 2, 3, 4, \dots$   $i = k \neq 1$  (A.10b)

$$h_n^{(+i)} = \sum_{k=n+1}^{+\infty} h_k^{(i-1)}$$
 for  $i = 1, 2, 3, 4, \dots$  and  $k = 1, 2, 3, 4, \dots$   $i = k \neq 1$  (A.10c)

If we decide to use the first order approximation of  $R_N$ , we conclude that  $R_N$  could be written as

$$R_{M,N} = \widetilde{G}_{M,N}^{(-1,-1)} f_{M-1}^{(+2)} h_{N-1}^{(+2)}$$
(A.11)

where

$$\widetilde{G}_{m,n}^{(-1,1)} = \widetilde{G}_{m,n} \Big|_{\substack{m=M\\n=N}}$$
 (A.12a)

$$f_{M-1}^{(+2)} = \sum_{k=m+1}^{+\infty} f_k^{(+1)} \bigg|_{m=M-1}$$
(A.12b)

$$h_{N-1}^{(+2)} = \sum_{k=n+1}^{+\infty} h_k^{(+1)} \bigg|_{n=N-1}$$
(A.12c)

It should be pointed out that the terms M and N, which divide the series, have to be optimally adjusted according to the specific case.

The transformation presented in this subappendix has been used when we apply the summation by parts technique to accelerate the 2-D Green function with 2-D periodicity in Subsection 2.3.4.

# A.2 Green's Functions of Parallel-Plate and Rectangular Waveguides and 2-D Cavities

In this second appendix, we focus on why the summation of the exponential  $e^{-jk_xx}$  evaluated in m between  $(-\infty, +\infty)$  can be written as either  $2\epsilon_m \cos(k_x x)$  or  $-2j\sin(k_x x)$  evaluated in m between  $(0, +\infty)$  depending on whether the function is even or odd respect to  $k_x$ .

This is used in Subsection 1.2.1 when we transform the summation of two Green's functions into one single summation to obtain the total Green's function of a parallel-plate waveguide. We also use this in Subsection 2.4.1 when we carry out the same transformation for the case of rectangular waveguide and cavity Green's functions.

To this end, we use the sine and the cosine transforms to express the series that depend on the exponential  $e^{-jk_xx}$ . This can be understood by using Euler's formula  $e^{-jk_xx} = \cos(k_xx) - j\sin(k_xx)$ . Recalling that  $k_x$  was defined as  $k_x = \frac{\pi m}{a}$ , we can write the following equality

$$\sum_{m=-\infty}^{+\infty} f(k_x) e^{-jk_x x} = \sum_{m=-\infty}^{+\infty} f(k_x) \cos(k_x x) - j \sum_{m=-\infty}^{+\infty} f(k_x) \sin(k_x x)$$
 (A.13)

Firstly, we detail the steps used for an even function. If the function  $f(k_x)$  is even with respect to  $k_x$ , its sine transform will be null. Therefore, the previous series remains

$$\sum_{m=-\infty}^{+\infty} f(k_x)e^{-jk_x x} = \sum_{m=-\infty}^{+\infty} f(k_x)\cos(k_x x)$$
(A.14)

On the other hand, as the function  $f(k_x)$  and  $\cos(k_x x)$  are even with respect to  $k_x$ , the positive m and the negative m will produce the same result.

According to this, we can write this summation in m between  $(-\infty, +\infty)$  like twice the summation between  $(0, +\infty)$ , taking into account that then, the term m = 0 is summed twice. So, if we wish to write the summation between  $(0, +\infty)$ , we have to add a factor

 $\epsilon_m$  which is 1/2 in m=0 in order to sum the term m=0 once.

$$\sum_{m=-\infty}^{+\infty} f(k_x)e^{-jk_x x} = 2\epsilon_m \sum_{m=0}^{+\infty} f(k_x)\cos(k_x x)$$
(A.15)

Where  $\epsilon_m$  is defined as  $\epsilon_m = 1$  for  $m \neq 0$  and  $\epsilon_0 = 1/2$ .

