Numerical integration methods for fast evaluation of the acoustic quasi-periodic Green's function

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Declaration

I declare that the work submitted is my own, except where indicated by referencing, and this work has not been submitted for any other degree.

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Abstract

The purpose of this thesis is to investigate efficient calculation methods for integrals of the form

$$I := \int_{-\infty}^{\infty} e^{-\rho v^2} F(v) dv,$$

where $\rho > 0$ and F is a given analytic function, and to apply these calculation methods to particular integrals of this type that arise in applications in acoustics. It is well known that the simplest integration rule, the midpoint rule, is exponentially convergent as the step-size $h \to 0$, if F is bounded and analytic in a strip surrounding the real axis, and that the contour integration arguments used to prove this lead to modifications to the midpoint rule that retain this exponential convergence in the case that F has pole singularities that may lie close to the real axis. In practice this midpoint rule has to be truncated. In the first part of this thesis we derive, by contour integration arguments, a new error estimate for a truncated version of the midpoint rule, modified with a correction factor to take into account simple poles of the integrand near the real axis. This estimate assumes that F is bounded on the real axis but not necessarily in a strip surrounding the real axis. In the second, larger part of the thesis, we consider the evaluation of the 2D acoustic quasi-periodic Green's function, the solution to the problem of acoustic propagation from an infinite array of line sources in free space. We derive a new representation for this Green's function, in terms of integrals of the above form, and apply the truncated modified midpoint rule to obtain concrete approximations. We compare our new approximations for this Green's function with existing methods of evaluation, for the test examples selected in the review paper of Linton (*J. Eng. Math.* **33**, 377-401, 1998), and through more systematic testing over the full range of parameter values. We also use our general error estimate to derive a rigorous error estimate, as a function of the various parameters, for our new approximations to this Green's function.

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Chapter 1

Introduction

This thesis is concerned with efficient computational methods for integrals of the form

$$I := \int_{-\infty}^{\infty} f(v)dv \tag{1.1}$$

where, for some $\rho > 0$,

$$f(v) = e^{-\rho v^2} F(v), \quad v \in \mathbb{R}, \tag{1.2}$$

and F is an analytic function with simple poles which may lie close to the real line. Numerical integration (numerical quadrature) is a well-known topic of numerical analysis that deals with approximating integrals that are difficult to compute. Different numerical methods are available and introduced in [11], [27], and [18] for computing different types of integrals and equations of scientific and engineering problems. We will study for (1.1) arguably the simplest of all methods, but we will see that it is a very efficient method. This approximation is called the truncated midpoint rule approximation with step size h, given by

$$I_h^N := h \sum_{k=-N}^{N+1} f((k-1/2)h), \quad h > 0. \tag{1.3}$$

In the case where F is analytic in a region near the real axis except for simple poles, the midpoint rule (1.3) can be replaced by a modified version of I_h^N which we denote by I_h^{*N}, given by

$$\begin{aligned} I_h^{*N} &:= I_h^N + C_F \\ &= h \sum_{k=-N}^{N+1} f((k-1/2)h) + i\pi \sum_{k=1}^{n} (\mathrm{sgn}(\mathrm{Im} v_k) - g(v_k))R_k, \end{aligned} \tag{1.4}$$

(see [7], [2], [26]), which includes an additional finite sum C_F, called a correction factor, arising from the residues R_k of the function $F(v)$ at its poles v_k lying near the real axis; the function g in (1.4) is defined by

$$g(v) := i \cot\left(\pi \left(\frac{v}{h} + \frac{1}{2}\right)\right) = -i \tan(\pi v/h).$$

This thesis focuses on the truncated midpoint rule applied to approximating I; we initially follow the previous work of Goodwin [17], LaPorte [26] and Al Azah [2] to introduce propositions, which this thesis is based on (see §1.1 for detail of our original contributions). In Chapter 2 we present two propositions and a theorem and the proofs of these propositions using contour integration and Cauchy's residue theorem (see Propositions 2.3, 2.4, and Theorem 2.9). In Chapter 3, we consider a specific application of the integral (1.1) in the area of acoustics, in particular the accurate computation of Green's functions for time-harmonic acoustic propagation, where the source of acoustic excitation is a coherent line source in free space in two-dimensional problems. In section 3.3 we present an integral formula for a particular Green's function G_β^d, that has been written as an integral of the form (1.1). The problem is to calculate the Green's function G_β^d for an infinite array of line sources at (x_n, y_n) for $n \in \mathbb{Z}$, where $x_n = x_0$, $y_n = y_0 + nd$, β is the quasi-periodicity coefficient, and d is the period, so that G_β^d is the unique solution of

$$(\nabla^2 + k^2)G_\beta^d = \delta(X) \sum_{n=-\infty}^{\infty} \delta(Y - nd)e^{in\beta d} \tag{1.5}$$

that satisfies appropriate radiation conditions. In section 3.4, we divide our numerical implementations into 3 parts. In part A, we show how G^d_β can be approximated by using the standard midpoint rule; the numerical approximation obtained agrees with the result given in [28]. A similar test is performed to approximate G^d_β by the modified midpoint rule. By comparing the results of the two tests, we find that the modified midpoint method we propose is more accurate in approximation to the solution of this problem than the original midpoint rule. In part B, we turn our attention to including contributions related to all the poles in the domain $S_H := \{v \in \mathbb{C} : |\mathrm{Im}(v)| < H\}$. We have presented a formula for the correction factor in this case. In part C, we derive a new integral formula for the Green's function, involving a natural number M, namely

$$G^d_\beta(X,Y) = \frac{-i}{4} \sum_{n=1-M}^{M-1} H^1_0(kr_n)e^{in\beta d} + R_M \tag{1.6}$$

where the remainder R_M can be expressed as a sum of integrals of two forms, the first form is given by (1.1) while the second form, obtained by a simple substitution, is

$$\widetilde{I} = \int_{-\infty}^{\infty} \widetilde{f}(v)dv, \tag{1.7}$$

where

$$\widetilde{f}(v) = e^{-v^2} F(\frac{v}{\sqrt{\rho}}).$$

We apply the standard and the modified midpoint rules to both forms and the numerical results show the efficiency of using the modified version of the midpoint rule and that, for a fixed number of quadrature points, the accuracy increases significantly with increasing M. In section 3.5, we compare our numerical results with the results given in [28] and [30] with the same values of X, Y, k, β, and d, given in [28]. We show that our approximation is more accurate than the results given in [28] and [30] with much less computation. In our practical implementation we use Python, which is an excellent programming language for developing scientific and engineering applications, which provides numerous packages (such as, Numpy, Sympy, Scipy, and Matplotlib...etc); see [8], [25], and [23].

In Chapter 4, we present a bound on $|E_h^{*N}|$ (the error in approximating (1.1) by (1.4)) based on our new Theorem 2.9, choosing an appropriate value of H (in the definition of S_H) and an appropriate value of the step size h. We also test our approximation systematically in test A using a wide range of values for d and in test B, restricting to $d \geq 1$. From these two tests, we see that the modified midpoint rule approximation is accurate and efficient, provided X is not too large and d is not too small.

Many authors have studied this type of approximation or, more commonly, have studied the related trapezium rule approximation to (1.1) with a quadrature point at zero. That is, they have studied the evaluation of I by the trapezium rule approximation with an infinite summation given by

$$I_h := h \sum_{j=-\infty}^{\infty} f(jh), \quad h > 0, \tag{1.8}$$

the modified trapezium rule,

$$I_h^* := I_h + C_F, \tag{1.9}$$

where C_F is the correction factor, and the further approximation of the sum (1.8) by the truncated trapezium rule given by

$$I_{h,N} := h \sum_{j=-N}^{N} f(jh), \quad h > 0; \tag{1.10}$$

see [17], [39], [20], [34], [16] and [37]. A comprehensive introduction to the trapezium rule can be found in the review paper by Trefethen and Weideman [38]. If F is analytic in the strip $-H < \mathrm{Im} z < H$, for some $H > 0$, then I_h converges to I

exponentially, as $h \to 0$, precisely, for some $C > 0$,

$$|I - I_h| \leq Ce^{-2\pi H/h}. \tag{1.11}$$

(see e.g. [17] and [20]). When the singularities of the integrand F are poles, precisely F is analytic in $-H < \mathrm{Im} z < H$ apart from a finite number of poles, then (1.11) still holds, as long as I_h is replaced by a modified version of the trapezium rule which we indicate by I_h^*, which includes an additional finite sum depending on the residues of the function F at its poles. That this is true is clear from the main derivation of (1.8) in Goodwin [17] (and see Turing, p.181, [39]), but this seems to be explicitly noted first by Reichel and Chiarella [15] when computing an integral representation for the complementary error function (also see Reichel and Matta [32], Hunter and Regan [22], and Al Azah and Chandler-Wilde [3], [4]). This modification was developed later for a more general case in Bialecki (see [7],Theorem 2.2), where it is shown that the error bound of the modified trapezium rule is given by

$$|I - I_h^*| \leq \frac{e^{-2\pi H/h}}{1 - e^{-2\pi H/h}} \int_{-\infty}^{\infty} (|f(t+iH))| + |f(t-iH)|dt, \tag{1.12}$$

(see also [26], [2], and [3]). In a practical implementation we have to truncate the trapezium sum, approximating the modified trapezium rule approximation by the truncated modified trapezium rule approximation, given by

$$I_{h,N}^* := h \sum_{j=-N}^{N} f(jh) + C_F, \quad h > 0, \tag{1.13}$$

where C_F is the same correction factor as defined in (1.4).

Remark 1.1. *Many authors study a generalized trapezium rule formula, given by*

$$I(h, \alpha)[f] := h \sum_{j \in \mathbb{Z}} f((j - \alpha)h), \tag{1.14}$$

for $h > 0$ and $\alpha \in [0, 1)$, as an approximation to I. Note that $I(h, \alpha)[f] = I(h, 0)[\tilde{f}]$, where $\tilde{f}(t) := f(t - \alpha h)$, for $t \in \mathbb{R}$, i.e., $I(h, \alpha)[f]$ is the trapezium rule in the standard sense for a shifted function $\tilde{f}(t)$. Note further that $I(h, 0)[f]$ and $I(h, 1/2)[f]$ are the standard trapezium and midpoint rule.

1.1 The contributions of this thesis

The contributions of this thesis are of two types. Firstly, we derive new rigorous error bounds on the error in the truncated modified midpoint rule. Let us compare our work with previous work in [26], [2], [38], and [3]. As we discuss in more detail in Chapter 2, previous authors [3] and [2] split the total error into two primary sources of error to derive the bound on the error in the truncated modified trapezium rule approximation. The first source of error is the discretization error which is the difference between I, given in (1.1), and the infinite sum of the modified trapezium rule I_h^*, given in (1.9). For F defined as in (1.2), in the case that F is even, the bound on this error obtained in [2] and [3] is given by

$$|I - I_h^*| \leq \frac{2\sqrt{\pi} M_H(F) e^{\rho H^2 - 2\pi \frac{H}{h}}}{\sqrt{\rho}(1 - e^{-2\pi \frac{H}{h}})} \tag{1.15}$$

on the assumption [Assumption 1.2.1, [2]], that F is analytic except for simple poles and is O(1) at infinity in the strip S_H, and where $M_H(F)$ is the supremum of the function F on $\Gamma_H = \{z \in \mathbb{C} : \mathrm{Im}(z) = H\}$. The second source of error is the so-called truncation error, which is the difference between the infinite sum of the trapezium rule (1.9) and the truncated sum of the modified trapezium rule (1.13), given (in the case that F and f are even) by

$$|I_h^* - I_{N,h}^*| = |2h \sum_{k=N+1}^{\infty} f(kh)|. \tag{1.16}$$

The bound [Eq. (57), [3]] implies that

$$|I_h^* - I_{N,h}^*| \leq M^{(N+1)h}(F)e^{-\rho h^2(N+1)^2}\left(\frac{1+2\rho h^2(N+1)}{\rho h(N+1)}\right), \tag{1.17}$$

where $M^A(F) := \sup_{t\geq A}|F(t)|$ for $A > 0$. The sum of (1.15) and (1.17) gives the total error in approximating the integral (1.1) by the truncated modified trapezium rule, i.e.,

$$|E_N^*| \leq |I - I_h^*| + |I_h^* - I_{N,h}^*|.$$

In this thesis, we bound $E_h^{*N} = I - I_h^{*N}$ by a more direct, one step approach (see Theorem 2.9). In more detail, we approximate I in (1.1) by the truncated modified midpoint rule I_h^{*N}, given by (1.4), the error in this approximation is given by

$$E_h^{*N} = I - I_h^{*N},$$

and our error estimate is

$$\begin{aligned} |E_h^{*N}| \leq{} & \frac{2\sqrt{\pi}M_3(H,(N+1)h)e^{\rho H^2 - 2\pi H/h}}{\sqrt{\rho}(1-e^{-2\pi H/h})} \\ & + e^{-\rho(N+1)^2h^2}\left(\frac{M_1((N+1)h)}{\rho(N+1)h} + 2HM_2(H,(N+1)h)\right) \end{aligned} \tag{1.18}$$

where, for $A > 0$,

$$M_1(A) := \sup_{t\geq A}|F(t)|. \tag{1.19}$$

$$M_2(H,A) := \sup_{0\leq y\leq H}[|F(-A+iy)| + |F((A+iy)|],$$

and

$$M_3(H,A) := \sup_{-A\leq t\leq A}|F(t+iH)|. \tag{1.20}$$

Note that, importantly, the bound (1.15) requires that F is bounded on Γ_H (which implies that the even function F is also bounded on Γ_{-H}), so that also $F(z) = O(1)$ as $\mathrm{Re}(z) \to \infty$ with $z \in \overline{S_H}$, uniformly in $\mathrm{Im}(z)$, for $-H \leq \mathrm{Im}(z) \leq H$. In contrast, our new bound (1.18) only requires that F satisfies Assumption 2.1 below, so that F need not to be bounded on Γ_H, we need only that F is bounded on $\mathbb{R}$. Thus our new theory applies to Example 3 in §2.2.3, while the bound (1.15) does not. More significantly, our new theory applies to the Green function example in chapters 3 and 4. The bound (1.15) does not apply to this application.

In Chapter 3, we propose an approximation to evaluate the 2D quasi-periodic Green's function. We provide a new integral representation of the quasi-periodic Green's function, which involves a number of sources M, given by (3.108). The standard midpoint rule and modification of the midpoint rule are techniques that can be used in the approximation of the integral representation of Green's function for a problem involving wave propagation in the periodic structure. We apply these techniques, and we show, through numerical calculations when simple poles lie close to the real axis, that the modified midpoint rule approximation is significantly more accurate than the midpoint rule (see the results in Table 3.9). We compare our approximation with the best known techniques given in [28], notably Ewald's method, and with the asymptotic correction term method in [30]. Our approximation achieves high accuracy with $N = 6$ quadrature points, and $M = 3$ (see the results of comparison in Tables 3.12 and 3.13). The results in Parts A and B suggest that it is enough, to achieve high accuracy, to include in our correction factor in the modified midpoint rule only residues associated to the poles nearest to the real axis. The results of Part C make clear that it is advantageous, in terms of accuracy and efficiency, to use our new representation (3.108) with $M > 1$, rather than the existing representation ($M = 1$).

In Chapter 4 we apply our new Theorem 2.9, showing how the theoretical bound on the actual error is obtained, by choosing an appropriate value of H (in the definition of S_H) and an appropriate value of h to minimize the bound on the error. We provide a completely explicit error bound in Theorem 4.10. Linton in [28, p.394] suggests that accurate computation in the case when $X = 0$ is particularly challenging. Theorem 4.10 reduces to a simpler statement in that case (see Corollary 4.11).

Chapter 2

Modified Midpoint Rule Approximation

2.1 A modified midpoint rule approximation rule for when F has simple poles near the real-axis

In this chapter we are concerned with understanding the error in the midpoint rule approximation (2.11), modifying this approximation in the case when F has poles that lie close to the real line, and with deriving a new representation and error bound for the error in these approximations. The derivation of (1.8), using contour integration and Cauchy's residue theorem, dates back in a special case at least to Turing in [39], and was analysed in more general cases in Goodwin [17], Schwartz [34], and Stenger [37]. The exponential convergence rate (1.11) of the trapezium rule approximation depends on the width, H, of the analytic strip around the real axis, and the accuracy of the trapezium rule approximation deteriorates when the function f has singularities near the real line. But, when the singularities are poles, the contour integration argument used to derive the exponential convergence of the trapezium rule approximation, leads to a modification of the trapezium rule approximation by a correction factor which depends on the residues of f at the poles. This seems to have been noticed explicitly first by Chiarella and Reichel [15] in the context of evaluating an integral representation for the complementary error function (see also Matta and Reichel [32], Hunter and Regan [22], and Al Azah and Chandler-Wilde [3], [4]), and was developed into a general theory in Bialecki [7]. In practice, as we have discussed already in Chapter 1, the trapezium rule (1.8) and its modified version (1.9) have to be truncated to finite sums as (1.10) and (1.13), and the correct balance between N and h has to be made. This is not addressed in the above papers but is studied by Chandler-Wilde and Al Azah in [3], [4], and by La Porte [26] and Al Azah [2]. In all these works they represent the error in the truncated modified trapezium rule approximation as the sum of a discretization error and a truncation error. It is important to note, however, that the error estimates stated in [3], [2] and [26], involving the supremum $M_H(F)$, given by (1.15), are not helpful in cases where $M_H(F) = +\infty$. This is the case, in particular, for our function (3.33) in Chapter 3.

To solve this issue, in the first section we will, using the contour integral arguments of propositions 2.3 and 2.4, derive a new error estimate for the truncated modified midpoint rule (i.e., a new bound on $|I - I_h^{*N}|$), given in Theorem 2.9. In contrast to previous estimates:

- our contour integral method argument leads directly to a bound on $|I - I_h^{*N}|$, there is no need for additional argument to estimate $|I_h^* - I_h^{*N}|$ (cf. (1.17));
- except that F is required to be bounded on the real axis, we impose no constraint on the behaviour of F at infinity, making the following assumption:

Assumption 2.1. *For some* $H > 0$, *where* $S_H := \{v \in \mathbb{C} \colon |Im(v)| < H\}$, *we have that*

(i) F *is analytic in* S_H *except for finitely many simple poles at* $v_k \in S_H$, *with* $Im(v_k) \neq 0$ *for* $k = 1, 2, 3, ..., n$.

(ii) F *is continuous on* $\bar{S_H} \setminus \{v_1, v_2, ..., v_n\}$.

(iii) For $t \in \mathbb{R}$, $F(t) = O(1)$ as $t \to \pm\infty$.

In the second section, we will provide three numerical examples and estimate the error caused by the modified midpoint rule approximation. Note that all integrals of the examples in this chapter and the rest of the thesis are of the form of (2.10).

Given $h > 0$ define the function $g(v)$ by

$$g(v) := i \cot\left(\pi\left(\frac{v}{h} + \frac{1}{2}\right)\right) = -i\tan(\pi v/h), \tag{2.1}$$

which is an odd meromorphic function with simple poles at $v = (k - \frac{1}{2})h$, for $k \in \mathbb{Z}$. For $v = x + iy$, with x and y real with $y > 0$, we have

$$|1 - g(v)| = \frac{2e^{-2\pi y/h}}{1 - e^{-2\pi y/h}}; \tag{2.2}$$

similarly, for $y < 0$,

$$|1 + g(v)| = \frac{2e^{2\pi y/h}}{1 - e^{2\pi y/h}}. \tag{2.3}$$

It is convenient to state a bound here that is required for vertical integrals in Theorem 2.9. From the definition (2.1) of $g(v)$, for $v = nh + iy$ with $n \in \mathbb{Z}$ and $y \in \mathbb{R}$, we have that

$$g(v) = -\left(\frac{e^{i\pi(n+1/2)-\pi y/h} + e^{-i\pi(n+1/2)+\pi y/h}}{e^{i\pi(n+1/2)-\pi y/h} - e^{-i\pi(n+1/2)+\pi y/h}}\right) \tag{2.4}$$

Recalling that $e^{\pm i\pi(n+1/2)} = \pm i(-1)^n$, we have

$$g(v) = -\left(\frac{i(-1)^n e^{-\pi y/h} - i(-1)^n e^{\pi y/h}}{i(-1)^n e^{-\pi y/h} + i(-1)^n e^{\pi y/h}}\right) = \frac{e^{\pi y/h} - e^{-\pi y/h}}{e^{-\pi y/h} + e^{\pi y/h}} \tag{2.5}$$

so

$$|1 - g(v)| = \left|1 + \frac{e^{-\pi y/h} - e^{\pi y/h}}{e^{-\pi y/h} + e^{\pi y/h}}\right|. \tag{2.6}$$

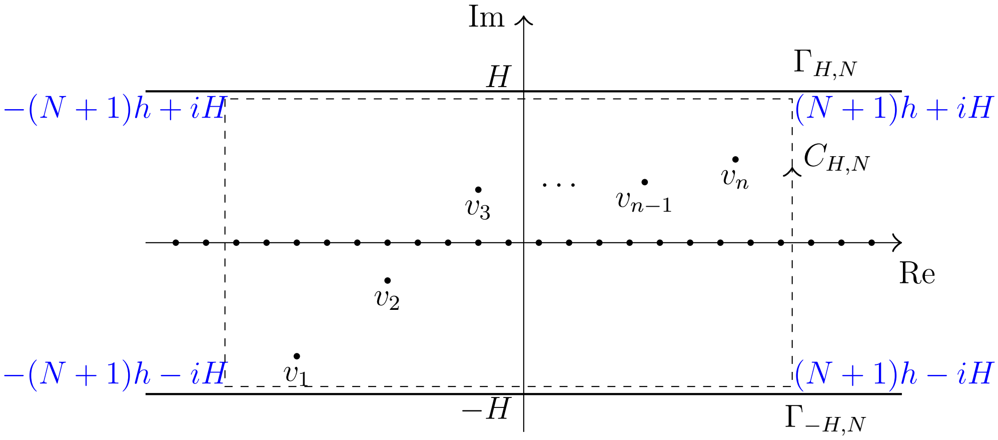

Figure 2.1: The contour $C_{H,N}$ used in the proof of Proposition 2.3. The dots on the real line are the poles of $g(v)$ at $(k-1/2)h$, for $k \in Z$.

Hence

$$|1-g(v)| \leq 2e^{-2\pi y/h} \quad \text{for} \quad y > 0, \tag{2.7}$$

and similarly

$$|1+g(v)| \leq 2e^{2\pi y/h}, \quad \text{for} \quad y < 0. \tag{2.8}$$

All of the integrals we consider in this thesis have an integrand of the form

$$f(v) = e^{-\rho v^2} F(v), \tag{2.9}$$

for some $\rho > 0$, with F satisfying Assumption 2.1, and we wish to compute the integral

$$I = \int_{-\infty}^{\infty} f(v)dv = \int_{-\infty}^{\infty} e^{-\rho v^2} F(v)dv. \tag{2.10}$$

Note that the function $f(v)$ is a product of the entire function $e^{-\rho v^2}$ and $F(v)$; if F satisfies Assumption 2.1 then f also satisfies Assumption 2.1. In the case that F satisfies Assumption 2.1, Figure 2.1 shows the poles (all simple poles) of the function f located above and below the real line, and the simple poles of g; these are all located on the real line. For any $h > 0$, we define the truncated midpoint rule formula by

$$I_h^N = h \sum_{k=-N}^{N+1} f((k-1/2)h). \tag{2.11}$$

Remark 2.2. *In the following propositions, starting with Proposition 2.3, we assume that Assumption 2.1 holds, which implies, in particular, that all the poles of f in S_H are simple. It is possible, with some increase in complexity, to allow also higher order poles. If the pole at v_k is of order n_k then the summation*

$$\sum_{k=1}^{n} g(v_k) R_k$$

in (2.12) *needs to be replaced by*

$$\sum_{k=1}^{n} \mathrm{Res}(gf, v_k) = \sum_{k=1}^{n} \frac{1}{(n_k-1)!} \lim_{v \to v_k} \frac{d^{n_k-1}}{dv^{n_k}} \left((v-v_k)^{n_k} g(v) f(v)\right),$$

and similar changes need to be made in the residue calculations in Proposition 2.4. For example, if $n_k = 2$, i.e f has a double pole at v_k so that

$$f(v) = \frac{f_{-2}}{(v-v_k)^2} + \frac{f_{-1}}{v-v_k} + \widehat{f}(v),$$

where f is analytic near v_k, then

$$\mathrm{Res}(gf, v_k) = g'(v_k) f_{-2} + g(v_k) f_{-1}.$$

We apply Cauchy's residue theorem to prove the following propositions.

Proposition 2.3. *If Assumption 2.1 holds and f is given by (2.9) then*

$$\begin{aligned} I_h^N = \frac{1}{2}\left(\int_{-(N+1)h}^{(N+1)h} f(t+iH)g(t+iH)dt - \int_{-(N+1)h}^{(N+1)h} f(t-iH)g(t-iH)dt\right) + i\pi\sum_{k=1}^{n} g(v_k)R_k \\ + \frac{i}{2}\int_0^H \left[f(-(N+1)h+iy)g(-(N+1)h+iy) - f((N+1)h+iy)g((N+1)h+iy)\right]dy \\ + \frac{i}{2}\int_{-H}^0 \left[f(-(N+1)h+iy)g(-(N+1)h+iy) - f((N+1)h+iy)g((N+1)h+iy)\right]dy, \end{aligned} \tag{2.12}$$

where $R_k := \mathrm{Res}(f, v_k) = \lim_{v\to v_k}(v-v_k)f(v)$, *provided* $(N+1)h > \max_{k=1,..,n} |Re(v_k)|$.

Proof. Let $C_{H,N}$ denote the positively oriented rectangular contour with vertices at $(N+1)h \pm iH$ and $-(N+1)h \pm iH$, with N large enough so that this contour encloses the poles $\{v_1, v_2, ..., v_n\}$. Applying Cauchy's residue theorem, we have, where g is defined by (2.1),

$$\int_{C_{H,N}} f(v)g(v)dv = 2\pi i\left(\sum_{k=-N}^{N+1} \mathrm{Res}(fg, (k-1/2)h) + \sum_{k=1}^{n}\mathrm{Res}(fg, v_k)\right) \tag{2.13}$$

where

$$\mathrm{Res}(fg, (k-1/2)h) = \frac{ih}{\pi} f((k-1/2)h),$$

and

$$\mathrm{Res}(fg, v_k) = g(v_k)R_k.$$

Thus

$$\frac{1}{2}\int_{C_{H,N}} f(v)g(v)dv = -h\sum_{k=-N}^{N+1} f((k-1/2)h) + i\pi\sum_{k=1}^{n} g(v_k)R_k, \tag{2.14}$$

i.e.

$$I_h^N = i\pi\sum_{k=1}^{n} g(v_k)R_k - \frac{1}{2}\int_{C_{H,N}} f(v)g(v)dv \tag{2.15}$$

where I_h^N is defined by (2.11). Now $C_{H,N}$ is the sum of four paths C_1, C_2, C_3, and

C_4, so that

$$\int_{C_{H,N}} f(v)g(v) = \left\{\int_{C_1} + \int_{C_2} + \int_{C_3} + \int_{C_4}\right\} f(v)g(v)dv, \tag{2.16}$$

where

$$\int_{C_1} f(v)g(v)dv = \int_{-(N+1)h-iH}^{(N+1)h-iH} f(v)g(v)dv = \int_{-(N+1)h}^{(N+1)h} f(t-iH)g(t-iH)dt,$$

$$\int_{C_2} f(v)g(v)dv = \int_{(N+1)h-iH}^{(N+1)h+iH} f(v)g(v)dv = \int_{-H}^{H} f((N+1)h+iy)g((N+1)h+iy)idy,$$

$$\int_{C_3} f(v)g(v)dv = \int_{(N+1)h+iH}^{-(N+1)h+iH} f(v)g(v)dv = -\int_{-(N+1)h}^{(N+1)h} f(t+iH)g(t+iH)dt,$$

and

$$\int_{C_4} f(v)g(v)dv = \int_{-(N+1)h+iH}^{-(N+1)h-iH} f(v)g(v)dv = -\int_{-H}^{H} f(-(N+1)h+iy)g(-(N+1)h+iy)idy.$$

Thus

$$\begin{aligned}\frac{-1}{2}\int_{C_{H,N}} f(v)g(v) = {} & \frac{1}{2}\left(\int_{-(N+1)h}^{(N+1)h} f(t+iH)g(t+iH)dt - \int_{-(N+1)h}^{(N+1)h} f(t-iH)g(t-iH)dt\right) \\ & + \frac{i}{2}\left(\int_{-H}^{H} f(-(N+1)h+iy)g(-(N+1)h+iy)dy\right. \\ & \left. - \int_{-H}^{H} f((N+1)h+iy)g((N+1)h+iy)dy\right).\end{aligned} \tag{2.17}$$

Hence (2.15) becomes

$$\begin{aligned}I_h^N = {} & \frac{1}{2}\left(\int_{-(N+1)h}^{(N+1)h} f(t+iH)g(t+iH)dt - \int_{-(N+1)h}^{(N+1)h} f(t-iH)g(t-iH)dt\right) + i\pi\sum_{k=1}^{n} g(v_k)R_k \\ & + \frac{i}{2}\int_0^H \left[f(-(N+1)h+iy)g(-(N+1)h+iy) - f((N+1)h+iy)g((N+1)h+iy)\right] dy \\ & + \frac{i}{2}\int_{-H}^0 \left[f(-(N+1)h+iy)g(-(N+1)h+iy) - f((N+1)h+iy)g((N+1)h+iy)\right] dy.\end{aligned} \tag{2.18}$$

□

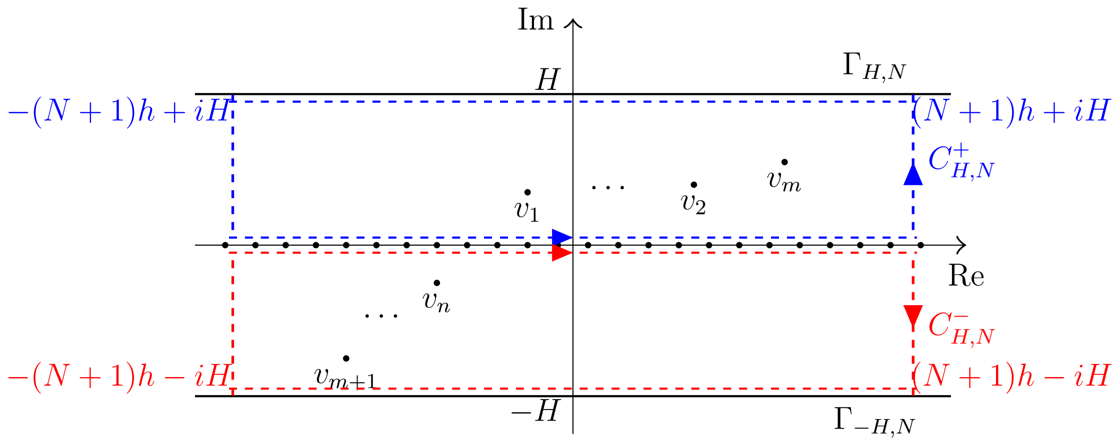

Figure 2.2: The blue contour $C^+_{H,N}$ encloses the poles $\{v_1, v_2, ..., v_m\}$ and the red contour $C^-_{H,N}$ encloses the poles $\{v_{m+1}, ..., v_n\}$, these contours used in the proof of Proposition 2.4

Proposition 2.4. *If Assumption (2.1) holds and f is given by (2.9) then*

$$I = \int_{-\infty}^{\infty} f(v)dv = \int_{-(N+1)h}^{(N+1)h} f(v)dv + \int_{-\infty}^{-(N+1)h} f(v)dv + \int_{(N+1)h}^{\infty} f(v)dv, \quad (2.19)$$

and

$$\begin{aligned}\int_{-(N+1)h}^{(N+1)h} f(v)dv &= \frac{1}{2}\int_{-(N+1)h}^{(N+1)h} [f(t-iH)dt + f(t+iH)]dt \\ &\quad - \frac{i}{2}\int_0^H [f((N+1)h+iy) - f(-(N+1)h+iy)]dy \\ &\quad - \frac{i}{2}\int_{-H}^0 [f(-(N+1)h+iy) - f((N+1)h+iy)]dy + \pi i \sum_{k=1}^{n} sgn(Imv_k)R_k,\end{aligned}$$

provided $(N+1)h > \max_{k=1,..,n} |Re(v_k)|$.

Proof. Let $C^{\pm}_{H,N}$ be defined as in Figure 1.2, and consider

$$\int_{C^{\pm}_{H,N}} f(v)dv. \quad (2.20)$$

$C^+_{H,N}$ is the positively oriented rectangular contour with vertices $-(N+1)h, (N+1)h, \pm(N+1)h + iH$, and N large enough so that $C^+_{H,N}$ encloses the simple poles $\{v_1, v_2, ..., v_m\}$ (see Figure 2.2). By applying Cauchy's residue theorem, we have

$$\int_{C^+_{H,N}} f(v)dv = 2\pi i \sum_{k=1}^{m} R_k, \tag{2.21}$$

where $R_k := Res(f, v_k)$, for $k = 1, 2, ..., m$. Note that

$$\int_{C^+_{H,N}} f(v)dv = \left\{ \int_{C^+_{1,H,N}} + \int_{C^+_{2,H,N}} + \int_{C^+_{3,H,N}} + \int_{C^+_{4,H,N}} \right\} f(v)dv \tag{2.22}$$

where

$$\int_{C^+_{1,H,N}} f(v)dv = \int_{-(N+1)h}^{(N+1)h} f(v)dv,$$

$$\int_{C^+_{2,H,N}} f(v)dv = \int_{(N+1)h}^{(N+1)h+iH} f(v)dv = \int_0^H f((N+1)h + iy)idy$$

$$\int_{C^+_{3,H,N}} f(v)dv = -\int_{-(N+1)h+iH}^{(N+1)h+iH} f(v)dv = -\int_{-(N+1)h}^{(N+1)h} f(t+iH)dt,$$

and

$$\int_{C^+_{4,H,N}} f(v)dv = -\int_{-(N+1)h}^{-(N+1)h+iH} f(v)dv = -\int_0^H f(-(N+1)h + iy)idy.$$

Similarly, $C^-_{H,N}$ is the negatively oriented rectangular contour with vertices $-(N+1)h, (N+1)h, \pm(N+1)h - iH$, and N large enough so that $C^-_{H,N}$ encloses the simple poles $\{v_{m+1}, ..., v_n\}$ (see Figure 2.2). Making a similar application of Cauchy's residue theorem, we have

$$\int_{C^-_{H,N}} f(v)dv = -2\pi i \sum_{k=m+1}^{n} R_k, \tag{2.23}$$

where $R_k = Res(f, v_k)$, for $k = m+1, ..., n$. Note that

$$\int_{C^-_{H,N}} f(v)dv = \left\{ \int_{C^-_{1,H,N}} + \int_{C^-_{2,H,N}} + \int_{C^-_{3,H,N}} + \int_{C^-_{4,H,N}} \right\} f(v)dv,$$

where

$$\int_{C^-_{1,H,N}} f(v)dv = \int_{-(N+1)h}^{(N+1)h} f(v)dv,$$

$$\int_{C^-_{2,H,N}} f(v)dv = \int_{(N+1)h}^{(N+1)h-iH} f(v)dv = -\int_{-H}^{0} f((N+1)h+iy)idy,$$

$$\int_{C^-_{3,H,N}} f(v)dv = \int_{(N+1)h-iH}^{-(N+1)h-iH} f(v)dv = -\int_{-(N+1)h}^{(N+1)h} f(t-iH)dt,$$

and

$$\int_{C^-_{4,H,N}} f(v)dv = \int_{-(N+1)h-iH}^{-(N+1)h} f(v)dv = \int_{-H}^{0} f(-(N+1)h+iy)idy.$$

Now we have

$$\int_{C^+_{H,N}} f(v)dv = \int_{-(N+1)h}^{(N+1)h} f(t)dt - \int_{-(N+1)h}^{(N+1)h} f(t+iH)dt + \int_{0}^{H} [f((N+1)h+iy) - f(-(N+1)h+iy)]idy \tag{2.24}$$

and

$$\int_{C^-_{H,N}} f(v)dv = \int_{-(N+1)h}^{(N+1)h} f(t)dt - \int_{-(N+1)h}^{(N+1)h} f(t-iH)dt + \int_{-H}^{0} [f(-(N+1)h+iy) - f((N+1)h+iy)]idy. \tag{2.25}$$

Combining (2.24) and (2.25) we obtain

$$\begin{aligned} \frac{1}{2}\left(\int_{C^+_{H,N}} f(v)dv + \int_{C^-_{H,N}} f(v)dv\right) &= \int_{-(N+1)h}^{(N+1)h} f(t)dt - \frac{1}{2}\int_{-(N+1)h}^{(N+1)h} [f(t-iH)dt + f(t+iH)]dt \\ &+ \frac{1}{2}\int_{0}^{H} [f((N+1)h+iy) - f(-(N+1)h+iy)]idy \\ &+ \frac{1}{2}\int_{-H}^{0} [f(-(N+1)h+iy) - f((N+1)h+iy)]idy, \end{aligned} \tag{2.26}$$

Also, from (2.21) and (2.23) we have that

$$\frac{1}{2}\left(\int_{C^+_{H,N}} f(v)dv + \int_{C^-_{H,N}} f(v)dv\right) = \pi i \sum_{k=1}^{n} sgn(\text{Im}v_k)R_k, \tag{2.27}$$

and this equals the right-hand side of (2.26). Hence,

$$\begin{aligned}\int_{-(N+1)h}^{(N+1)h} f(t)dt = \frac{1}{2}\int_{-(N+1)h}^{(N+1)h}&[f(t+iH)+f(t-iH)]dt + \pi i \sum_{k=1}^{n} sgn(\text{Im}(v_k))R_k\\ &-\frac{i}{2}\int_0^H [f((N+1)h+iy)-f(-(N+1)h+iy)]dy\\ &-\frac{i}{2}\int_{-H}^0 [f(-(N+1)h+iy)-f((N+1)h+iy)]dy.\end{aligned} \tag{2.28}$$

□

Corollary 2.5. *In the case that f is given by (2.9), and Assumption 2.1 holds, then the error,*

$$E_h^N := I - I_h^N, \tag{2.29}$$

is given by

$$\begin{aligned}E_h^N = &\frac{1}{2}\left(\int_{-(N+1)h}^{(N+1)h} f(t+iH)(1-g(t+iH))dt + \int_{-(N+1)h}^{(N+1)h} f(t-iH)(1+g(t-iH))dt\right)\\ &+\frac{i}{2}\int_0^H [f(-(N+1)h+iy)(1-g(-(N+1)h+iy))\\ &-f((N+1)h+iy)(1-g((N+1)h+iy))]dy\\ &+\frac{i}{2}\int_{-H}^0 [f((N+1)h+iy)(1+g((N+1)h+iy))\\ &-f(-(N+1)h+iy)(1+g(-(N+1)h+iy))]dy + \int_{-\infty}^{-(N+1)h} f(v)dv\\ &+\int_{(N+1)h}^{\infty} f(v)dv + C_F,\end{aligned} \tag{2.30}$$

where

$$C_F := i\pi \sum_{k=1}^{n} (\text{sgn}(Im(v_k)) - g(v_k))R_k, \tag{2.31}$$

will be known as the correction factor.