Finally, we detail the steps used for an odd function. If the function  $f(k_x)$  is odd with respect to  $k_x$ , its cosine transform will be null

$$\sum_{m=-\infty}^{+\infty} f(k_x)e^{-jk_x x} = -j\sum_{m=-\infty}^{+\infty} f(k_x)\sin(k_x x)$$
(A.16)

As the function  $f(k_x)$  and  $\sin(k_x x)$  are odd with respect to  $k_x$ ,  $f(k_x) = -f(-k_x)$  and  $\sin(k_x x) = -\sin(-k_x x)$ . Therefore, the product of  $f(k_x)\sin(k_x x)$  for positive m has the same value as the product of  $f(k_x)\sin(k_x x)$  for negative m.

According to this, we can write this summation in m between  $(-\infty, +\infty)$  like twice the summation between  $(0, +\infty)$ , taking into account that then, the term m = 0 is null due to  $\sin(0) = 0$ . So, if we wish to write the summation between  $(0, +\infty)$ , we can remove it from the summation as follows

$$\sum_{m=-\infty}^{+\infty} f(k_x)e^{-jk_x x} = -2j \sum_{m=1}^{+\infty} f(k_x)\sin(k_x x)$$
 (A.17)

The relations proved in (A.15) and (A.17) have been used in the proofs of the parallelplate waveguide, rectangular waveguide and 2-D cavity Green's functions in Chapter 1 and Chapter 2.

#### A.3 Kummer's Transformation in Parallel-Plate Waveguide

In this first appendix, we detail how to transform the infinite series that appear in Subsection 1.2.1 when we apply Kummer's technique to the Green's functions involved in parallel-plate waveguide problems. This transformation is formulated for both the logarithm and the generic s-th order polylogarithm.

The idea is, starting from the definition of logarithm and polylogarithm, to demonstrate that the series that appear in parallel-plate waveguide problems can be summed using these functions. • Transformation using the logarithm.

In first place, we begin with the logarithm. The logarithm can be defined as the following infinite series

$$\sum_{m=1}^{+\infty} \frac{e^{am}}{m} = -\ln(1 - e^a) \tag{A.18}$$

We are interested in finding a relation to write analytically the series

$$\sum_{m=1}^{+\infty} \frac{e^{bm} \cos(cm)}{m} \tag{A.19}$$

For this purpose, if we define a as complex number a = b + jc, then the summation in (A.18) can be written as

$$\sum_{m=1}^{+\infty} \frac{e^{am}}{m} = \sum_{m=1}^{+\infty} \frac{e^{(b+jc)m}}{m} = \sum_{m=1}^{+\infty} \frac{e^{bm}e^{jcm}}{m} = \sum_{m=1}^{+\infty} \frac{e^{bm} \left[\cos(cm) + j\sin(cm)\right]}{m}$$

$$= \sum_{m=1}^{+\infty} \frac{e^{bm} \cos(cm)}{m} + j \sum_{m=1}^{+\infty} \frac{e^{bm} \sin(cm)}{m}$$
(A.20)

Using the relation given in (A.18), we can proceed as follows

$$\sum_{m=1}^{+\infty} \frac{e^{am}}{m} = -\ln\left(1 - e^{a}\right) \; ; \; \sum_{m=1}^{+\infty} \frac{e^{(b+jc)m}}{m} = -\ln\left(1 - e^{(b+jc)}\right)$$

$$\sum_{m=1}^{+\infty} \frac{e^{bm}\cos(cm)}{m} + j \sum_{m=1}^{+\infty} \frac{e^{bm}\sin(cm)}{m} = -\ln\left(1 - e^{(b+jc)}\right)$$

$$\sum_{m=1}^{+\infty} \frac{e^{bm}\cos(cm)}{m} + j \sum_{m=1}^{+\infty} \frac{e^{bm}\sin(cm)}{m}$$

$$= \mathbb{R}e\left\{-\ln\left(1 - e^{(b+jc)}\right)\right\} + j \mathbb{I}m\left\{-\ln\left(1 - e^{(b+jc)}\right)\right\}$$
(A.21)