Proof. Subtracting (2.12) from (2.19) gives

$$\begin{aligned}
E_h^N &= \frac{1}{2}\int_{-(N+1)h}^{(N+1)h}[f(t-iH)dt+f(t+iH)]dt+\pi i\sum_{k=1}^{n} sgn(\mathrm{Im}(v_k))R_k+\int_{-\infty}^{-(N+1)h} f(v)dv \\
&+\int_{(N+1)h}^{\infty} f(v)dv-\frac{i}{2}\int_0^H[f((N+1)h+iy)-f(-(N+1)h+iy)]dy \\
&-\frac{i}{2}\int_{-H}^{0}[f(-(N+1)h+iy)-f((N+1)h+iy)]dy \\
&-\frac{1}{2}\left(\int_{-(N+1)h}^{(N+1)h} f(t+iH)g(t+iH)dt-\int_{-(N+1)h}^{(N+1)h} f(t-iH)g(t-iH)dt\right)-i\pi\sum_{k=1}^{n} g(v_k)R_k \\
&-\frac{i}{2}\int_0^H[f(-(N+1)h+iy)g(-(N+1)h+iy)dy-f((N+1)h+iy)g((N+1)h+iy)]dy \\
&-\frac{i}{2}\int_{-H}^{0}[f(-(N+1)h+iy)g(-(N+1)h+iy)dy-f((N+1)h+iy)g((N+1)h+iy)]dy,
\end{aligned} \tag{2.32}$$

which simplifies to give (2.30) □

Remark 2.6. *We can rewrite the formula for C_F in (2.31) as*

$$C_F = \pi i \sum_{k=1}^{n} G(v_k) \tag{2.33}$$

where

$$G(v_k) := \frac{2R_k}{1+e^{-2\pi i(v_k/h)}}\begin{cases} -e^{-2\pi i(v_k/h)}, & Im(v_k) < 0, \\ 1, & Im(v_k) > 0. \end{cases}$$

Corollary 2.7. *If the conditions of Corollary 2.1 are satisfied and also F (and so f) are even, in which case n is even and exactly $m = n/2$ the poles of F are in the upper half-plane, then (2.11) simplifies to*

$$I_h^N = 2h\sum_{k=1}^{N+1} f((k-1/2)h)$$

and (2.30) simplifies to

$$\begin{aligned} E_h^N &= \int_{-(N+1)h}^{(N+1)h} f(t+iH)(1-g(t+iH))dt \\ &+ i\int_0^H [f(-(N+1)h+iy)(1-g(-(N+1)h+iy)) \\ &- f((N+1)h+iy)(1-g((N+1)h+iy))]dy \\ &+ 2\int_{(N+1)h}^{\infty} f(v)dv + 2\pi i\sum_{k=1}^{m}(1-g(v_k))R_k, \end{aligned} \tag{2.34}$$

where the sum is over the poles in the upper half-plane.

Proof. Substituting $t=-s$, the second term in (2.30) is, recalling that g is odd,

$$\begin{aligned} -\int_{(N+1)h}^{-(N+1)h} f(-s-iH)(1+g(-s-iH))ds &= \int_{-(N+1)h}^{(N+1)h} f(-s-iH)(1+g(-s-iH))ds, \\ &= \int_{-(N+1)h}^{(N+1)h} f(s+iH)(1-g(s+iH))ds, \end{aligned}$$

i.e.

$$\int_{-(N+1)h}^{(N+1)h} f(t+iH)(1-g(t+iH))dt = \int_{-(N+1)h}^{(N+1)h} f(t-iH)(1+g(t-iH))dt.$$

Similarly, substituting $t=-y$ into

$$-\int_{-H}^{0}[f(-(N+1)h+iy)(1+g(-(N+1)h+iy))-f((N+1)h+iy)(1+g((N+1)h+iy))]dy,$$

we have, in the case when f is even, that

$$-\int_0^H [f(-(N+1)-it)(1+g(-(N+1)h-it))-f((N+1)h-it)(1+g((N+1)h-it))]dt,$$

$$= -\int_0^H [f((N+1)h+it)(1-g((N+1)h+it)-f(-(N+1)h+it)(1-g(-(N+1)h+it)))]dt,$$

$$= \int_0^H [f(-(N+1)h+it)(1-g(-(N+1)h+it)-f((N+1)h+it)(1-g((N+1)h+it)))]dt.$$

Also, substituting $t = -v$ in $\int_{-\infty}^{-(N+1)h} f(v)dv$, we have

$$\int_{-\infty}^{-(N+1)h} f(v)dv = -\int_{\infty}^{(N+1)h} f(-t)dt = \int_{(N+1)h}^{\infty} f(-t)dt$$
$$= \int_{(N+1)h}^{\infty} f(v)dv,$$

so

$$\int_{-\infty}^{-(N+1)h} f(v)dv + \int_{(N+1)h}^{\infty} f(v)dv = 2\int_{(N+1)h}^{\infty} f(v)dv.$$

In the case when F is even, then every pole in the upper half plane has a corresponding pole in the lower half plane (i.e. if v_k is pole in the upper half plane, then $-v_k$ is a pole in the lower half plane). So there is an even number of poles (i.e. $n = 2m$, for some $m \in \mathbb{N}$), and, if we order the poles so that the first m poles are in the upper half plane, then

$$C_F = i\pi \sum_{k=1}^{m} [sgn(\text{Im}(v_k)) - g(v_k)]R_k + [sgn(\text{-Im}(v_k)) - g(-v_k)]\widetilde{R}_k$$

$$= i\pi \sum_{k=1}^{m} [1 - g(v_k)]R_k + [-1 + g(v_k)]\widetilde{R}_k$$
$$= i\pi \sum_{k=1}^{m} (1 - g(v_k))(R_k - \widetilde{R}_k)$$

where

$$\widetilde{R}_k := \text{Res}(f, -v_k).$$

Now, we will show that $\widetilde{R}_k = -R_k$, where $\widetilde{R}_k$ and R_k are the residues of $f(v)$ at $-v_k$ and v_k respectively. Explicitly,

$$R_k = \lim_{v \to v_k} (v - v_k)f(v) \tag{2.35}$$

and

$$\widetilde{R}_k = \lim_{v \to -v_k} (v + v_k)f(v). \tag{2.36}$$

In the case when f is even, $\widetilde{R}_k$ can be written as

$$\widetilde{R}_k = \lim_{v \to -v_k} (v + v_k) f(-v)$$

$$= - \lim_{-v \to v_k} (-v - v_k) f(-v).$$

This is obviously

$$\widetilde{R}_k = -R_k.$$

Therefore the formula (2.31) simplifies to

$$C_F = 2\pi i \sum_{k=1}^{m} (1 - g(v_k)) R_k.$$

Hence (2.30) becomes

$$\begin{aligned} E_h^N = & \int_{-(N+1)h}^{(N+1)h} f(t + iH)(1 - g(t + iH))dt \\ & + i \int_0^H [f(-(N+1)h + iy)(1 - g(-(N+1)h + iy)) \\ & - f((N+1)h + iy)(1 - g((N+1)h + iy))]dy \\ & + 2 \int_{(N+1)h}^{\infty} f(v)dv + 2\pi i \sum_{k=1}^{m} (1 - g(v_k)) R_k. \end{aligned} \tag{2.37}$$

□

Definition 2.8. *In the case that Assumption (2.1) holds, let the modification of the truncated midpoint rule, denoted by I_h^{*N}, be the formula (2.11) with the addition of the correction factor (2.31), that is define*

$$\begin{aligned} I_h^{*N} & := I_h^N + C_F \\ & = h \sum_{k=-N}^{N+1} f((k - 1/2)h) + i\pi \sum_{k=1}^{n} [sgn(Im(v_k)) - g(v_k)] R_k, \end{aligned} \tag{2.38}$$

and let E_h^{*N} be the error in this approximation, that is

$$E_h^{*N} := I - I_h^{*N}. \tag{2.39}$$

Next we will propose a theorem for bounding the error of the modified truncated midpoint approximation, defined by (2.39).

Theorem 2.9. *If Assumption 2.1 holds and f is given by (2.9) and f is even, then, for $0 < h < \frac{2\pi}{\rho H}$, so that $\rho H^2 - \frac{2\pi H}{h} \leq 0$, it holds that*

$$\begin{aligned} |E_h^{*N}| \leq & \frac{2\sqrt{\pi} M_3(H,(N+1)h) e^{\rho H^2 - 2\pi H/h}}{\sqrt{\rho}(1-e^{-2\pi H/h})} \\ & + e^{-\rho(N+1)^2 h^2} \left(\frac{M_1((N+1)h)}{\rho(N+1)h} + 2HM_2(H,(N+1)h) \right) \end{aligned} \tag{2.40}$$

where, for $A > 0$,

$$M_1(A) := \sup_{t \geq A} |F(t)|. \tag{2.41}$$

$$M_2(H,A) := \sup_{0 \leq y \leq H} [|F(-A+iy)| + |F(A+iy)|] \tag{2.42}$$

and

$$M_3(H,A) := \sup_{-A \leq t \leq A} |F(t+iH)|, \tag{2.43}$$

Proof. Since $E_h^N := I - I_h^N$ and $I_h^{*N} := I_h^N + C_F$, from Corollary 2.7 we have

$$\begin{aligned} E_h^{*N} = & \int_{-(N+1)h}^{(N+1)h} f(t+iH)(1-g(t+iH))dt \\ & + i \int_0^H [f(-(N+1)h+iy)(1-g(-(N+1)h+iy)) \\ & - f((N+1)h+iy)(1-g((N+1)h+iy))]dy \\ & + 2\int_{(N+1)h}^{\infty} f(v)dv. \end{aligned} \tag{2.44}$$

Using the bound (2.2) for the first integral and the bound (2.7) in the second integral gives

$$\begin{aligned}|E_h^{*N}| \leq \frac{2e^{-2\pi H/h}}{1-e^{-2\pi H/h}} \left(\int_{-(N+1)h}^{(N+1)h} |f(t+iH)|dt \right) + 2\int_{(N+1)h}^{\infty} |f(v)|dv, \\ + 2\int_0^H e^{-2\pi y/h}[|f(-(N+1)h+iy)| + |f((N+1)h+iy)|]dy.\end{aligned} \tag{2.45}$$

Using (2.9), then

$$\begin{aligned}\left| \int_{-(N+1)h}^{(N+1)h} f(t+iH)dt \right| &= \left| \int_{-(N+1)h}^{(N+1)h} e^{-\rho(t+iH)^2} F(t+iH)dt \right| \\ &\leq M_3(H,(N+1)h)e^{\rho H^2} \int_{-(N+1)h}^{(N+1)h} e^{-\rho t^2} dt \\ &\leq M_3(H,(N+1)h)\sqrt{\frac{\pi}{\rho}} e^{\rho H^2}.\end{aligned} \tag{2.46}$$

We have also

$$\begin{aligned}2\left| \int_{(N+1)h}^{\infty} f(t)dt \right| &= 2\left| \int_{(N+1)h}^{\infty} e^{-\rho t^2} F(t)dt \right| \\ &\leq 2M_1((N+1)h) \int_{(N+1)h}^{\infty} e^{-\rho t^2} dt.\end{aligned} \tag{2.47}$$

Using integration by parts, we find that

$$2\int_{(N+1)h}^{\infty} e^{-\rho t^2} dt < \frac{e^{-\rho(N+1)^2h^2}}{\rho(N+1)h} \tag{2.48}$$

so

$$2\left| \int_{(N+1)h}^{\infty} f(t)dt \right| < M_1((N+1)h)\frac{e^{-\rho(N+1)^2h^2}}{\rho(N+1)h}. \tag{2.49}$$

Also, $2\int_0^H e^{-2\pi y/h}[|f(-(N+1)h+iy)| + |f((N+1)h+iy)|]dy$

$$\begin{aligned}&\leq 2e^{-\rho(N+1)^2h^2} \sup_{0\leq y\leq H} [|F(-(N+1)h+iy)| + |F((N+1)h+iy)|] \int_0^H e^{\rho y^2 - 2\pi y/h} dy \\ &\leq 2He^{-\rho(N+1)^2h^2} \sup_{0\leq y\leq H} [|F(-(N+1)h+iy)| + |F((N+1)h+iy)|],\end{aligned} \tag{2.50}$$

since $\rho H^2 - \frac{2\pi}{\rho H} \leq 0$, for $0 \leq y \leq H$. Hence

$$
\begin{aligned}
|E_h^{*N}| \leq & \frac{2\sqrt{\pi} M_3(H,(N+1)h) e^{\rho H^2 - 2\pi H/h}}{\sqrt{\rho}(1-e^{-2\pi H/h})} \\
& + e^{-\rho(N+1)^2 h^2} \left(\frac{M_1((N+1)h)}{\rho(N+1)h} + 2HM_2(H,(N+1)h) \right).
\end{aligned}
\tag{2.51}
$$

□

Note that if we use the bound (2.2) for the second integral in (2.44), this term will blow up at $y = 0$. For this reason we choose the bound (2.7).

2.2 Numerical examples

Now, we will consider three numerical examples. These examples are presented to show the accuracy and efficiency of the modified truncated midpoint rule. The first example will be the simplest case when the function $F = 1$ in (2.10), the second example will be the complementary error function, and the function in the third example is given by (2.76). All integrands in these examples are entire and meromorphic functions. Practically, the integrals in these examples will be approximated by the modified midpoint rule defined by (2.38). Theoretically, we will test the error estimate, proved in Theorem 2.1.

2.2.1 Example 1:

Let

$$I = \int_{-\infty}^{\infty} e^{-x^2} dx = \sqrt{\pi} = 1.7724538509055159, \tag{2.52}$$

i.e. I is defined by (2.10) with $f(v) = e^{-v^2}, \rho = 1, F(v) = 1$. The integrand in this example is an entire function. The example demonstrates the approximation by the truncated midpoint rule (2.11),

$$I_h^N = h \sum_{k=-N}^{N+1} e^{-(k-1/2)^2 h^2} = 2h \sum_{k=1}^{N+1} e^{-(k-1/2)^2 h^2}. \tag{2.53}$$

Since f does not have singularities we do not need to apply the modified midpoint rule (i.e. in this case, the midpoint rule = the modified midpoint rule). For numerical results, we let $N = 4, 6, 8, 10, 12$, and compute I_h^N, the actual error $E_h^N = I - I_h^N$, and the theoretical bound on the error E_h^N given by (2.57) below. Table 2.1 below shows the calculation of the truncated midpoint rule I_h^N with different numbers of quadrature points N and step size $h = \sqrt{\pi/(N+1)}$; see the discussion in §2.2.1.1 below. From the table we can see that I_h^N gives 7 correct digits with four quadrature points for $h = 0.7926$ and 16-digit accuracy with 12 quadrature points with $h = 0.4915$.

N	$h = \sqrt{\pi/(N+1)}$	I_h^N	$\lvert I - I_h^N \rvert$	RHS of (2.57)
4	0.7926	**1.7724533**078535685	5.430×10^{-7}	2.961×10^{-6}
6	0.6699	**1.77245384**9893308	1.012×10^{-9}	6.336×10^{-9}
8	0.5908	**1.77245385090**36283	1.887×10^{-12}	1.313×10^{-11}
10	0.5344	**1.7724538509055**13	2.886×10^{-15}	2.672×10^{-14}
12	0.4915	**1.7724538509055159**	0	5.363×10^{-16}

Table 2.1: Approximating the integral (2.52) using the truncated midpoint rule

For completeness, let us also approximate the integral I by the composite trapezoidal rule, i.e., approximate I by $I_{h,N}$ given by (1.10). As in the above calculations for the midpoint rule we take, as recommended in [2] and [26], $h = \sqrt{\pi/(N+1)}$. Since the integral has no pole in this example, $C_F = 0$ and $I_{h,N} = I^*_{h,N}$, where $I^*_{h,N}$ is given by (1.13). From (1.15) and (1.17) it follows, since $M_H(F) = M^{(N+1)h}(F) = 1$ and $\rho = 1$ for this example, that

$$\begin{aligned} |I - I_{N,h}| &= |I - I^*_{N,h}| \\ &\le |I - I^*_h| + |I^*_h - I^*_{N,h}| \end{aligned}$$

$$\leq e^{-\pi(N+1)} \left(\frac{2\sqrt{\pi}}{1 - e^{-2\pi(N+1)}} + \frac{1+2\pi}{\sqrt{\pi(N+1)}} \right). \qquad (2.54)$$

N	$h = \sqrt{\pi/(N+1)}$	$I_{h,N}$	$\|I - I_{h,N}\|$	RHS of (2.54)
4	0.7926	**1.77245**41459790366	2.950 $\times 10^{-7}$	8.111$\times 10^{-7}$
6	0.6699	**1.77245385**15256285	6.201 $\times 10^{-10}$	1.434 $\times 10^{-9}$
8	0.5908	**1.7724538509**067571	1.241 $\times 10^{-12}$	2.582 $\times 10^{-12}$
10	0.5344	**1.772453850905518**3	2.442 $\times 10^{-15}$	4.695 $\times 10^{-15}$
12	0.4915	**1.772453850905516**	2.220 $\times 10^{-16}$	8.585$\times 10^{-16}$

Table 2.2: Approximating the integral (2.52) using the truncated trapezium rule

In Table 2.2 we plot $I_{h,N}$, $|I - I_{h,N}|$, and the right hand side of (2.54) against N. Comparing Tables 2.1 and 2.2 we see that:

- For $N \leq 10$, the trapezium rule error, $|I - I_{h,N}|$, is slightly smaller, by a factor $c_N \in [1.181, 1.840]$, than the midpoint rule error, $|I - I_h^N|$.
- Similarly, the error bound for the trapezium rule (the RHS of (2.54)) is smaller, by a factor $c_N{}' \in [3.650, 6.246]$, than the error bound for the midpoint rule (the RHS of (2.57)).

Recall, as discussed in §1.1, that these error bounds are obtained by somewhat different arguments.

2.2.1.1 Theoretical error estimate using theorem 2.1

In this case Assumption 2.1 is satisfied for every $H > 0$, and for every $H > 0$, $E_h^N = I - I_h^N = I - I_h^{*N} = E_h^{*N}$. For our example 1 we have $\rho = 1$, $F = 1$, and, for $H \geq 0$, and $A > 0$, $M_1(A) = 1, M_3(H, A) = 1$, and $M_2(H, A) = 2$, so by Theorem 2.1, provided $h < 2\pi/H$,

$$|I - I_h^N| = |E_h^N| = |E_h^{*N}| \leq \frac{2\sqrt{\pi}e^{H^2 - 2\pi H/h}}{1 - e^{-2\pi H/h}} + e^{-(N+1)^2h^2} \left(\frac{1}{(N+1)h} + 4H \right). \qquad (2.55)$$

For simplicity, we choose specific values of H and h as follows:

- We choose $H = \pi/h$ to minimize the expression $H^2 - 2\pi H/h$ (this choice also ensures that $h = \frac{\pi}{H} < \frac{2\pi}{H}$), to obtain

$$|E_h^{*N}| \leq \frac{2\sqrt{\pi}e^{-\pi^2/h^2}}{1 - e^{-2\pi^2/h^2}} + e^{-(N+1)^2h^2}\left(\frac{1}{(N+1)h} + \frac{4\pi}{h}\right). \tag{2.56}$$

- We choose $h = \sqrt{\frac{\pi}{N+1}}$ (as recommended in [26] and [2]), so that $\frac{\pi^2}{h^2} = (N+1)^2h^2$ in the above bound (2.52), so that we equalise the exponents of $e^{-\pi^2/h^2}$ and $e^{-(N+1)^2h^2}$ in (2.56). With this choice of h (2.56) becomes

$$|I - I_h^N| = |E_h^N| = |E_h^{*N}| \leq e^{-\pi(N+1)}\left(\frac{2\sqrt{\pi}}{1 - e^{-2\pi(N+1)}} + \frac{1}{\sqrt{\pi(N+1)}} + 4\sqrt{\pi(N+1)}\right). \tag{2.57}$$

In Table 2.1 we tabulate $|I - I_h^N|$ for these choices of H and h, and also tabulate the right-hand side of (2.57), showing that, indeed the bound (2.57) is satisfied.

2.2.2 Example 2:

The complementary error function, erfc, is defined by

$$\text{erfc(a)} := \frac{2}{\sqrt{\pi}}\int_a^\infty e^{-t^2}dt, \quad a \in \mathbb{R}. \tag{2.58}$$

It is also well known that, for $a > 0$,

$$\text{erfc(a)} = \frac{ae^{-a^2}}{\pi}I, \tag{2.59}$$

where

$$I := \int_{-\infty}^{\infty}\frac{e^{-t^2}}{t^2 + a^2}dt, \tag{2.60}$$

i.e. I is given by (2.10) with $f(t) = \frac{e^{-t^2}}{t^2+a^2}$, $\rho = 1$, $F(t) = \frac{1}{t^2+a^2}$. The integrand here is a meromorphic function with two simple poles at $t = \pm ia$. The function erfc(a) is implemented in the Python library Scipy as the function Scipy.special.erfc(a).

Evaluating erfc(a) for $a = 0.1$, we find that

$$I = \mathbf{0.8875370839817152}....$$

Note that Chiarella and Reichel [15] were the first to bound the error of the modified trapezium rule for this example. Since then Matta and Reichel [32] proposed to use the modified trapezoidal rule using the quadrature points kh, $k \in \mathbb{Z}$, and $H = \pi/h$, i.e, approximating

$$\text{erfc(a)} \approx \frac{ahe^{-a^2}}{\pi}\left(\frac{1}{a^2} + \sum_{k=1}^{N} \frac{e^{-(k)^2h^2}}{k^2h^2 + a^2}\right) + \frac{2}{1 - e^{2\pi a/h}}, \quad \text{for} \quad 0 < a < H. \quad (2.61)$$

This formula blows up when a is close to zero. Hunter and Regan [22] proposed, alternatively, to use the midpoint rule to resolve this difficulty, i.e, to define

$$I_h^N = \frac{ahe^{-a^2}}{\pi} \sum_{k=-N}^{N+1} \frac{e^{-(k-\frac{1}{2})^2h^2}}{(k-\frac{1}{2})^2h^2 + a^2} = \frac{2ahe^{-a^2}}{\pi} \sum_{k=1}^{N+1} \frac{e^{-(k-\frac{1}{2})^2h^2}}{(k-\frac{1}{2})^2h^2 + a^2}, \qquad (2.62)$$

take $H = \pi/h$, and to approximate erfc(a) by the truncated modified midpoint rule given by the expression

$$I_h^{*N} := \begin{cases} I_h^N + \frac{2}{1+e^{2\pi a/h}}, & \text{if} \quad a < H, \\ I_h^N, & \text{if} \quad H < a \end{cases} \qquad (2.63)$$

Note that the expression

$$C_F = \frac{2e^{-2\pi a/h}}{1 + e^{-2\pi a/h}} = \frac{2}{1 + e^{2\pi a/h}}, \qquad (2.64)$$

is the correction factor term.

Table 2.3 below shows the calculation of I_h^N for different values of N and h; we selected the value of h by arguing as in (§6, Table 1, [38]). Our version of this argument is as follows. Noting that $E_h^N = E_h^{*N}$, for $H < a$, by Theorem 2.1 for

$H < a$ with $\rho = 1$, we have that,

$$|E_h^N| = |E_h^{*N}| \leq \frac{2\sqrt{\pi} M_3(H,(N+1)h) e^{H^2 - 2\pi H/h}}{(1 - e^{-2\pi H/h})} + e^{-(N+1)^2 h^2} \left(\frac{M_1((N+1)h)}{(N+1)h} + 2H M_2(H,(N+1)h) \right). \tag{2.65}$$

We choose H as large as possible i.e., $H = a - \epsilon$ with ϵ very small, and then choose h to approximately equalise the exponents in (2.65), i.e. so that

$$-(N+1)^2 h^2 \approx H^2 - 2\pi H/h.$$

Precisely, we choose $h > 0$ so that

$$-(N+1)^2 h^2 = -2\pi a/h,$$

i.e. we choose

$$h = \left(\frac{2\pi a}{(N+1)^2} \right)^{1/3} = (2\pi a)^{1/3} (N+1)^{-2/3}. \tag{2.66}$$

In the case $a = 0.1$, this gives

$$h = C(N+1)^{-2/3}, \quad \text{where} \quad C = (0.2\pi)^{1/3} = 0.856498... \tag{2.67}$$

From Table 2.3 we see that the midpoint rule gives 2-digits accuracy with 30 quadrature points for $h = 0.0867$, while it gives 15-digits accuracy for $h = 0.008$ with $N = 1000$. Also from table 2.3 we can see that the error decreases with increasing N.

N	$h = (0.2\pi)^{1/3}(N+1)^{-2/3}$	I_h^N	$\lvert I - I_h^N \rvert$
15	0.134	**0.8**687219048806953	1.881 $\times 10^{-2}$
30	0.0867	**0.88**61014678620067	1.435$\times 10^{-3}$
45	0.066	**0.887**3745231948752	1.625 $\times 10^{-4}$
65	0.052	**0.8875**245520535163	1.253 $\times 10^{-5}$
95	0.040	**0.88753**66656566775	4.183 $\times 10^{-7}$
1000	0.008	**0.887537083981715**	3.330 $\times 10^{-16}$

Table 2.3: Approximating the integral (2.59) using the truncated midpoint rule.

2.2.2.1 Theoretical error estimate using Theorem 2.1

In Example 2 Assumption 2.1 is satisfied for all $H > 0$ with $H \neq a$; choosing $H = \pi/h$ and $h = \sqrt{\pi/(N+1)}$, equation (2.40) becomes

$$|E_h^{*N}| \leq e^{-\pi(N+1)} \left(\frac{2\sqrt{\pi} M_3(H,(N+1)h)}{1 - e^{-2\pi(N+1)}} + \frac{M_1((N+1)h)}{\sqrt{\pi(N+1)}} + 2M_2(H,(N+1)h)\sqrt{\pi(N+1)} \right). \tag{2.68}$$

where $M_2(H,A)$,$M_3(H,A)$, and $M_1(A)$ are given for $A > 0$, by (2.41) (2.42) and (2.43) respectively. Let us compute now these upper bounds:

1. First we compute $M_3(H,A) = \sup_{-A \leq t \leq A} |F(t+iH)|$, for $H > 0$, $H \neq a$, and $A > 0$. We have, for $t \in \mathbb{R}$,

$$|F(t+iH)| = \frac{1}{|(t+iH)^2 + a^2|} = \frac{1}{|(t+iH) - (ia)|^2}$$
$$= \frac{1}{|t + i(H-a)||t + i(H+a)|}.$$

Further,

$$|t + i(H-a)||t + i(H+a)| = \sqrt{t^2 + (H-a)^2}\sqrt{t^2 + (H+a)^2}$$
$$\geq |H-a||H+a| = |H^2 - a^2|.$$

Hence

$$|F(t+iH)| \leq \frac{1}{|H^2 - a^2|}. \tag{2.69}$$

Thus

$$M_3(H, A) \leq \frac{1}{|H^2 - a^2|}, \tag{2.70}$$

for $a > 0, H > 0$, with $H \neq a$, and $A > 0$.

2. Secondly, we calculate $M_1(A) = \sup_{t \geq A} |F(t)|$, for $A, a > 0$. We have, for $A > 0$ and $t \geq A$,

$$|F(t)| = \frac{1}{|t^2 + a^2|} \leq \frac{1}{t^2}. \tag{2.71}$$

Thus, for $t \geq A > 0$, we have

$$|F(t)| \leq \frac{1}{A^2}, \tag{2.72}$$

$$M_1(A) \leq \frac{1}{A^2}. \tag{2.73}$$

3. Finally we compute $M_2(H, A) = \sup_{0 \leq y \leq H} |F(A+iy) + F(-A+iy)|$, for $A, H > 0$. For $0 \leq y \leq H$,

$$|F(A + iy)| = \frac{1}{|(A + iy)^2 + a^2|} = \frac{1}{|(A + iy)^2 - (ia)^2|}$$

$$= \frac{1}{|A + i(y - a)||A + i(y + a)|}$$

and

$$|A + i(y - a)||A + i(y + a)| = \sqrt{A^2 + (y - a)^2}\sqrt{A^2 + (y + a)^2},$$

$$\geq |A||A| = A^2,$$

so

$$|F(A + iy)| \leq \frac{1}{A^2}. \tag{2.74}$$

Similarly

$$|F(-A + iy)| \leq \frac{1}{A^2}$$

so

$$M_2(H,A) \leq \frac{2}{A^2}. \tag{2.75}$$

Hence by (2.68), and (2.70), (2.73), and (2.75), for $N \in \mathbb{N}$, if the step size is chosen as $h = \sqrt{\pi/(N+1)}$ and $H \neq a$, then, where $A = (N+1)h = \sqrt{(N+1)\pi}$, the actual error of the modified midpoint rule is bounded by

$$\begin{aligned} |E_h^{*N}| = |I - I_h^{*N}| &\leq e^{-\pi(N+1)} \left(\frac{2\sqrt{\pi} M_3(H,A)}{(1-e^{-2\pi(N+1)})} + \frac{M_1(A)}{\sqrt{\pi(N+1)}} + 2M_2(H,A)\sqrt{\pi(N+1)} \right), \\ &\leq e^{-\pi(N+1)} \left(\frac{2\sqrt{\pi}}{|H^2-a^2|(1-e^{-2\pi(N+1)})} + \frac{1}{A^2\sqrt{\pi(N+1)}} + \frac{4\sqrt{\pi(N+1)}}{A^2} \right) \\ &\leq e^{-\pi(N+1)} \left(\frac{2\sqrt{\pi}}{|H^2-a^2|(1-e^{-2\pi(N+1)})} + \frac{1+4\pi(N+1)}{(\pi(N+1))^{3/2}} \right). \end{aligned} \tag{2.76}$$

In Python we calculate the actual error of the modified midpoint rule and the theoretical bound on the error using (2.76), choosing $a = 0.1$, and $H = \pi/h$ and the results are shown in the Table 2.4 below.

N	$h = \sqrt{\pi/(N+1)}$	I_h^{*N}	$\lvert E_h^{*N}\rvert$	RHS of (2.76)	RHS/ $\lvert E_h^{*N}\rvert$
2	1.02	**0.887537**9054906791	8.215×10^{-7}	1.129×10^{-4}	137.43
4	0.79	**0.887537084**9504878	9.687×10^{-10}	1.859×10^{-7}	191.94
6	0.66	**0.887537083983**0392	1.324×10^{-12}	3.279×10^{-10}	247.70
8	0.59	**0.88753708398171**72	1.998×10^{-15}	5.927×10^{-13}	296.62
10	0.53	**0.8875370839817152**	0	1.083×10^{-15}	

Table 2.4: Approximating the integral (2.60) using the modified truncated midpoint rule.

From Tables 2.3 and 2.4 above, we can see that the truncated midpoint rule is less efficient than the modified truncated midpoint rule. From Table 2.4 we can see that the convergence is amazingly fast, with 6 digits accuracy for $h = 1.02$ with only two quadrature points and 16 digits accuracy for $h = 0.53$ with 10 quadrature points. Also from Table 2.4 we can see that the RHS of (2.76) is greater than the actual error, providing a check for the validity of (2.76).

2.2.3 Example 3

Given $a > 0$, let us consider now the evaluation of the integral

$$I = \int_{-\infty}^{\infty} e^{-v^2} F(v)dv = \frac{a}{\pi} \int_{-\infty}^{\infty} \frac{e^{-v^2}\cos(v^2)}{v^2 + a^2} dv \approx \mathbf{0.88554505848746}, \tag{2.77}$$

where

$$F(v) := \frac{a\cos(v^2)}{\pi(v^2 + a^2)}. \tag{2.78}$$

This function has simple poles at $v = \pm ia$. The truncated midpoint rule is

$$I_h^N = \frac{ah}{\pi} \sum_{k=-N}^{N+1} \frac{e^{-t_k^2}\cos(t_k^2)}{t_k^2 + a^2}, \tag{2.79}$$

where $t_k = (k - 1/2)h$. In cases, as here, where a is the distance to the nearest

N	h	I_h^N	$\lvert E_h^N \rvert$
25	0.0975	**0.88**2318615701214	3.2×10^{-3}
50	0.0622	**0.8854**611392879025	8.3×10^{-5}
100	0.0394	**0.88554**48097583446	2.4×10^{-7}
200	0.0249	**0.8855450584**638402	2.3×10^{-11}
500	0.0135	**0.88554505848746**	0

Table 2.5: Approximating the integral (2.77) by truncated midpoint rule.

singularity to the real axis, a choice of h proportional to $N^{-2/3}$ is, recommended as optimal in Trefethen and Weideman [38], and we make the specific choice (2.64) giving,

$$|I - I_h^N| = \mathcal{O}(e^{-(2\pi a(N+1))^{2/3}}), \tag{2.80}$$

see the results in Table 2.5. The truncated modified midpoint rule is

$$I_h^{*N} = \frac{ah}{\pi} \sum_{k=-N}^{N+1} \frac{e^{-(t_k)^2}\cos(t_k^2)}{t_k^2 + a^2} + \frac{2\cos(a^2)e^{a^2 - 2\pi a/h}}{1 + e^{-2\pi a/h}}. \tag{2.81}$$

We use for this rule, first of all the choice $h = \sqrt{\pi/(N+1)}$ used in Example 2 (see the results in Table 2.6), and secondly the different choice $h = \sqrt{\pi/(\sqrt{2}(N+1))}$ motivated by the theoretical error analysis below (see the results in Table 2.7).

N	h	I_h^{*N}	$\lvert E_h^{*N}\rvert$
2	1.0233	**0.885**6811311523397	1.3×10^{-4}
5	0.7236	**0.885544**725476039	3.3×10^{-7}
20	0.3867	**0.88554505848746**2	8.8×10^{-16}

Table 2.6: Approximating the integral (2.77) by I_h^{*N}.

N	h	I_h^{*N}	$\lvert E_h^{*N}\rvert$	R.H.S of 2.85
2	0.860	**0.88554**73331714725	2.2×10^{-6}	3.8×10^{-2}
5	0.608	**0.885545055**4333251	3.05×10^{-9}	6.5×10^{-3}
20	0.325	**0.88554505848746**1	1.1×10^{-16}	7.29×10^{-6}

Table 2.7: Approximating the integral (2.77) by I_h^{*N}.

From Tables 2.6 and 2.7 we see that our approximation with $h = \sqrt{\pi/(\sqrt{2}(N+1))}$ is more accurate than our approximation with $h = \sqrt{\pi/(N+1)}$, for instance, when $N = 2$ in Table 2.7, we obtain 5-digits accuracy, while we only obtain 3 correct digits for the same number of quadrature points in Table 2.6.

Now let us find the upper bounds on F defined by (2.78) that are needed for the error bound (2.40). We start with the simplest upper bound

$$M_1(A) = \sup_{t\geq A}\left|\frac{a\cos(t^2)}{\pi(t^2+a^2)}\right|.$$

It is clear that $|\cos(t)| \leq 1$ for all real numbers, and also

$$|t^2+a^2| \geq t^2 \geq A^2,$$

for $t \geq A$. Thus

$$M_1(A) \leq \frac{a}{\pi A^2}. \tag{2.82}$$

The second upper bound on F is

$$M_3(H, A) = \sup_{-A \le t \le A} \left| \frac{a\cos(v^2)}{\pi(v^2 + a^2)} \right|,$$

where $v = t + iH$. Now

$$\begin{aligned} \cos((t+iH)^2) &= \frac{e^{i(t+iH)^2} + e^{-i(t+iH)^2}}{2} \\ &= \frac{e^{it^2 - 2Ht - iH^2} + e^{-it^2 + 2Ht + iH^2}}{2} \end{aligned}$$

so

$$\begin{aligned} |\cos((t+iH)^2)| &\le \frac{e^{-2Ht} + e^{2Ht}}{2} = \cosh(2Ht) \\ &\le e^{2HA}, \end{aligned}$$

for $-A \le t \le A$. Also we have

$$\begin{aligned} |(t+iH)^2 + a^2| = |(t+iH)^2 - (ia)^2| &= |t + i(H-a)||t + i(H+a)| \\ &= \sqrt{t^2 + (H-a)^2}\sqrt{t^2 + (H+a)^2} \\ &\ge |H-a||H+a| = |H^2 - a^2|. \end{aligned}$$

Thus

$$M_3(H, A) \le \frac{ae^{2HA}}{\pi|H^2 - a^2|}. \tag{2.83}$$

The third upper bound is

$$M_2(H, A) = \sup_{0 \le y \le H} \left| \frac{a\cos((-A+iy)^2)}{\pi((-A+iy)^2 + a^2)} + \frac{a\cos((A+iy)^2)}{\pi((A+iy)^2 + a^2)} \right|$$

For $y \le H$, $|\cos((A+iy)^2)| \le \cosh(2Ay) \le e^{2AH}$. Also,

$$\begin{aligned} |(A+iy)^2 + a^2| = |(A+iy)^2 - (ia)^2| &= |(A + i(y-a))||(A + i(y+a))| \\ &= \sqrt{A^2 + (y-a)^2}\sqrt{A^2 + (y+a)^2} \\ &\ge |A||A| = A^2. \end{aligned}$$

Thus

$$M_2(H, A) \leq \frac{2ae^{2HA}}{\pi A^2}. \tag{2.84}$$

So choosing $H = \sqrt{\pi(N+1)}(2^{1/4} - 2^{-1/4})$ and $h = \sqrt{\pi/(\sqrt{2}(N+1))}$, to approximately minimize the error bound, so $A = h(N+1) = \sqrt{\pi(N+1)/\sqrt{2}}$, we get

$$|E_h^{*N}| \leq e^{\frac{-\pi(N+1)}{4+3\sqrt{2}}} \left(\frac{2\sqrt{\pi}\, a}{\pi|H^2 - a^2|(1 - e^{-2\pi H/h})} + \frac{ae^{-2HA}}{\pi A^3} + \frac{4H\, a}{\pi A^2} \right), \tag{2.85}$$

with

$$2HA = 2\pi(N+1)(1 - 2^{-1/2}),$$

$$2\pi H/h = 2\pi(N+1)(2^{1/2} - 1),$$

and

$$\frac{H}{A^2} = \frac{1}{\sqrt{\pi(N+1)}}(2^{3/4} - 2^{1/4}).$$

Note that the error bound (2.85) suggests that when N increases by 1, the error in the approximation decreases by at least a factor

$$e^{\frac{-\pi}{4+3\sqrt{2}}} \approx 0.683. \tag{2.86}$$

2.2.4 Conclusions regarding the numerical examples

The new error bound proposed in Theorem 2.1 was tested by examples 1, 2, and 3, and we have shown how fast the actual error decreases with increasing N. From the above results, we see that the standard midpoint rule and the modified midpoint rule give accurate results. But with the suggested modification, the numerical approximation is improved greatly and we achieve significant levels of accuracy in each example with small numbers of quadrature points. In Example 1, where I is defined by (2.10) with $F = 1$, we applied the midpoint rule approximation and the trapezium rule approximation; the results are shown in Tables 2.1 and 2.2.

We derived the error bounds (2.57) and (2.54) for the midpoint rule approximation and the trapezium rule, respectively. As discussed in §1.1, these error bounds are obtained by somewhat different arguments. In Example 3 the bound on the error in the trapezium rule approximation (1.15) does not apply, because the function (2.78) is only bounded on the real axis.

Chapter 3

Quasi-Periodic Green's Function

3.1 Introduction

In scattering theory, the boundary integral equation method is a widely used technique in many branches of physics and engineering. In the numerical calculations for solving these integral equations, a large number of evaluations of some relevant Green's function are required. Many mathematics researchers have been interested in the topic of electromagnetic and acoustic fields scattered by periodic surfaces (diffraction gratings) with quasi-periodic incident plane waves, where the corresponding Green's function of the 2D Helmholtz equation is also quasi-periodic. The obvious sum of sources and Fourier series representations for this Green's function contain series which converge very slowly and so are inappropriate for numerical work.

In this chapter we will present an integral representation for the quasi-periodic Green's function in the form

$$I = \int_{-\infty}^{\infty} e^{-\rho v^2} F(v), \tag{3.1}$$

where F is analytic in a neighborhood of the real axis except for simple poles. We will apply the numerical method proposed in chapter 2, namely the truncated modified midpoint rule, to evaluate this quasi-periodic Green's function for the 2D Helmholtz equation. We will show that our new methods are effective, indeed that they appear to be competitive in operation counts and accuracy compared with other effective ways of evaluating the Green's function. In particular, we make a comparison in section 3.5 with Ewald's method, recommended as the most efficient computational method in the review paper [28], and with another new method proposed in [30].