Consequently, we have proved that the following identity is fulfilled.

$$\sum_{m=1}^{+\infty} \frac{e^{bm}\cos(cm)}{m} = \mathbb{R}e\left\{-\ln\left(1 - e^{(b+jc)}\right)\right\} = \mathbb{R}e\left\{\frac{1}{\ln\left(1 - e^{(b+jc)}\right)}\right\}$$
(A.22)

As commented before, this relation is useful to write in a closed form the series that remains when we extract one term to the spectral parallel-plate waveguide Green's

functions in the application of Kummer's transformation. This has been applied in Subsection 1.2.1 in the extraction of one term.

• Transformation using the s-th order polylogarithm.

Once we have obtained the relation between the previous infinite series and the logarithm, we proceed in the same way for the polylogarithm. The polylogarithm can be defined as the following infinite series

$$\sum_{m=1}^{+\infty} \frac{e^{am}}{m^s} = \operatorname{Li}_s(e^a) \tag{A.23}$$

where s is the order and  $e^a$  is the argument of the polylogarithm. If we define a as complex number a = b + jc, then the summation in the previous equation can be written as

$$\sum_{m=1}^{+\infty} \frac{e^{(b+jc)m}}{m^s} = \sum_{m=1}^{+\infty} \frac{e^{bm}e^{jcm}}{m^s} = \sum_{m=1}^{+\infty} \frac{e^{bm} \left[\cos(cm) + j\sin(cm)\right]}{m^s}$$

$$= \sum_{m=1}^{+\infty} \frac{e^{bm}\cos(cm)}{m^s} + j\sum_{m=1}^{+\infty} \frac{e^{bm}\sin(cm)}{m^s}$$
(A.24)

Using the relation given in (A.23), we can proceed as follows

$$\sum_{m=1}^{+\infty} \frac{e^{(b+jc)m}}{m^s} = \operatorname{Li}_s\left(e^{(b+jc)}\right)$$

$$\sum_{m=1}^{+\infty} \frac{e^{bm} \cos(cm)}{m^s} + j \sum_{m=1}^{+\infty} \frac{e^{bm} \sin(cm)}{m^s} = \operatorname{Li}_s\left(e^{(b+jc)}\right)$$

$$\sum_{m=1}^{+\infty} \frac{e^{bm} \cos(cm)}{m^s} + j \sum_{m=1}^{+\infty} \frac{e^{bm} \sin(cm)}{m^s} = \operatorname{Re}\left\{\operatorname{Li}_s\left(e^{(b+jc)}\right)\right\} + j \operatorname{Im}\left\{\operatorname{Li}_s\left(e^{(b+jc)}\right)\right\}$$
Real part

(A.25)

Consequently, we have proved that the following identity is fulfilled.

$$\sum_{m=1}^{+\infty} \frac{e^{bm} \cos(cm)}{m^s} = \mathbb{R}e\left\{ \operatorname{Li}_s\left(e^{(b+jc)}\right) \right\}$$
 (A.26)

As stated above, this relation is useful to write in a semi-closed form the series that remain when we extract more than one term to the spectral parallel-plate waveguide

Green's functions in the application of Kummer's transformation. This has been applied in Subsection 1.2.1 in the extraction of two, three and Q terms.

### A.4 2-D Poisson's Formula and Non-orthogonal Mapping of Fourier Transform

In this appendix, 2-D Poisson's formula is obtained through the theory of non-orthogonal mapping of the Fourier transform. Despite the fact that some authors have already suggested the 2-D Poisson's formula [2,3] before, the obtaining of this through the arbitrary mapping of the Fourier transform has not been discussed yet.