This chapter is organized as follows. In section 3.2 we introduce some notations relating to the Green's function and the Helmholtz equation, using the notations in [28] and [14]. In section 3.3 we introduce the problem; our starting point is the notations and formulas for the quasi-periodic Green's function from [28]. We present three formulas for the quasi-periodic Green's function and the main focus is on the integral representation. We show an integral representation for the quasi-periodic Green's function in the form (3.1), and we calculate a correction factor term $G^{\pm}_{F_{m,m+1}}$ which depends on the residues of functions $F_{\pm}$ at their poles $v^{-}_{\pm,n}$ and $v^{+}_{\pm,n}$. We divide section 3.4 into 3 parts. In part A we apply the truncated midpoint rule and the modified truncated midpoint rule to approximate (3.30), where the number of sources represented explicitly is $M = 1$; the results show increases in the accuracy with increasing N (see Tables 3.5 and 3.6). In part B we turn our attention to including contributions related to all the poles in the domain $S_H := \{v \in \mathbb{C} : |\mathrm{Im}(v)| < H\}$ and present a formula for the correction factor in this case. The results are slightly more accurate than Part A. In Part C, we derive a new integral representation for the quasi-periodic Green's function written in the form (3.1), where $2M - 1$ sources are computed explicitly, for some $M \in \mathbb{N}$. We apply the modification of the truncated midpoint rule in this part (see the numerical results in the Tables 3.9 and 3.10). In section 3.5 we compare our method with other methods, presented in [28], namely Ewald's method and the asymptotic correction term method of [30], and we show that the proposed numerical method is robust, accurate and efficient.

3.2 The Green's function for the 2D Helmholtz equation in free space.

We will adopt notations to introduce our problem and the equations that are the same as used in [14] and [28]. All implementations are done in Python in this chapter, as discussed in the introduction. Before finding the Green's function for periodic structures we need to clarify some important concepts that we use in our case. In 2D problems we will use Cartesian coordinates $Oxyz$; everything in the $z-$direction will be constant, so our mathematical problem to be solved just depends on x and y. Also, $\mathbf{r}$ will be the vector $\mathbf{r} = (x, y) \in \mathbb{R}^2$. Let the pressure U at time t at the point whose position vector is $\mathbf{r}$ be given by $U(\mathbf{r}, t)$. Then U satisfies

$$\Delta U = \frac{1}{c^2}\frac{\partial^2 U}{\partial t^2}, \tag{3.2}$$

which is the wave equation, where $\Delta = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}$ in 2D. If time-dependence is **time harmonic**, i.e. $U(\mathbf{r}, t)$ is given by

$$U(\mathbf{r}, t) = A(\mathbf{r})\cos(\phi(\mathbf{r}) - \omega\mathbf{t}),$$

for some **angular frequency** $\omega = 2\pi f > 0$, with f = **frequency**, the pressure is given by

$$U(\mathbf{r}, t) = \Re(u(\mathbf{r})e^{-i\omega t}), \tag{3.3}$$

where $u(\mathbf{r}) = A(\mathbf{r})e^{i\phi(r)}$ satisfies the **Helmholtz equation**

$$(\Delta + k^2)u = 0, \tag{3.4}$$

where $k = \omega/c = 2\pi/\lambda$ **is the wave number**, and λ is **the wavelength**. In the case when the domain is unbounded, the acoustic pressure u should satisfy the

Sommerfeld radiation conditions,

$$u = O(r^{-1/2}), \tag{3.5}$$

$$\left(\frac{\partial}{\partial r} - ik\right) u = o(r^{-1/2}), \tag{3.6}$$

as $r := |\mathbf{r}| = \sqrt{x^2 + y^2} \longrightarrow \infty$; r is the radial direction. A line source generates an acoustic pressure that depends on its location. When the line source is **along the z-axis**, the solution to equation (3.4) depends only on $\mathbf{r}$; at the receiver position $\mathbf{r} = (x, y)$ the solution is

$$u(\mathbf{r}) = \frac{-i}{4} H_0^{(1)}(kr), \tag{3.7}$$

where $H_0^{(1)}$ is the **Hankel function of the first kind of order zero**. To within multiplication by a constant, this is the unique solution to (3.4) in $\mathbb{R}^2 \setminus \{0\}$ that satisfies (3.5)-(3.6) and depends only on r. The constant $(-i/4)$ in (3.7) is chosen so that

$$\Delta u + k^2 u = \delta(x)\delta(y),$$

where δ is the one-dimensional Dirac delta function. When the line source is **parallel to the z-axis** through what we will refer to as the source position, $\mathbf{r_0} = (x_0, y_0)$, the solution to equation (3.4) is

$$u(\mathbf{r}) = G(\mathbf{r}, \mathbf{r_0}) := \frac{-i}{4} H_0^{(1)}(k|\mathbf{r} - \mathbf{r_0}|) = \frac{-i}{4} H_0^{(1)}(kR), \tag{3.8}$$

where $R = |\mathbf{r} - \mathbf{r_0}|$ is the distance from the source to the receiver. The function $G(\mathbf{r}, \mathbf{r_0})$ is **called the fundamental solution of equation (3.4)**. Denote the source point by $\mathbf{r_0} = (x_0, y_0)$, and the field point by $\mathbf{r} = (x, y)$. The Green's function G satisfies **the Helmholtz equation**

$$(\nabla^2 + k^2)G = \delta(X)\delta(Y) \tag{3.9}$$

where $X = x - x_0$, $Y = y - y_0$, so $R = \sqrt{X^2 + Y^2}$.

3.3 The free space quasi-periodic Green's function $G_\beta^d(X, Y)$ for the 2D Helmholtz equation

We turn now to the main topic of this chapter, the derivation and computation of representations for the two-dimensional quasi-periodic Green's function for the Helmholtz equation. This function $G_\beta^d(X, Y)$, defined for $k > 0$ and $\beta \in [-k, k]$, is the unique solution of the inhomogeneous Helmholtz equation

$$(\nabla^2 + k^2)G_\beta^d = \delta(X) \sum_{n=-\infty}^{\infty} \delta(Y - nd)e^{in\beta d} \tag{3.10}$$

that satisfies appropriate outgoing radiation conditions implying that (cf., (3.8) and [28]),

$$G_\beta^d(X, Y) = \frac{-i}{4} \sum_{m=-\infty}^{\infty} H_0^{(1)}(kr_m)e^{idm\beta}, \tag{3.11}$$

where $r_m = \sqrt{X^2 + (Y - md)^2}$. This representation for G_β^d is commonly known as **a spatial representation**.

To explain the physical meaning of this Green's function, let $\mathbf{r} = (x, y)$, and let $\mathbf{r_0} = (x_0, y_0)$ be an initial source position, and consider an infinite array of line sources in free space at the positions $\mathbf{r_n} = (x_n, y_n)$, for $n \in \mathbb{Z}$, where $x_n = x_0$, and $y_n = y_0 + nd$. Setting $X = x - x_0$, $Y = y - y_0$, $G_\beta^d(X, Y)$, given by (3.11), is the field at $\mathbf{r}$ due to an infinite array of sources at $\mathbf{r_n}$, $n \in \mathbb{Z}$, with a phase shift $e^{i\beta d}$ from one source to next. Note that (3.10) and (3.11) imply that $G_\beta^d(X, Y)$ is *quasi-periodic* as a function of d, meaning that

$$e^{-i\beta d}G_\beta^d(X, Y+d) = \frac{-i}{4} \sum_{n=-\infty}^{\infty} H_0^{(1)}(kr_{n-1})e^{i(n-1)\beta d} = \frac{-i}{4} \sum_{n=-\infty}^{\infty} H_0^{(1)}(kr_n)e^{in\beta d} = G_\beta^d(X, Y). \tag{3.12}$$

As we noted in §3.1, this Green's function arises in the integral equation formulation of two-dimensional problems of scattering by diffraction gratings, where a plane wave

$$u^i(\mathbf{r}) = e^{ik\mathbf{r}.\hat{d}}, \quad \mathbf{r} = (x, y) \in \mathbb{R}^2, \tag{3.13}$$

with $\hat{d} = (-\cos\theta, \sin\theta)$ and $\theta \in [-\pi/2, \pi/2]$, is incident on a diffraction grating, a surface S that is the graph of a function $\mathfrak{f}$, periodic with some period d, taking the form

$$S = \{(x, y) : y \in \mathbb{R}, x = \mathfrak{f}(y)\}.$$

In this application, as u^i is quasi-periodic with period d, i.e.

$$u^i(x, y + d) = e^{id\beta} u^i(x, y), \tag{3.14}$$

with

$$\beta = k \sin\theta \in [-k, k], \tag{3.15}$$

it is natural to look for a solution to the problem of scattering by the diffraction grating S that is also quasi-periodic with the same period d, i.e. that satisfies

$$u^s(x, y + d) = e^{id\beta} u^s(x, y), \tag{3.16}$$

where u^s is the field scattered by S. The quasi-periodicity (3.16) can be achieved by looking for the scattered field as the integral

$$u^s(\mathbf{r}) = \int_{S_1} G^d_\beta(x - x_0, y - y_0)\phi(\mathbf{r_0})ds(\mathbf{r_0}), \tag{3.17}$$

where $S_1 = \{(x, y) : 0 \le y \le d, x \in \mathfrak{f}(y)\}$ is a single period of S, $(x_0, y_0) = \mathbf{r_0}$, and $\phi \in C(S_1)$ is an unknown density that can be determined by enforcing the boundary conditions on S_1. E.g., in the case of a sound-soft surface S, $u^s = -u^i$ on S_1 so that

ϕ satisfies the boundary integral equation

$$\int_{S_1} G^d_\beta(x - x_0, y - y_0)\phi(\mathbf{r_0})ds(\mathbf{r_0}) = -u^i(\mathbf{r}), \quad \mathbf{r} \in S_1. \tag{3.18}$$

Note that the quasi-periodicity (3.12) of G^d_β ensures that u^s, given by (3.17), satisfies the quasi-periodicity (3.16).

The Green' function $G^d_\beta(X, Y)$ can also be expressed as an eigenfunction expansion, **the spectral representation** ([28] and [10]):

$$G^d_\beta(X, Y) = -\frac{1}{2d}\sum_{n=-\infty}^{\infty}\frac{e^{-\gamma_n|X|}e^{i\beta_n Y}}{\gamma_n}, \tag{3.19}$$

where $\beta_n := \beta + n2\pi/d$,

$$\gamma_n := \begin{cases} \sqrt{\beta_n^2 - k^2}, \text{ if } & |\beta_n| > k \\ -i\sqrt{k^2 - \beta_n^2}, \text{ if } & |\beta_n| \leq k. \end{cases} \tag{3.20}$$

As is well known, the expressions for the quasi-periodic Green's function which are given in (3.11) and (3.19) converge extremely slowly, and many analytical methods have therefore been developed to produce fast convergent periodic Green-function formulas, including Kummer's transformation (see [28], [35], [40], [41]), Ewald's method (see [28], [12], [5], [13], [40], [24], [33]), lattice sum methods [28], and [33], the fast Fourier transformation method [43], and integral representations (see [28], [24]). Singh in [36] evaluated the 2D periodic Green's function efficiently using the ρ-Algorithm, and the results are shown to speed up the convergence of the free space periodic Green's function in both spatial and spectral domains. Yasumoto and Yoshitomi in [42] have shown that the lattice sums for the free-space periodic Green's function can be evaluated by an efficient method based on recurrence relations for Hankel functions and a Fourier integral representation, leading to a highly accurate evaluation of the periodic Green's function without costing more time in computation.

In the 1998 review paper by Linton [28], a number of analytical methods are employed to derive suitable expressions for computation of the 2D periodic Green's function. One of the techniques given in this paper that seems well-suited for efficient computation is the integral representation. The integral representation method was originally presented in [31] for converting the infinite sum in a spatial representation of the Green's function to an improper integral. Twelve years later, Linton has shown an alternative integral representation for the 2D quasi-periodic Green's function with 1D periodicity and he has highlighted that "[while the] integral representations [(2.14) and (2.15), in [29]] can be used for the accurate and efficient computation of [the Green's function], the numerical implementation needs care due to the singular and/or oscillatory integrals" [29, p 10].

Both the spatial and spectral representations, (3.11) and (3.19) above are slowly convergent sums. Next, we will compute these representations in Python with the same sets of parameters values, taken from [28]. Also we will present an integral representation for the quasi-periodic Green's function.

3.3.1 Spatial representation

This is (see (3.11))

$$G_{\beta}^{d}(X,Y) = \frac{-i}{4}\sum_{n=-\infty}^{\infty} H_0^{(1)}(kr_n)e^{in\beta d}, \tag{3.21}$$

where $r_n = \sqrt{(X^2 + (Y - nd)^2}$. This formula is known to converge very slowly, requiring a partial sum with many terms to obtain acceptable accuracy [9]. We code up the function (3.21) (see Appendix A.1) using Python to study the behaviour of the partial sum

$$b_N = \frac{-i}{4}\sum_{n=-N}^{N} H_0^{(1)}(kr_n)e^{in\beta d}, \tag{3.22}$$

as N takes larger and larger values. The results are shown below in Table 3.1 for specific parameter values ($X = 0, Y = 0.04, \beta = \sqrt{2}/4,\ k = 0.5, d = 4$), taken from [Table 2, [28]].

N	Green's function values
5000	**-0.4634247357 - 0.3530848710** i

Table 3.1: Computing (3.21) with $N = 5000$.

Table 3.1 shows the Green's function calculation with $N = 5000$; the value of the quasi-periodic Green's function agrees with the value given in (Table 2, [28], p.397), also with $N = 5000$, to 10 significant figures.

3.3.2 Spectral representation

This is (see (3.19))

$$G_\beta^d(X,Y) = -\frac{1}{2d}\sum_{n=-\infty}^{\infty}\frac{e^{-\gamma_n|X|}e^{i\beta_n Y}}{\gamma_n} \tag{3.23}$$

$$\approx -\frac{1}{2d}\sum_{n=-N}^{N}\frac{e^{-\gamma_n|X|}e^{i\beta_n Y}}{\gamma_n}$$

where we have written, for $n \in \mathbb{Z}$,

$$\beta_n := \beta + n2\pi/d, \quad \gamma_n := \begin{cases} \sqrt{\beta_n^2 - k^2}, & \text{if} \quad |\beta_n| > k, \\ -i\sqrt{k^2 - \beta_n^2}, & \text{if} \quad |\beta_n| \le k. \end{cases} \tag{3.24}$$

The spectral form (3.23) has fast convergence when $|\beta_n| > k$, unless $|X|$ is small, due to the exponentially decaying term $e^{-\gamma_n|X|}$. If $|\beta_n| \le k$, then $\gamma_n = -i\sqrt{k^2 - \beta_n^2}$, and so the term $|e^{-\gamma_n|X|}| = |e^{i|X|\sqrt{k^2-\beta_n^2}}| = 1$ (see [9], [28]).

N	values of G_β^d
5000	**-0.4595441802 - 0.3509133120i**

Table 3.2: Computing (3.23) at $N = 5000$.

We code up (3.23) (see Appendix A.2) with the same values as in (Table 2, [28], p.397), and we obtain the same result, $G_\beta^d = \mathbf{-0.4595441802 - 0.3509133120i}$ with $N = 5000$, as in (Table 2, [28], method 2).

3.3.3 An integral representation of the form (1.1) for the 2D periodic Green's function

In [28], Linton transforms the Green's function spatial representation into a form more appropriate for computation. He obtains

$$\sum_{n=1}^{\infty} H_0^{(1)}(kr_n)e^{in\beta d} = -\frac{2ie^{-ikY}}{\pi}\int_0^\infty \frac{e^{k(Y-d)u}\cos[kX(u^2-2iu)^{1/2}]}{(e^{-i(\beta+k)d}-e^{-kdu})(u^2-2iu)^{1/2}}du, \quad (3.25)$$

by use of the Hankel function representation (3.99) and summing a geometric progression. (For more detail see §3.5.3.) It follows from (3.17) and (3.25) that the 2D periodic Green's function has an integral representation as (Eq. (2.37), [28])

$$\begin{aligned} G_\beta^d(X,Y) = \frac{-i}{4}H_0^{(1)}(kr) &- \frac{e^{-ikY}}{2\pi}\int_0^\infty \frac{e^{k(Y-d)u}\cos[kX(u^2-2iu)^{1/2}]}{(e^{-i(\beta+k)d}-e^{-kdu})(u^2-2iu)^{1/2}}du \\ &- \frac{e^{ikY}}{2\pi}\int_0^\infty \frac{e^{-k(Y+d)u}\cos[kX(u^2-2iu)^{1/2}]}{(e^{i(\beta-k)d}-e^{-kdu})(u^2-2iu)^{1/2}}du. \end{aligned} \quad (3.26)$$

To convert the integrals in (3.26) into the form

$$I = \int_{-\infty}^{\infty} e^{-\rho v^2}F(v)dv, \quad (3.27)$$

we first substitute $u = v^2$ into (3.26) to get, for $-d \le Y \le d$,

$$\begin{aligned} G_\beta^d(X,Y) = \frac{-i}{4}H_0^{(1)}(kr) &- \frac{e^{-ikY}}{\pi}\int_0^\infty \frac{e^{k(Y-d)v^2}\cos[kXv(v^2-2i)^{1/2}]}{(e^{-i(\beta+k)d}-e^{-kdv^2})(v^2-2i)^{1/2}}dv \\ &- \frac{e^{ikY}}{\pi}\int_0^\infty \frac{e^{-k(Y+d)v^2}\cos[kXv(v^2-2i)^{1/2}]}{(e^{i(\beta-k)d}-e^{-kdv^2})(v^2-2i)^{1/2}}dv. \end{aligned} \quad (3.28)$$

We also substitute $u = v^2$ into (3.25) to obtain

$$\sum_{n=1}^{\infty} H_0^{(1)}(kr_n)e^{in\beta d} = -\frac{4ie^{-ikY}}{\pi}\int_0^{\infty} \frac{e^{k(Y-d)v^2}\cos[kX(v^2-2i)^{1/2}]}{(e^{-i(\beta+k)d}-e^{-kdv^2})(v^2-2i)^{1/2}}dv. \tag{3.29}$$

It follows from (3.28) that

$$G_\beta^d(X,Y) = \frac{-i}{4}H_0^{(1)}(kr) - \frac{e^{-ikY}}{2\pi}\int_{-\infty}^{\infty} e^{-\rho_- v^2}F_-(v)dv - \frac{e^{ikY}}{2\pi}\int_{-\infty}^{\infty} e^{-\rho_+ v^2}F_+(v)dv, \tag{3.30}$$

i.e.,

$$G_\beta^d(X,Y) = \frac{-i}{4}H_0^{(1)}(kr) - \frac{e^{-ikY}}{2\pi}I^- - \frac{e^{ikY}}{2\pi}I^+, \tag{3.31}$$

where

$$I^{\pm} := \int_{-\infty}^{\infty} e^{-\rho_\pm v^2}F_\pm(v)dv, \tag{3.32}$$

with $\rho_- = k(d-Y) \geq 0$ in the first integral and $\rho_+ = k(d+Y) \geq 0$ in the second integral, and with $F_\pm(v)$ given by

$$F_-(v) := \frac{\cos[kXv(v^2-2i)^{1/2}]}{(e^{-i(\beta+k)d}-e^{-kdv^2})(v^2-2i)^{1/2}}, \quad -\frac{\pi}{2} < \arg(\sqrt{v^2-2i}) \leq \frac{\pi}{2} \tag{3.33}$$

and

$$F_+(v) := \frac{\cos[kXv(v^2-2i)^{1/2}]}{(e^{i(\beta-k)d}-e^{-kdv^2})(v^2-2i)^{1/2}}, \quad -\frac{\pi}{2} < \arg(\sqrt{v^2-2i}) \leq \frac{\pi}{2}. \tag{3.34}$$

Let us examine the analyticity of the functions $F_\pm(v)$, starting with function $F_-(v)$. Clearly,

$$F_-(v) = \frac{f_3(v)}{f_2(v)f_1(v)},$$

where

$$f_1(v) = \sqrt{v^2-2i},$$

$$f_2(v) = e^{-i(\beta+k)d} - e^{-kdv^2},$$

$$f_3(v) = \cos(kXv\sqrt{v^2 - 2i}).$$

Now $f_1(v) = \sqrt{v^2 - 2i}$ is a multiple-valued function with two branches. Each branch is a single-valued function. Precisely, defining the function f_1 by $f_1(v) := \sqrt{v-(1+i)}\sqrt{v+(1+i)}$, where $\mathrm{Re}(\sqrt{v \pm (1+i)}) \geq 0$, so that $\mathrm{Re}(\sqrt{v^2 - 2i}) > 0$, for $v \in \mathbb{R}$, f_1 has branch points at $\pm(1+i)$, and branch cuts as in Figure 3.1. It is obvious from Figure 3.1 that, for $H \in (0, 1)$, f_1 is analytic in the domain

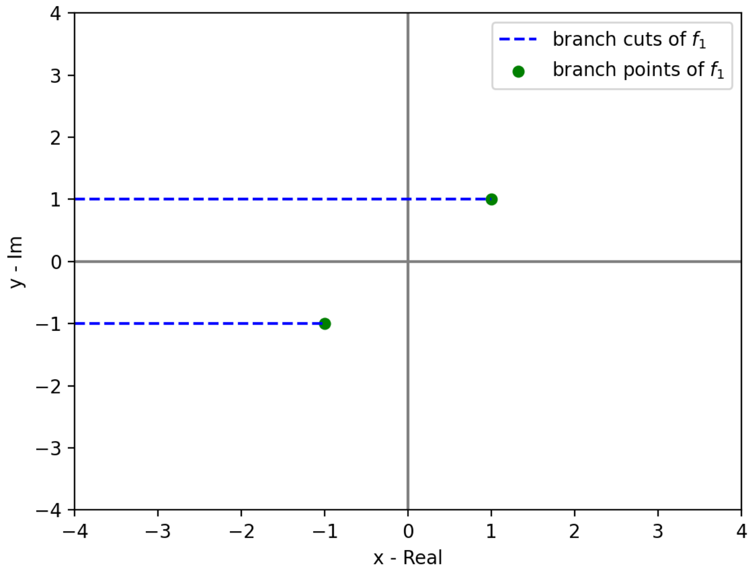

Figure 3.1: Corresponding branch cuts of $\sqrt{v^2 - 2i}$.

$S_H = \{v \in \mathbb{C} : \quad |\mathrm{Im}(v)| < H\}$. The function $f_2(v) = e^{-i(\beta+k)d} - e^{-kdv^2}$ is an entire function and

$$e^{-i(\beta+k)d} - e^{-kdv^2} = 0$$

$$\iff e^{-i(\beta+k)d} = e^{-kdv^2}.$$

This holds if and only if, for some $n \in \mathbb{Z}$,

$$-i(\beta + k)d + 2in\pi = -kdv^2$$

$$\iff v^2 = \frac{i(\beta + k)d - 2in\pi}{kd}$$

$$\iff v = \pm\sqrt{\frac{i(\beta+k)d - 2in\pi}{kd}}$$

$$\iff v = \pm\sqrt{iw_n^-}$$

$$\iff v = v_{\pm,n}^- := \pm e^{i\pi/4}\sqrt{w_n^-}, \tag{3.35}$$

where $\sqrt{w_n^-}$ denotes the principal square root and

$$w_n^- := \frac{(\beta+k)d - 2n\pi}{kd}, \quad \text{for} \quad n \in \mathbb{Z}. \tag{3.36}$$

From the definition of the principal square root, $\sqrt{w_n^-} \geq 0$ if $w_n^- \geq 0$, $\sqrt{w_n^-} = i\sqrt{-w_n^-}$ with $\sqrt{-w_n^-} \geq 0$ if $w_n^- < 0$. The function $f_3(v) = \cos(kXv\sqrt{v^2-2i})$ is an entire function because it has a convergent series everywhere, precisely

$$f_3(v) = \sum_{n=0}^{\infty} \frac{(-1)^n (kXv)^{2n}(v^2-2i)^n}{(2n)!}$$

and, using the ratio test,

$$\lim_{n\to\infty}\left|\frac{(-1)^{n+1}}{(2n+2)!}\frac{(2n)!}{(-1)^n}\right|$$

$$= \lim_{n\to\infty}\left(\frac{1}{(2n+2)(2n+1)}\right) = 0,$$

so that the series is absolutely convergent for all $v \in \mathbb{C}$. Thus, provided $(\beta+k)d \notin 2\pi\mathbb{Z}$, so there are no poles on the real line, then Assumption 2.1 is satisfied by $F_-(v)$, provided also $H \in (0,1)$ is chosen, so that $\Im(v_{+,n}^-) \neq H$, for $n \in \mathbb{Z}$.

Similarly, the function $F_+(v) = \frac{f_3(v)}{f_2(v)f_1(v)}$, with $f_1(v)$ and $f_3(v)$ as defined above and with $f_2(v) := e^{i(\beta-k)d} - e^{-kdv^2}$ so that $f_2(v) = 0$, if and only if

$$v_{\pm,n}^+ := \pm e^{i\pi/4}\sqrt{w_n^+}, \tag{3.37}$$

for some $n \in \mathbb{Z}$, where

$$w_n^+ := \frac{-(\beta - k)d - 2n\pi}{kd}, \quad \text{for} \quad n \in \mathbb{Z}. \tag{3.38}$$

We are concerned with approximating the integrals I^- and I^+ by using the truncated midpoint rule and modification of this rule discussed in Chapter 2. But, before applying the proposed numerical methods, we first find the closest poles of $F_\pm(v)$ to the origin and then calculate the residues of $F_\pm(v)$ at these poles.

3.3.3.1 The closest simple poles of $F_\pm(v)$ to the origin

Now $w_n^- := 1 + \frac{\beta}{k} - \frac{2\pi n}{kd}$, and since $\sqrt{i} = \pm(\frac{1}{\sqrt{2}} + i\frac{1}{\sqrt{2}}) = \pm e^{i\pi/4}$,

$$v_{\pm,n}^- := \pm e^{i\pi/4}\sqrt{w_n^-}, \quad \text{with} \quad 0 \le \arg\sqrt{w_n^-} \le \pi/2. \tag{3.39}$$

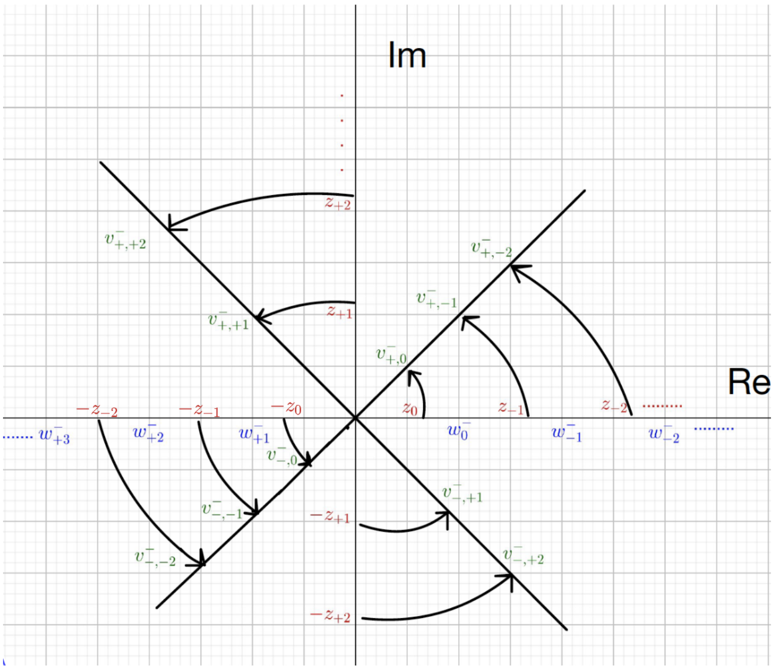

Figure 3.2: The position of $v_{\pm,n}^-$ in the complex plane where $w_n^- := 1 + \frac{\beta}{k} - \frac{2\pi n}{kd}$, $z_n := \sqrt{w_n^-}$, in the case when m, given by (3.44), has the value $m = 0$.

Clearly, given $H \in (0, 1)$, the poles $v_{\pm,n}^-$ lie in S_H if and only if $|\mathrm{Im}(v_{\mp,n}^-)| < H$.

Further

$$|v^-_{\pm,n}| = \sqrt{|w^-_n|}$$

and

$$\begin{aligned} |\mathrm{Im}(v^-_{\pm,n})| &= \frac{1}{\sqrt{2}}|v^-_{\pm,n}| \\ &= \frac{1}{\sqrt{2}}\sqrt{|w^-_n|}. \end{aligned} \tag{3.40}$$

As is illustrated in Figure 3.2, it follows from $w^-_n := 1 + \frac{\beta}{k} - \frac{2\pi n}{kd}$, with $-\pi/2 < \arg\sqrt{w^-_n} \leq \pi/2$, and from the definition of $v^-_{\pm,n}$ in (3.39), that $F_-(v)$ has infinitely many poles. Let us denote by P^- the set of all these poles so,

$$\begin{aligned} P^- : &= \{v^-_{-,n} : n \in \mathbb{Z}\} \cup \{v^-_{+,n} : n \in \mathbb{Z}\} \\ &= \{e^{i\pi/4}\sqrt{w^-_n} : n \in \mathbb{Z}\} \cup \{-e^{i\pi/4}\sqrt{w^-_n} : n \in \mathbb{Z}\}. \end{aligned} \tag{3.41}$$

For $H \in (0, 1]$, let P^-_H denote the set of poles in P^- which have imaginary part with modulus less than H, i.e,

$$P^-_H := \{v^-_{\pm,n} \in P^- : |\mathrm{Im}(v^-_{\pm,n})| < H\}. \tag{3.42}$$

From the definitions $w^-_n := 1 + \frac{\beta}{k} - \frac{2\pi n}{kd}$ and $\beta := k \sin\theta \in [-k, k]$, it is clear that

$$w^-_0 = 1 + \frac{\beta}{k},$$

$$= 1 + \sin\theta \in [0, 2].$$

Further, for general $n \in \mathbb{Z}$,

$$w^-_n = 1 + \frac{\beta}{k} - \frac{2\pi n}{kd} \geq 0$$

$$\iff n \leq \frac{kd}{2\pi}(1 + \sin\theta). \tag{3.43}$$

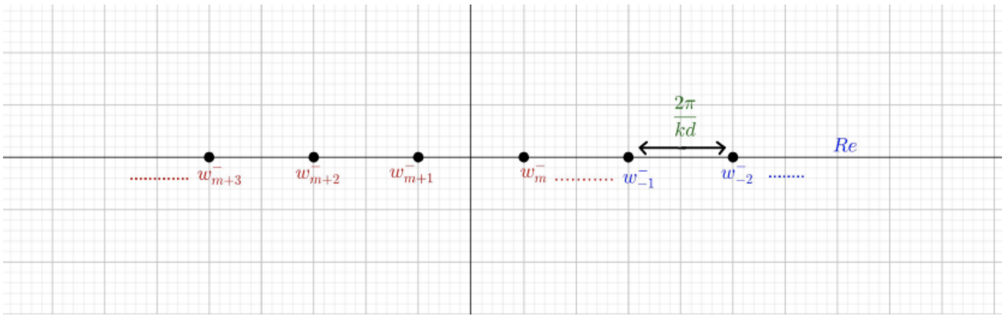

Figure 3.3: The position of the values of w_n^-, for $n \in \mathbb{Z}$; m is given by (3.44)

From Figure 3.3 (or the definition of w_n^-) we see that the distance between w_n^- and w_{n+1}^- is $2\pi/kd$. Let $m \in \mathbb{Z}$ be such that $|w_m^-|$ and $|w_{m+1}^-|$ are the two smallest values of $|w_n^-|$. In other words, $m \in \mathbb{Z}$ is the largest integer such that $w_m^- \geq 0$, so that, by (3.43),

$$m := \left\lfloor \frac{kd}{2\pi}(1+\sin\theta) \right\rfloor. \tag{3.44}$$

(Note that, for $x \in \mathbb{R}$, we denote by $\lfloor x \rfloor$ the largest integer $\leq x$). Thus, the closest poles to the real axis are $v_{\pm,m}^-$ and $v_{\pm,m+1}^-$, with m given by (3.44), which correspond to the smallest values of $|w_n^-|$ and also, by (3.40), correspond to the smallest values of $|\mathrm{Im}(v_{\pm,n}^-)|$; let's denote these poles by

$$s_0 := v_{+,m}^- \quad s_1 := v_{+,m+1}^- \quad s_2 := -s_0 = v_{-,m}^- \quad s_3 := -s_1 = v_{-,m+1}^-. \tag{3.45}$$

As an example, in Python, we work out (3.44) for the case $k = 0.5$, $\beta = 0.353$, $d = 4$, $X = 0$ and $Y = 0.04$, for which 3.44 gives $m = 0$ and, from Figure 3.4 (cf. Figure 3.2 and Figure 3.5), $w_m = w_0 \approx 1.706$ and $w_{m+1} = w_1 \approx -1.44$.

In like manner, defining $w_n^+ := 1 - \frac{\beta}{k} - \frac{2\pi n}{kd}$,

$$v_{\pm,n}^+ := \pm e^{i\pi/4}\sqrt{w_n^+}, \quad 0 \leq \arg\sqrt{w_n^+} \leq \pi/2, \tag{3.46}$$

the set of poles of $F_+(v)$ is

$$P^+ := \{v_{\pm,n}^+ : n \in \mathbb{Z}\} = \{\pm e^{i\pi/4}\sqrt{w_n^+} : n \in \mathbb{Z}\}, \tag{3.47}$$

```
from math import floor
from numpy.lib.scimath import *
d=4; k=0.5; beta= 0.353; Y=0.04; X=0
theta=pi/4
a=1+(beta/k)
m=floor(k*d*a/(2*pi))
print('m=',m)
print('m+1=', m+1)
n=m
w1=a-2*pi*n/(k*d)
print('w1=',w1)
vm=exp(1j*pi/4)*sqrt(w1)
print('v_m=',vm)
n=m+1
w2=a-2*pi*n/(k*d)
print('w2=',w2)
vm1=exp(1j*pi/4)*sqrt(w2)
print('v_{m+1}=', vm1)
```

```
m= 0
m+1= 1
w1= 1.706
v_m= (0.9235799911215055+0.9235799911215054j)
w2= -1.4355926535897932
v_{m+1}= (-0.847228615424961+0.8472286154249612j)
```

Figure 3.4: Computing w_m^-, w_{m+1}^- and v_m^-, v_{m+1}^-.

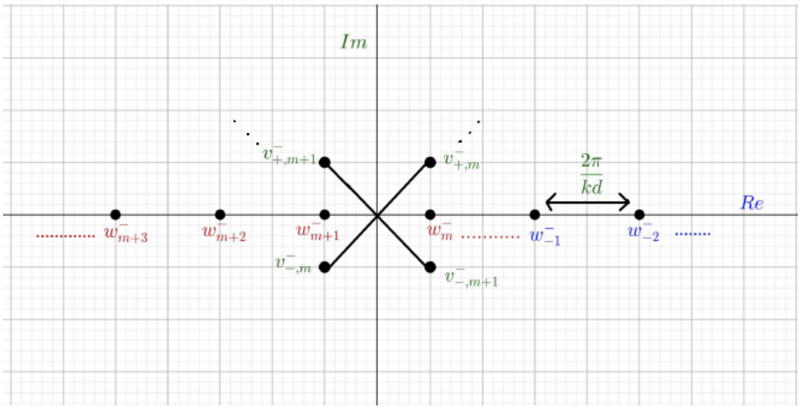

Figure 3.5: The positions of $v_{\pm,m}^-$ and $v_{\pm,m+1}^-$.

and the set of poles which have imaginary part with modulus less than H is

$$P_H^+ := \{v_{\pm,n}^+ : |\mathrm{Im}(v_{\pm,n}^+)| < H\}. \tag{3.48}$$

Similarly to (3.45), the poles closest to the real line are

$$s_0^+ := v_{+,m}^+, \quad s_1^+ := v_{+,m+1}^+, \quad s_2^+ := -s_0^+, \quad \text{and} \quad s_3^+ := -s_1^+, \tag{3.49}$$

where

$$m := \left\lfloor \frac{kd}{2\pi}(1 - \sin\theta) \right\rfloor. \tag{3.50}$$

3.3.3.2 Residues of $F_{\pm}(v)$ at the poles $v^-_{\pm,n}$ and $v^+_{\pm,n}$

Let $R^-_{\pm,n}$ denote the residue of f_- at $v^-_{\pm,n}$, where

$$f_-(v) := e^{-\rho_- v^2} F_-(v) \tag{3.51}$$

is meromorphic for $|\text{Im}(v)| < 1$ with poles at $v^-_{\pm,n}$, $n \in \mathbb{Z}$, i.e. at $v \in P^-$. Provided $|\text{Im}(v^-_{\pm,n})| \neq 0$, i.e. $v^-_{\pm,n} \neq 0$, the pole at $v^-_{\pm,n}$ is simple. The function F_- is of form p/q where q has zeros at $v^-_{\pm,n}$, and also $p(v^-_{\pm,n}) \neq 0$ and $q'(v^-_{\pm,n}) \neq 0$, provided $v^-_{\pm,n} \neq 0$. Thus we can use the formula

$$R^-_{\pm,n} = \text{Res}(f_-, v^-_{\pm,n}) = \frac{p(v^-_{\pm,n}) e^{-\rho_-(v^-_{\pm,n})^2}}{q'(v^-_{\pm,n})}, \tag{3.52}$$

where $p(v^-_{\pm,n}) = ((v^-_{\pm,n})^2 - 2i))^{-1/2} \cos(kXv^-_{\pm,n}\sqrt{(v^-_{\pm,n})^2 - 2i})$ and $q'(v^-_{\pm,n}) = 2kdv^-_{\pm,n} e^{-kd(v^-_{\pm,n})^2}$ so we have

$$R^-_{\pm,n} = \pm \frac{(i(w^-_n - 2))^{-1/2} \cos(kX\sqrt{iw^-_n}\sqrt{i(w^-_n - 2)}) e^{-i\rho_- w^-_n}}{2kde^{i\pi/4}\sqrt{w^-_n} e^{-ikdw^-_n}}. \tag{3.53}$$

Similarly, where $f_+(v) := e^{-\rho_+(v)^2} F_+(v)$, for $R^+_{\pm,n} = \text{Res}(f_+, v^+_{\pm,n})$ we get

$$R^+_{\pm,n} = \pm \frac{(i(w^+_n - 2))^{-1/2} \cos(kX\sqrt{iw^+_n}\sqrt{i(w^+_n - 2)}) e^{-i\rho_+ w^+_n}}{2kde^{i\pi/4}\sqrt{w^+_n} e^{-ikdw^+_n}}. \tag{3.54}$$

So the functions f_- and f_+ have residues $R^-_{\pm,n}$ and $R^+_{\pm,n}$ at $v^-_{\pm,n}$ and $v^+_{\pm,n}$, for each n. Since F_- and F_+ are even, then $R^-_{+,n} = -R^-_{-,n}$, $s_2 = -s_0$ and $s_3 = -s_1$, and $R^+_{+,n} = -R^+_{-,n}$, and $s^+_2 = -s^+_0$ and $s^+_3 = -s^+_1$.