Hence, we propose here how to obtain this generic Poisson's formula in the case of two-dimensional series with 2-D arbitrary periodicity. For this purpose, we base it on the theory of the non-orthogonal mapping of the Fourier transform. This formulation has been developed in collaboration with the professor doctor Rafael Verdú Monedero from Universidad Politécnica de Cartagena.

We start defining the vectors of periodic sampling as

$$\bar{a}_1 = (a_{1x} , a_{1y})$$
  
 $\bar{a}_2 = (a_{2x} , a_{2y})$ 
(A.27)

Using these vectors, the periodicity matrix can be written as

$$\bar{P} = (\bar{a}_1 \ \bar{a}_2) = \begin{pmatrix} a_{1x} & a_{2x} \\ a_{1y} & a_{2y} \end{pmatrix}$$
(A.28)

and the gain factor of the transformation is

$$G = \frac{1}{|\bar{P}|} = \frac{1}{\begin{vmatrix} a_{1x} & a_{2x} \\ a_{1y} & a_{2y} \end{vmatrix}} = \frac{1}{|\bar{a}_1 \times \bar{a}_2|} = \frac{1}{(\bar{a}_1 \times \bar{a}_2) \cdot \hat{z}} = \frac{1}{A}$$
 (A.29)

On the other hand, we have to calculate the pulse vectors, which are the basis of the periodicity in the spectral domain. These vectors are

$$\bar{u}_1 = (u_{1x} , u_{1y})$$

$$\bar{u}_2 = (u_{2x} , u_{2y})$$
(A.30)

Consequently, the pulse matrix is

$$\bar{\bar{U}} = (\bar{u}_1 \ \bar{u}_2) = \begin{pmatrix} u_{1x} & u_{2x} \\ u_{1y} & u_{2y} \end{pmatrix}$$
 (A.31)

where the values of these coordinates are given by the following transformation

$$\bar{\bar{U}} \times \bar{\bar{P}}^T = 2\pi \cdot \bar{\bar{I}}$$

$$\bar{\bar{U}} = 2\pi \cdot \bar{\bar{I}} \cdot \left(\bar{\bar{P}}^T\right)^{-1}$$
(A.32)

Firstly, we calculate the matrix resulted by  $\left(\bar{\bar{P}}^T\right)^{-1}$ 

$$\left(\bar{\bar{P}}^T\right)^{-1} = \begin{pmatrix} a_{1x} & a_{1y} \\ a_{2x} & a_{2y} \end{pmatrix}^{-1} \tag{A.33}$$

In the knowledge that the inverse of a generic matrix  $\bar{Q}$  can be obtained as

$$\left(\bar{\bar{Q}}\right)^{-1} = \begin{pmatrix} q_{1x} & q_{2x} \\ q_{1y} & q_{2y} \end{pmatrix} = \frac{1}{|\bar{\bar{Q}}|} \cdot \operatorname{Adj}(Q) = \frac{1}{|\bar{\bar{Q}}|} \cdot \begin{pmatrix} q_{2y} & -q_{2x} \\ -q_{1y} & q_{1x} \end{pmatrix}$$
(A.34)

we can rewrite (A.33) as

$$\left(\bar{\bar{P}}^T\right)^{-1} = \frac{1}{|\bar{\bar{P}}|} \begin{pmatrix} a_{2y} & -a_{1y} \\ -a_{2x} & a_{1x} \end{pmatrix}$$
 (A.35)

Using (A.35) in (A.32), we can express the pulse matrix as

$$\bar{\bar{U}} = \frac{2\pi}{A} \cdot \bar{\bar{I}} \begin{pmatrix} a_{2y} & -a_{1y} \\ -a_{2x} & a_{1x} \end{pmatrix} \tag{A.36}$$

and therefore the pulse vector are

$$\bar{u}_1 = (u_{1x} , u_{1y}) = \frac{2\pi}{A} [a_{2y}\hat{x} - a_{2x}\hat{y}]$$

$$\bar{u}_2 = (u_{2x} , u_{2y}) = \frac{2\pi}{A} [-a_{1y}\hat{x} + a_{1x}\hat{y}]$$
(A.37)

or, in x - y subspace, are

$$\bar{u}_x = \frac{2\pi}{A} [a_{2y} - a_{1y}] \hat{x}$$

$$\bar{u}_y = \frac{2\pi}{A} [-a_{2x} + a_{1x}] \hat{y}$$
(A.38)

If we include the following spatial shift in the arbitrary vectors of periodicity,

$$m\bar{a}_1 = ma_{1x}\hat{x} + ma_{1y}\hat{y}$$
  
 $n\bar{a}_2 = na_{2x}\hat{x} + na_{2y}\hat{y}$  (A.39)

it can be translated to the spectral domain as

$$m\bar{u}_{1} = (mu_{1x} , mu_{1y}) = \frac{2\pi}{A} [ma_{2y}\hat{x} - ma_{2x}\hat{y}]$$

$$n\bar{u}_{2} = (nu_{2x} , nu_{2y}) = \frac{2\pi}{A} [-na_{1y}\hat{x} + na_{1x}\hat{y}]$$
(A.40)

Thus, the periodicity in the spatial domain remains

$$d_x = ma_{1x} + na_{2x} d_y = ma_{1y} + na_{2y}$$
(A.41)

and in the spectral domain, remains

$$\widetilde{d}_{x} = \frac{2\pi}{A} [ma_{2y} - na_{1y}] 
\widetilde{d}_{y} = \frac{2\pi}{A} [-ma_{2x} + na_{1x}]$$
(A.42)

Finally, through this development we can suggest that the 2-D Poisson's formula for a non-orthogonal mapping of the Fourier transform is

$$\sum_{m=-\infty}^{+\infty} \sum_{n=-\infty}^{+\infty} f(m\bar{a}_{1}, n\bar{a}_{2}) = \frac{1}{A} \sum_{m=-\infty}^{+\infty} \sum_{n=-\infty}^{+\infty} \tilde{f}(m\bar{u}_{1}, n\bar{u}_{2})$$

$$\sum_{m=-\infty}^{+\infty} \sum_{n=-\infty}^{+\infty} f(ma_{1x}\hat{x} + ma_{1y}\hat{y}, na_{2x}\hat{x} + na_{2y}\hat{y})$$

$$= \frac{1}{A} \tilde{f} \left( \frac{2\pi}{A} [ma_{2y}\hat{x} - ma_{2x}\hat{y}], \frac{2\pi}{A} [-na_{1y}\hat{x} + na_{1x}\hat{y}] \right)$$
(A.43)

Or, in x - y subspace, is

$$\sum_{m=-\infty}^{+\infty} \sum_{n=-\infty}^{+\infty} f(d_x, d_y) = \frac{1}{A} \sum_{m=-\infty}^{+\infty} \sum_{n=-\infty}^{+\infty} \tilde{f}\left(\tilde{d}_x, \tilde{d}_y\right)$$

$$\sum_{m=-\infty}^{+\infty} \sum_{n=-\infty}^{+\infty} f(ma_{1x} + na_{2x}, ma_{1y} + na_{2y}) = \frac{1}{A} \tilde{f}\left(\frac{2\pi}{A}[ma_{2y} - na_{1y}], \frac{2\pi}{A}[-ma_{2x} + na_{1x}]\right)$$
(A.44)

As can be noted, the obtained 2-D Poisson's formula is the same that the suggested in [2]. This has been used in Subsection 2.1.1 and Subsection 2.2.1 to go from a double spatial series with an arbitrary basis of periodicity to a its corresponding double series in the spectral domain.

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