3.3.3.3 The correction factors

Now we derive the formulas for the correction factors which arise from the residues of $F_{\pm}(v)$ of its poles. The correction factor C_F, given by (2.31), for $F = F_-$ is

$$C_{F_-} = G_F^- := i\pi \sum_{v^- \in P_H^-} (\text{sgn}(\text{Im}v^-) - g(v^-))R_{+,n}^- \tag{3.55}$$

where $R_{+,n}^- = \text{Res}(f_-, v_{+,n}^-)$ is given by (3.52) and (3.53). The correction factor for $F = F_+$ is

$$C_{F_+} = G_F^+ := i\pi \sum_{v^+ \in P_H^+} (\text{sgn}(\text{Im}v^+) - g(v^+))R_{+,n}^+, \tag{3.56}$$

where $R_{+,n}^+ = \text{Res}(f_+, v_{+,n}^+)$ is given by (3.54).Thus the modified truncated midpoint approximations to I^- and I^+ are

$$I_{h,N}^{*,-} = h \sum_{j=-N}^{N+1} e^{-\rho_-(j-1/2)^2h^2} F_-((j-1/2)h) + G_F^- \tag{3.57}$$

and

$$I_{h,N}^{*,+} = h \sum_{j=-N}^{N+1} e^{-\rho_+(j-1/2)^2h^2} F_+((j-1/2)h) + G_F^+. \tag{3.58}$$

Now, let us choose $H \in (0,1)$ so that only the closest poles to the real line are included in the correction factor. Recall that s_0, s_2, s_1, and s_3 are the nearest poles to the origin, let $G_{F_{m,m+1}}^-$ denote the total of the sum (3.55) for the two pairs of poles s_0, s_1, s_2, s_3, and let $G_{F_m}^-$ and $G_{F_{m+1}}^-$ denote the contributions from the pairs s_0, s_2 and s_1, s_3, respectively, so that

$$G_{F_{m,m+1}}^- = G_{F_m}^- + G_{F_{m+1}}^-. \tag{3.59}$$

By using the facts that $s_2 = -s_0$, $s_3 = -s_1$, $R^-_{+,m} = -R^-_{-,m}$, and $R^-_{+,m+1} = -R^-_{-,m+1}$,

$$\begin{aligned} G^-_{F_m} &= i\pi R^-_m(\text{sgn}(\text{Im}(s_0)) - g(s_0)) - i\pi R^-_m(-\text{sgn}(\text{Im}(s_0)) - g(-s_0)) \\ &= i\pi R^-_m(\text{sgn}(\text{Im}(s_0)) - g(s_0)) - i\pi R^-_m(-\text{sgn}(\text{Im}(s_0)) + g(s_0)) \\ &= 2\pi i R^-_m(\text{sgn}(\text{Im}(s_0)) - g(s_0)) \end{aligned}$$

i.e.

$$G^-_{F_m} = 2\pi i R^-_m(\text{sgn}(\text{Im}s_0) - i\text{cot}(\pi s_0/h + \pi/2)). \tag{3.60}$$

Similarly,

$$G^-_{F_{m+1}} = 2\pi i R^-_{m+1}(\text{sgn}(\text{Im}s_1) - i\cot(\pi s_1/h + \pi/2)). \tag{3.61}$$

Since $\text{Im}(s_0) > 0$ and $\text{Im}(s_1) > 0$, these simplify to

$$G^-_{F_m} = 2\pi i R^-_m(1 - i\cot(\pi s_0/h + \frac{\pi}{2})), \tag{3.62}$$

$$G^-_{F_{m+1}} = 2\pi i R^-_m(1 - i\cot(\pi s_1/h + \frac{\pi}{2})). \tag{3.63}$$

Now, we derive a formula for $G^-_{F_m}$ that is well suited to numerical calculation, but before that, it is necessary to find the residue of f_- at the poles s_0 and s_1, since $R^-_{+,m} = -R^-_{-,m}$ and, by (3.53),

$$R^-_{+,m} = \frac{(i(w^-_m - 2))^{-1/2}\cos(kX\sqrt{iw^-_m}\sqrt{i(w^-_m - 2)})e^{-i\rho_- w^-_m}}{2kde^{i\pi/4}\sqrt{w^-_m}e^{-ikdw^-_m}} \tag{3.64}$$

and

$$R^-_{+,m+1} = \frac{(i(w^-_{m+1} - 2))^{-1/2}\cos(kX\sqrt{iw^-_{m+1}}\sqrt{i(w^-_{m+1} - 2)})e^{-i\rho_- w^-_{m+1}}}{2kde^{i\pi/4}\sqrt{w^-_{m+1}}e^{-ikdw^-_{m+1}}}. \tag{3.65}$$

It is convenient to use the formula that

$$i\cot(\pi(s_0/h+1/2)) = \frac{1+e^{2i\pi(s_0/h+1/2)}}{1-e^{2i\pi(s_0/h+1/2)}}$$

which implies that

$$1-i\cot(\pi(s_0/h+1/2)) \equiv \frac{-2e^{2i\pi(s_0/h+1/2)}}{1-e^{2i\pi(s_0/h+1/2)}}. \tag{3.66}$$

so (3.60) may be written as

$$G^-_{F_m} = 2\pi i R^-_{+,m}\frac{-2e^{2i\pi(s_0/h+1/2)}}{1-e^{2i\pi(s_0/h+1/2)}}. \tag{3.67}$$

Thus

$$G^-_{F_m} = -\pi i\frac{e^{-i\rho_- w^-_m}(i(w^-_m-2))^{-1/2}\cos(kX\sqrt{iw^-_m}\sqrt{i(w^-_m-2)})}{kde^{i\pi/4}\sqrt{w^-_m}e^{-ikdw^-_m}}\frac{2e^{2i\pi(s_0/h+1/2)}}{1-e^{2i\pi(s_0/h+1/2)}}, \tag{3.68}$$

and similarly

$$G^-_{F_{m+1}} = -\pi i\frac{e^{-i\rho_- w^-_{m+1}}(i(w^-_{m+1}-2))^{-1/2}\cos(kX\sqrt{iw^-_{m+1}}\sqrt{i(w^-_{m+1}-2)})}{kde^{i\pi/4}\sqrt{w^-_{m+1}}e^{-ikdw^-_{m+1}}}\cdot\frac{2e^{2i\pi(s_1/h+1/2)}}{1-e^{2i\pi(s_1/h+1/2)}}. \tag{3.69}$$

Combining (3.68) and (3.69), we obtain that

$$\begin{aligned} G^-_{F_{m,m+1}} = \frac{-2\pi i}{kde^{i\pi/4}}&\left(\frac{e^{-i\rho_- w^-_m}(i(w^-_m-2))^{-1/2}\cos(kX\sqrt{iw^-_m}\sqrt{i(w^-_m-2)})}{e^{-ikdw^-_m}\sqrt{w^-_m}}\frac{e^{2i(\pi s_0/h+\frac{\pi}{2})}}{1-e^{2i(\pi s_0/h+\frac{\pi}{2})}}\right.\\ &+\left.\frac{e^{-i\rho_- w^-_{m+1}}(i(w^-_{m+1}-2))^{-1/2}\cos(kX\sqrt{iw^-_{m+1}}\sqrt{i(w^-_{m+1}-2)})}{e^{-ikdw^-_{m+1}}\sqrt{w^-_{m+1}}}\frac{e^{2i(\pi s_1/h+\frac{\pi}{2})}}{1-e^{2i(\pi s_1/h+\frac{\pi}{2})}}\right). \end{aligned} \tag{3.70}$$

Similarly,

$$G^+_{F_{m,m+1}} = \frac{-2\pi i}{kde^{i\pi/4}} \left(\frac{e^{-i\rho_+ w^+_m}(i(w^+_m - 2))^{-1/2} \cos(kX\sqrt{iw^+_m}\sqrt{i(w^+_m - 2)})}{e^{-ikdw^+_m}\sqrt{w^+_m}} \frac{e^{2i(\pi s^+_0/h + \pi/2)}}{1 - e^{2i(\pi s^+_0/h+\pi/2)}} \right.$$
$$\left. + \frac{e^{-i\rho_+ w^+_{m+1}}(i(w^+_{m+1} - 2))^{-1/2} \cos(kX\sqrt{iw^+_{m+1}}\sqrt{i(w^+_{m+1} - 2)})}{e^{-ikdw^+_{m+1}}\sqrt{w^+_{m+1}}} \frac{e^{2i(\pi s^+_1/h + \pi/2)}}{1 - e^{2i(\pi s^+_1/h+\pi/2)}} \right). \tag{3.71}$$

Let us relate (3.70) and (3.71) to the general formulas (3.55) and (3.56). Suppose that $s_0, s_1, s_2, s_3 \in S_1$ and $H \in (0,1)$ is chosen so that

$$P^-_H = \{s_0, s_1, s_2, s_3\}$$

in which case (since $s_2 = -s_0$ and $s_3 = -s_1$)

$$P^-_H = \{s_0, s_1, -s_0, -s_1\}.$$

Then $G^-_F = G^-_{F_{m,m+1}}$. Similarly, if $s^+_0, s^+_1, s^+_2, s^+_3 \in S_1$ then $G^+_F = G^+_{F_{m,m+1}}$ if $H \in (0,1)$ is chosen so that

$$P^+_H = \{s^+_0, s^+_1, s^+_2, s^+_3\} = \{s^+_0, s^+_1, -s^+_0, -s^+_1\}.$$

But it may or may not be the case that s_0, s_1, s^+_0, s^+_1 are contained in S_1. To ensure that contributions from these poles are included in the correction factors only when these poles lie in S_1 we modify the above formulas. Let $\mathbf{H}$ denote the Heaviside step function defined by

$$\mathbf{H}(t) := \begin{cases} 1, \text{ if } & t \geq 0 \\ 0, \text{ if } & t < 0. \end{cases} \tag{3.72}$$

Then we modify (3.70) and (3.71) to

$$G^-_{F_{m,m+1}} = A_- \left(\frac{\mathbf{H}(1-|\mathrm{Im} v^-_{+,m}|)e^{-i\rho_- w^-_m}(i(w^-_m-2))^{-1/2}\cos(kX\sqrt{iw^-_m}\sqrt{i(w^-_m-2)})}{e^{-ikdw^-_m}\sqrt{w^-_m}} \frac{e^{2i(\pi s_0/h+\frac{\pi}{2})}}{1-e^{2i(\pi s_0/h+\frac{\pi}{2})}} \right.$$
$$+ \frac{\mathbf{H}(1-|\mathrm{Im} v^-_{+,m+1}|)e^{-i\rho_- w^-_{m+1}}(i(w^-_{m+1}-2))^{-1/2}\cos(kX\sqrt{iw^-_{m+1}}\sqrt{i(w^-_{m+1}-2)})}{e^{-ikdw^-_{m+1}}\sqrt{w^-_{m+1}}}$$
$$\left. \frac{e^{2i(\pi s_1/h+\frac{\pi}{2})}}{1-e^{2i(\pi s_1/h+\frac{\pi}{2})}} \right). \tag{3.73}$$

and

$$G^+_{F_{m,m+1}} = A_+ \left(\frac{\mathbf{H}(1-|\mathrm{Im} v^+_{+,m}|)e^{-i\rho_+ w^+_m}(i(w^+_m-2))^{-1/2}\cos(kX\sqrt{iw^+_m}\sqrt{i(w^+_m-2)})}{e^{-ikdw^+_m}\sqrt{w^+_m}} \frac{e^{2i(\pi s^+_0/h+\pi/2)}}{1-e^{2i(\pi s^+_0/h+\pi/2)}} \right.$$
$$+ \frac{\mathbf{H}(1-|\mathrm{Im} v^+_{+,m+1}|)e^{-i\rho_+ w^+_{m+1}}(i(w^+_{m+1}-2))^{-1/2}\cos(kX\sqrt{iw^+_{m+1}}\sqrt{i(w^+_{m+1}-2)})}{e^{-ikdw^+_{m+1}}\sqrt{w^+_{m+1}}}$$
$$\left. \frac{e^{2i(\pi s^+_1/h+\pi/2)}}{1-e^{2i(\pi s^+_1/h+\pi/2)}} \right), \tag{3.74}$$

where $A_\pm = \frac{-2\pi i}{kde^{i\pi/4}}$.

3.3.3.4 The positions of simple poles $v^-_{\pm,n}$ and $v^+_{\pm,n}$ of the functions $f_\pm$

To illustrate the formulas (3.35) and (3.37) the poles $v^-_{\pm,n}$ and $v^+_{\pm,n}$ have been calculated with the same parameter values we used in Tables 3.1 and 3.2, which are $k = 0.5, d = 4, \beta = 0.353$; $v^-_{\pm,n}$, w^-_n, $v^+_{\pm,n}$, and w^+_n are defined respectively in (3.35),(3.36),(3.37) and (3.38). The results are shown in Table 3.3 below, and as plotted in Figures 3.6 and 3.7.

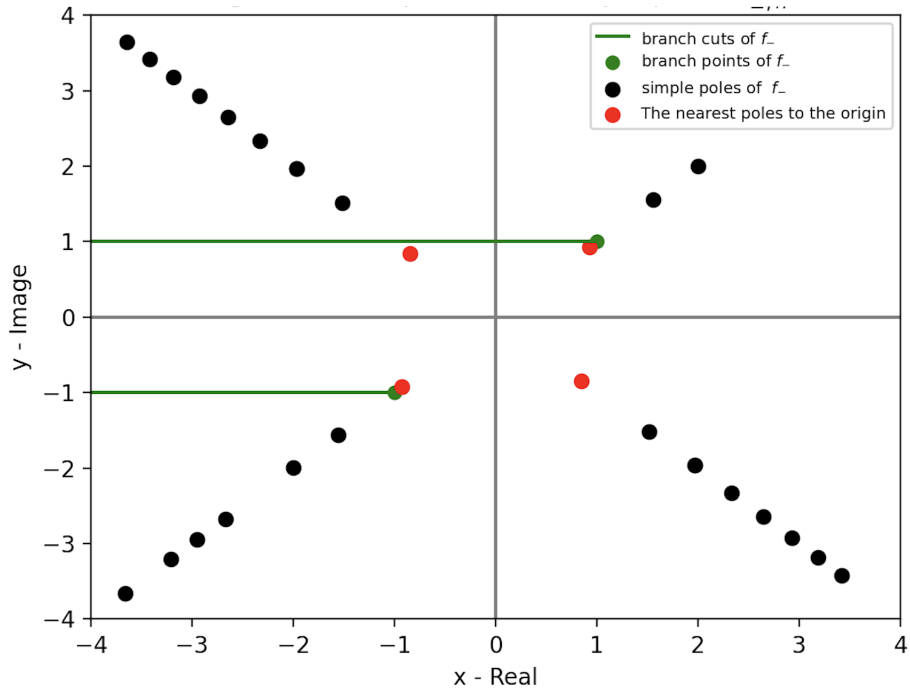

Figure 3.6: The positions of the poles $v^-_{\pm,n}$.

Figures 3.6 and 3.7 illustrate that there are infinitely many poles. These poles lie on the lines $y = x$ and $y = -x$. In the horizontal strip $|\text{Im}(v)| < 1$, there are finitely many simple poles. In particular, in Figure 3.6 there are 4 simple poles inside the strip, the poles with $n = 0, 1$, which are plotted with red points. In Figure 3.7 the only poles located inside the strip are the poles at $\pm(0.3826834323+0.3826834323$ i), with $n = 0$, which are plotted with red points.

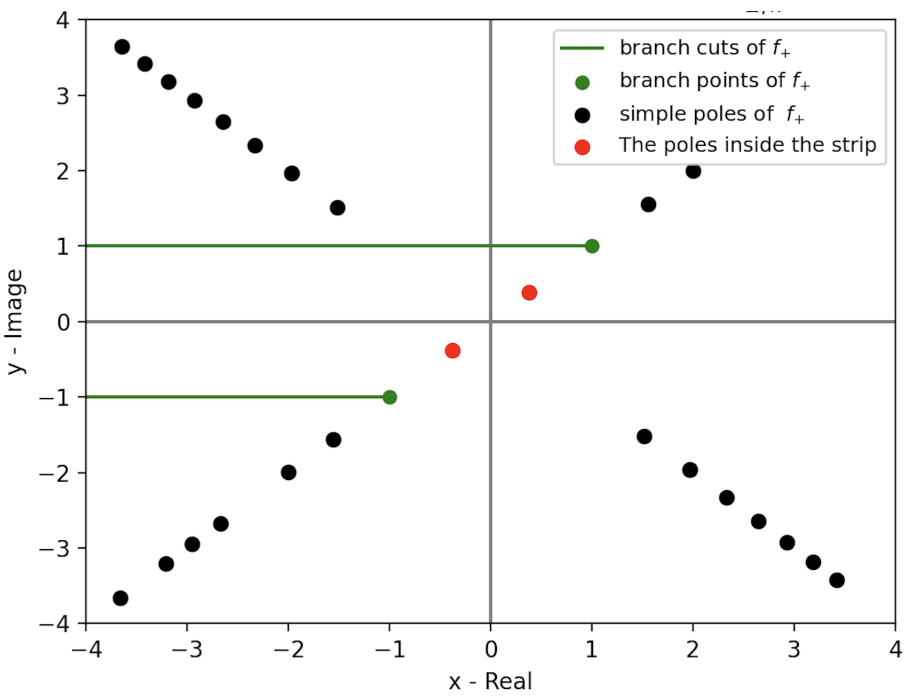

Figure 3.7: The positions of the poles $v^{+}_{\pm,n}$.

n	$v^{-}_{\pm,n}$	$v^{+}_{\pm,n}$
0	±(0.9238795325+0.9238795325 i)	± (0.3826834323+0.3826834323 i)
1	±(-0.8469019637 + 0.8469019637 i)	±(-1.1934612341 + 1.1934612341 i)
2	±(-1.5126266105 + 1.5126266105 i)	± (-1.7306490239 +1.7306490239 i)
3	±(-1.9643919134+1.9643919134 i)	± (-2.1368065824 + 2.1368065824i)
4	±(-2.3301570583 + 2.3301570583i)	± (-2.4772441740 + 2.4772441740 i)
5	±(-2.6458322402 + 2.6458322402i)	± (-2.7762447702 + 2.7762447702 i)
6	± (-2.9276653787 + 2.9276653787i)	±(-3.0460353496 + 3.0460353496j)
7	± (-3.1846539681 + 3.184653968i)	± (-3.2938014023 + 3.2938014023i)
8	± (-3.4223993372 + 3.4223993372i)	± (-3.5241912554 + 3.5241912554i)
9	± (-3.6446691963 + 3.6446691963 i)	± (-3.7404171333 + 3.7404171333 i)
-1	± (1.5570323430 + 1.5570323430 i)	± (1.3104361625 + 1.3104361625 i)
-2	± (1.9987861426 + 1.9987861426 i)	± (1.8132951395 +1.8132951395 i)
-3	±(2.3592249513 + 2.3592249513 i)	±(2.2042766590 + 2.2042766590 i)
-4	±(2.6714675176 + 2.6714675176 i)	±(2.5356718866 + 2.5356718866 i)
-5	±(2.9508532705 + 2.9508532705 i)	± (2.8285028271 + 2.8285028271 i)
-6	± (3.2059836792 + 3.2059836792i)	± (3.0937395769 + 3.0937395769 i)
-7	± (3.4422561900 + 3.4422561900i)	± (3.3379665811 + 3.3379665811i)
-8	± (3.6633214443 + 3.66332144443i)	± (3.5655037826 + 3.5655037826i)

Table 3.3: The positions of the poles $v^{-}_{\pm,n}$ and $v^{+}_{\pm,n}$ for the parameter values $k = 0.5, d = 4, \beta = 0.353$.

3.4 Numerical implementations

3.4.1 Part A

In this section, we will utilize our numerical integration method stated in Chapter 2, namely the truncated midpoint rule I_h^N, given by (2.11), and the modified truncated midpoint rule approximation I_h^{*N}, given by (2.38). These approximations I_h^N and I_h^{*N} to the integrals $I^{\pm}$ in (3.31) will be denoted $I_{N,h}^{\pm}$ and $I_{N,h}^{*\pm}$, respectively.

Firstly, we apply the truncated midpoint rule approximation $I_{N,h}^{\pm}$ to approximate (3.31) to speed up the convergence of the 2D quasi-periodic Green's function; the results agree with the results given in [Table 2, [28]]. Secondly, we apply the modification of the truncated midpoint rule to (3.31) with two sets of parameter values, taken from (Table 2, and Table 3 [28]). We obtain more accurate results than the results by the truncated midpoint rule (see Tables 3.4, 3.5 and 3.6).

3.4.1.1 Approximating $G_\beta^d(X,Y)$ using $I_{N,h}^{\pm}$

Let $G_\beta^d(X,Y)$ be given by (3.31) and let $I_{N,h}^{-}$ and $I_{N,h}^{+}$ be the truncated midpoint rule approximation to $I^{\pm}$, given by

$$I_{N,h}^{-} = h \sum_{j=-N}^{N+1} f_-(t_j), \tag{3.75}$$

$$I_{N,h}^{+} = h \sum_{j=-N}^{N+1} f_+(t_j), \tag{3.76}$$

where $t_j = (j-1/2)h$. We denote the corresponding approximation function, our approximation to $G_\beta^d = G_\beta^d(X,Y)$, as $G_\beta^{h,N,d}$. Thus our approximation becomes

$$G_\beta^d \approx G_\beta^{h,N,d} := \frac{-i}{4} H_0^{(1)}(kr) - \frac{e^{-ikY}}{2\pi} I_{N,h}^{-} - \frac{e^{ikY}}{2\pi} I_{N,h}^{+}, \tag{3.77}$$

i.e.

$$
\begin{aligned}
G_\beta^{h,N,d} = \frac{-i}{4} H_0^{(1)}(kr) - \frac{he^{-ikY}}{2\pi} \sum_{j=-N}^{N+1} e^{-\rho_-(j^2-1/2)h^2} F_-((j-1/2)h) \\
- \frac{he^{ikY}}{2\pi} \sum_{j=-N}^{N+1} e^{-\rho_+(j^2-1/2)h^2} F_+((j-1/2)h),
\end{aligned}
\tag{3.78}
$$

with $h > 0$ and $N \in \mathbb{N}$. As an example, we approximate G_β^d by $G_\beta^{h,N,d}$ with specific parameter values, those selected in (Table 2, [28]), namely $X = 0, Y = 0.04, d = 4, \beta = \sqrt{2}/4$, and $k = 0.5$. The results are shown in Table 3.4 below. Table 3.4

N	$h = 1/\sqrt{N}$	Computed values of $G_\beta^d(X,Y)$	
20	0.2236	**-0.4595**1515467317416	**-0.35091**65080999708 i
40	0.1581	**-0.459529**9616985824	**-0.350913**2423529163 i
60	0.1290	**-0.45952987**827307495	**-0.35091308**13007889 i
80	0.1118	**-0.459529879**62395764	**-0.35091308** 722624115i
100	0.1	**-0.4595298794**549343	**-0.3509130869**2604817 i
120	0.0912	**-0.4595298794**797906	**-0.35091308693**73357 i
140	0.0845	**-0.45952987947773**1505	**-0.350913086938**5231 i
160	0.0790	**-0.4595298794773**376	**-0.35091308693**8193 i
180	0.0745	**-0.45952987947737**92	**-0.350913086938212**55i
200	0.0707	**-0.459529879477374**56	**-0.3509130869382**181 i
500	0.0447	**-0.459529879477374**	**-0.3509130869382171 i**

Table 3.4: Approximating the integrals (3.30) using the truncated midpoint rule.

shows the computed values of $G_\beta^{h,N,d}$ for different values of N and we have chosen h as $1/\sqrt{N}$. As can be seen from Table 3.4 the value of $G_\beta^{h,N,d}$ with $N = 100$, agrees with the result given in (Table 2, [28]) to 10 significant figures.

3.4.1.2 Approximating $G_\beta^d(X,Y)$ using $I_{N,h}^{*,\pm}$

We have concerned ourselves so far with approximating the quasi-periodic Green's function by means of the truncated midpoint method. To speed up the convergence of this method and obtain more accurate results (at least 3 digits accuracy when $N = 2$ for the same parameter values), we use $I_{N,h}^{*-}$ and $I_{N,h}^{*+}$, the truncated modified midpoint rule approximations to $I^{\pm}$, given as follows:

$$I^{*-}_{N,h} := I^{-}_{N,h} + G^{-}_{F_{m,m+1}} \tag{3.79}$$

for the first integral in (3.30), and

$$I^{*+}_{N,h} := I^{+}_{N,h} + G^{+}_{F_{m,m+1}} \tag{3.80}$$

for the second integral in (3.30), where $G^{-}_{F_{m,m+1}}$ and $G^{+}_{F_{m,m+1}}$ are given by (3.73) and (3.74) respectively. Let $G^{*h,N,d}_{\beta}$ denote the corresponding approximation to G^{d}_{β}, so

$$G^{d}_{\beta} \approx G^{*h,N,d}_{\beta} := \frac{-i}{4} H^{(1)}_{0}(kr) - \frac{e^{-ikY}}{2\pi} I^{*-}_{N,h} - \frac{e^{ikY}}{2\pi} I^{*+}_{N,h} \tag{3.81}$$

$$= \frac{-i}{4} H^{(1)}_{0}(kr) - \frac{e^{-ikY}}{2\pi} \left(I^{-}_{N,h} + G^{-}_{F_{m,m+1}} \right) - \frac{e^{ikY}}{2\pi} \left(I^{+}_{N,h} + G^{+}_{F_{m,m+1}} \right). \tag{3.82}$$

Thus our approximation to the quasi-periodic Green's function is given by

$$\begin{aligned} G^{*h,N,d}_{\beta} &= \frac{-i}{4} H^{(1)}_{0}(kr) - \frac{e^{-ikY}}{2\pi} \left(h \sum_{j=-N}^{N+1} e^{-\rho_{-}((j-1/2)^2)h^2} F_{-}((j-1/2)h) + G^{-}_{F_{m,m+1}} \right) \\ &- \frac{e^{ikY}}{2\pi} \left(h \sum_{j=-N}^{N+1} e^{-\rho_{+}((j-1/2)^2)h^2} F_{+}((j-1/2)h) + G^{+}_{F_{m,m+1}} \right). \end{aligned} \tag{3.83}$$

Table 3.5 below shows results for the same values of X, Y, k and β, as in Table 3.4, the values selected in (Table 2, [28]), with $h = 1/\sqrt{N}$.

Comparing our approximation in Table 3.4 with the approximation in Table 3.5 we see that:

1. For $N = 10$ in Table 3.5, the accuracy of our approximation reaches 9 digits using the modified truncated midpoint rule, while in Table 3.4 the original truncated midpoint rule needs 80 quadrature points to reach the same level of accuracy.

N	h	M.M.R approximation to $G^d_\beta(X,Y)$		$\lvert I - I^{*,-}_{N,h}\rvert$
2	0.70	**-0.459**4854212614863	**-0.350**88663343756266 i	5.173 $\times 10^{-5}$
5	0.44	**-0.45952**966230238584	**-0.350913**1961459821i	2.430 $\times 10^{-7}$
10	0.31	**-0.459529879**08298915	**-0.35091308**74116392i	6.161 $\times 10^{-10}$
15	0.25	**-0.4595298794**831383	**-0.3509130869**411522i	6.468 $\times 10^{-12}$
20	0.22	**-0.4595298794773**115	**-0.350913086938**09115i	1.406 $\times 10^{-13}$
25	0.20	**-0.45952987947737**534	**-0.3509130869382**2176i	4.834 $\times 10^{-15}$
30	0.18	**-0.459529879477374**	**-0.350913086938217i**	1.241 $\times 10^{-16}$

Table 3.5: Approximating the integrals (3.30) using the modified truncated midpoint rule with $k = 0.5,\ X = 0, Y = 0.04, \beta = 0.353$ and $d = 4$.

2. In Table 3.5 the approximation achieves 10 digits accuracy for $N = 15$, and 13 correct digits for $N = 20$.

3. The computed value of the Green's function in Table 3.4 by using the modified truncated midpoint rule when $N = 30$ is the same as the value of the Green's function given in Table 3.4 with $N = 500$ quadrature points.

4. In Table 3.4 the truncated midpoint rule needs 20 quadrature points to obtain 4 digits accuracy, while the modified truncated midpoint rule achieves 3 correct digits in Table 3.5 with only two quadrature points.

These results support our proposed modified method, illustrating that when a simple pole lies close to the real line, the modification greatly improves the accuracy of the midpoint rule.

Now we carry out a calculation with the modified truncated midpoint rule approximation with another set of values of the parameters, taken from (see Table 3, [28]), which are $X = 0,\ Y = 0,04,\ k = 2.5,\ \beta = 5\sqrt{2}/4$. Again we choose $h = 1/\sqrt{N}$. The true value, obtained with $N = 500$, is

$$G^d_\beta(X,Y) = -\mathbf{0.3538172307170537} - \mathbf{0.1769332382522048i}.$$

The results are shown in Table 3.6 below.

From Table 3.6 we see that, also with higher values of the parameters k and β, the

N	$h = 1/\sqrt{N}$	M.M.R approximation to $G^d_\beta(X,Y)$		$\lvert I - I^{*,-}_{N,h}\rvert$
5	0.447	**-0.3538**25286089919	**-0.17694**408693174565 i	1.351 $\times 10^{-05}$
15	0.258	**-0.35381723**88682319	**-0.1769332**4073820155 i	8.521 $\times 10^{-09}$
25	0.2	**-0.3538172307**191948	**-0.176933238**446288 i	1.940 $\times 10^{-10}$
35	0.169	**-0.3538172307**1614285	**-0.1769332382**4769377 i	4.602 $\times 10^{-12}$
45	0.149	**-0.353817230717**085	**-0.17693323825**23834 i	1.813 $\times 10^{-13}$
55	0.134	**-0.3538172307170**5284	**-0.176933238252**19695 i	1.08 $\times 10^{-14}$

Table 3.6: Approximating the integrals (3.30) using the modified midpoint rule with $k = 2.5,\ X = 0, Y = 0.04, \beta = 5\sqrt{2}/4$ and $d = 4$.

modified midpoint rule works well and, again, the accuracy increases with increasing the number of quadrature points.

3.4.2 Part B

Now we turn our attention as in (3.57) and (3.58) to including contributions related to all the poles in the domain $S_H = \{v \in \mathbb{C} : |\mathrm{Im} v| < H\}$, given $H \in (0,1)$. In particular we have in mind to define H as

$$H := \min(\frac{\pi}{\rho h}, 0.9). \qquad (3.84)$$

Recall that the poles are given by $v^-_{\pm,j} = \pm e^{i\pi/4}\sqrt{w^-_j}$, for $j \in \mathbb{Z}$, with w^-_j defined by

$$w^-_j := 1 + \frac{\beta}{k} - \frac{2\pi j}{kd}. \qquad (3.85)$$

Recall also from the previous section that the magnitude of the imaginary part of the poles is $|\mathrm{Im}(v^-_{\pm,j})| = \sqrt{\frac{|w^-_j|}{2}}$. Assuming that H is large enough so that S_H contains at least one pole, the poles $v^-_{\pm,j}$ are in S_H if and only if $j = n^- + 1, ..., N^-$, for some integers $n^-, N^- \in \mathbb{Z}$, with $n^- + 1 < N^-$. Here n^- and N^- are the unique integers

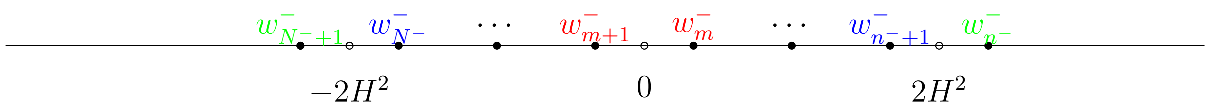

Figure 3.8: Illustration of (3.86)-(3.89)

satisfying

$$\sqrt{\frac{|w_j^-|}{2}} < H, \quad \text{for} \quad j = n^- + 1 \tag{3.86}$$

$$\sqrt{\frac{|w_j^-|}{2}} \geq H, \quad \text{for} \quad j = n^- \tag{3.87}$$

$$\sqrt{\frac{|w_j^-|}{2}} < H, \quad \text{for} \quad j = N^- \tag{3.88}$$

$$\sqrt{\frac{|w_j^-|}{2}} \geq H, \quad \text{for} \quad j = N^- + 1 \tag{3.89}$$

From (3.87), $w_{n^-}^- \geq 2H^2$, i.e.

$$1 + \frac{\beta}{k} - \frac{2\pi n^-}{kd} \geq 2H^2.$$

Since $\beta = k\text{sin}\theta$ (see (3.43)) this is equivalent to

$$n^- \leq \frac{kd}{2\pi}(1 + \sin\theta - 2H^2).$$

Further from (3.86) we have

$$n^- + 1 > \frac{kd}{2\pi}(1 + \sin\theta - 2H^2),$$

so

$$n^- = \left\lfloor \frac{kd}{2\pi}(1 + \sin\theta - 2H^2) \right\rfloor. \tag{3.90}$$

Similarly, from (3.88)-(3.89), $-w_{N^-}^- < 2H^2 \leq -w_{N^-+1}^-$, so that

$$N^- = \left\lfloor \frac{kd}{2\pi}(1 + \sin\theta + 2H^2) \right\rfloor. \tag{3.91}$$

Arguing exactly as we did when deriving (3.70) and (3.71), G_F^- and G_F^+, given by (3.55) and (3.56), can be written as follows:

$$G_F^- = \frac{-2\pi i}{kde^{i\pi/4}} \sum_{j=n^-+1}^{N^-} \frac{e^{-i\rho_- w_j^-}(i(w_j^- - 2))^{-1/2}\cos(kX\sqrt{iw_j^-}\sqrt{i(w_j^- - 2)})}{e^{-ikdw_j^-}\sqrt{w_j^-}} \frac{e^{2i\pi(v_{+,j}^-/h+1/2)}}{1-e^{2i\pi(v_{+,j}^-/h+1/2)}} \tag{3.92}$$

and

$$G_F^+ = \frac{-2\pi i}{kde^{i\pi/4}} \sum_{j=n^++1}^{N^+} \frac{e^{-i\rho_+ w_j^+}(i(w_j^+ - 2))^{-1/2}\cos(kX\sqrt{iw_j^+}\sqrt{i(w_j^+ - 2)})}{e^{-ikdw_j^+}\sqrt{w_j^+}} \frac{e^{2i\pi(v_{+,j}^+/h+1/2)}}{1-e^{2i\pi(v_{+,j}^+/h+1/2)}}, \tag{3.93}$$

where

$$n^+ := \left\lfloor \frac{kd}{2\pi}(1-\sin\theta - 2H^2) \right\rfloor$$

and

$$N^+ := \left\lfloor \frac{kd}{2\pi}(1-\sin\theta + 2H^2) \right\rfloor.$$

We implement a similar test to our approximation in Part A for the proposed approximation of G_β^d given by

$$\begin{aligned} G_\beta^d \approx G_\beta^{*h,N,d} := \frac{-i}{4}H_0^{(1)}(kr) - \frac{e^{-ikY}}{2\pi}\left(h\sum_{j=-N}^{N+1} e^{-\rho_-((j-1/2)^2)h^2}F_-((j-1/2)h) + G_F^-\right) \\ - \frac{e^{ikY}}{2\pi}\left(h\sum_{j=-N}^{N+1} e^{-\rho_+((j-\frac{1}{2})^2)h^2}F_+((j-1/2)h) + G_F^+\right), \end{aligned} \tag{3.94}$$

where $\rho_- = k(d-Y)$ and $\rho_+ = k(d+Y)$.

Let's compare the approximations of Part A with those of Part B. In both parts, we apply the modified truncated midpoint rule approximation to (3.30). In Part A the correction factors arise from the residues of $F_\pm$ at the nearest poles to the origin (up to 4 poles, see the formulas (3.73) and (3.74)). In Part B the correction factor is expressed as a sum of the residues of the $F_\pm$ at all the finite number of poles in S_H, given by (3.92) and (3.93).

N	$h = 1/\sqrt{N}$	M.M.R approximation to $G^d_\beta(X,Y)$		$\lvert I - I^{*,-}_{N,h}\rvert$
2	0.707	**-0.459**48692526488744	- **0.350**8836557209456i	5.20×10^{-5}
5	0.447	**-0.45952**966620006297	- **0.350913**1903000088i	2.37×10^{-7}
10	0.316	**-0.459529879**08248777	- **0.35091308**740489124i	6.11×10^{-10}
15	0.258	**-0.4595298794**831636	- **0.3509130869**411313i	6.48×10^{-12}
25	0.20	**-0.459529879477737**534	- **0.35091308693822**176i	4.83×10^{-15}
30	0.182	**-0.459529879477374**	- **0.350913086938217i**	1.24×10^{-16}

Table 3.7: Approximating the integrals (3.30) by the modified truncated midpoint rule using all the poles in S_H, with $k = 0.5$, $X = 0, Y = 0.04, \beta = \sqrt{2}/4$ and $d = 4$.

As a first test of our Part B implementation, we make a computation in Table 3.7 for the same parameter values used in Table 3.5. In this first test the results in Table 3.7 are identical to those in Table 3.5. This is to be expected as there are, for each N, at most four poles in S_H, so the Part A and Part B approximations should be identical.

N	$h = 1/\sqrt{N}$	M.M.R approximation to $G^d_\beta(X,Y)$		$\lvert I - I^{*,-}_{N,h}\rvert$
5	0.447	**-0.353**0494857481016	**-0.176**28333487515266 i	1.0×10^{-3}
15	0.258	**-0.35381722**5845444	**-0.17693324**291877913 i	6.746×10^{-09}
25	0.2	**-0.3538172307**510323	**-0.1769332382**9580487i	5.527×10^{-11}
35	0.169	**-0.35381723071716**836	**-0.17693323825**110102 i	1.109×10^{-12}
45	0.149	**-0.35381723071704**113	**-0.1769332382522**4047 i	3.780×10^{-14}
55	0.134	**-0.353817230717054**1	**-0.17693323825220**297 i	1.88×10^{-15}

Table 3.8: Approximating the integrals (3.30) by the modified truncated midpoint rule using all the poles in S_H with $k = 2.5$, $X = 0, Y = 0.04, \beta = 5\sqrt{2}/4$ and $d = 4$.

Tables 3.6 and 3.8 show results corresponding to higher values of k and β, namely the parameter values $X = 0$, $Y = 0.04$, $k = 2.5$ and $\beta = 5\sqrt{2}/4$. For these parameter values the approximations (3.82) and (3.94) are different. For the results in Table 3.6 in Part A, we have 2 terms in the correction factor, while in Table 3.8, when $N = 5$ we have 3 terms in the first sum (3.92) and 4 in (3.93), and from $N = 15$ to $N = 55$, we obtain 6 terms in each sum in (3.92) and (3.93). Of course, in Table 3.8 we are including all the poles in S_H with $H = \min(0.9, \pi/\rho h)$; and note that $H = 0.9$ for all small enough h.

Let us comment on the benefit or otherwise of the Part B approximation (the correction factor accounts for all the poles in S_H), compared to the Part A approximation (the correction factor accounts only for the poles closest to the real axis). In some cases (e.g., Tables 3.5 and 3.7) there is no difference between these approaches because the Part A approach already takes into account all the poles in S_H. Table 3.8 and 3.6 are results for parameter values where the approximations are different, but the Part B approximation is only marginally more accurate, and only for $N \geq 15$. It would be good to do a more thorough numerical investigation, but based on these limited results our recommendation is to use the more efficient Part A approximation.

3.4.3 Part C

In this part we, first of all, derive a new integral representation for the quasi-periodic Green's function. We follow the same steps as used in [28] to derive (3.26) which represents one of the sources in (3.11) explicitly and the rest of the sources as integrals of the form (3.1). In this part we show a new formula for the quasi-periodic Green's function which, for any $M \in \mathbb{N}$, represents the first $2M-1$ of these sources explicitly, with the remainder of the sources represented as integrals of the form (3.1), see (3.108). (Note that (3.108) reduces to (3.26) when $M = 1$.) The point of this new representation for computation is that the integrals in (3.108) can be evaluated by the same modified midpoint rule approximation as we used in Part A, but we shall see that, for the same amount of work, we obtain much more accurate results with values of $M > 1$ than for $M = 1$.

Let us now derive (3.108). Our method of proof is an extension of the argument used to prove (3.26) in [28] and [31]. We begin with the geometric series that, for $M \in \mathbb{N}$,

$$\sum_{n=M}^{\infty} z^n = z^M(1 + z + z^2 + z^3 + ...) = \frac{z^M}{1-z}, \tag{3.95}$$

provided $|z| < 1$. Let $z = e^{i(\beta+k)d-kdu}$ so that $|z| = e^{-kdu} \leq 1$, for all $u \geq 0$, with equality if and only if $u = 0$. Then, by (3.95),

$$\sum_{n=M}^{\infty} e^{in(\beta+k)d}e^{-nkdu} = \frac{e^{iM(\beta+k)d-(M-1)kdu}}{e^{kdu} - e^{i(\beta+k)d}}, \quad u > 0. \tag{3.96}$$

Multiplying both sides in (3.96) by $\frac{-2ie^{-ikY}e^{kYu}\cos[kX\sqrt{(u^2-2iu)}]}{\pi\sqrt{u^2-2iu}}$, we obtain that

$$\begin{aligned} &\frac{-2ie^{-ikY}}{\pi}\sum_{n=M}^{\infty}\frac{e^{in(\beta+k)d}e^{ku(Y-nd)}\cos[kX\sqrt{(u^2-2ui)}]}{\sqrt{u^2-2ui}} \\ &= \frac{-2ie^{-ikY}}{\pi}\frac{e^{iM(\beta+k)d}e^{ku(Y-(M-1)d)}\cos[kX\sqrt{(u^2-2iu)}]}{(e^{kdu}-e^{i(\beta+k)d})\sqrt{u^2-2iu}}. \end{aligned} \tag{3.97}$$

Integrating both sides in (3.97) with respect to u from 0 to ∞, we see that

$$\begin{aligned} J :&= \int_0^{\infty}\sum_{n=M}^{\infty}\frac{-2ie^{-ikY}}{\pi}\frac{e^{in(\beta+k)d}e^{ku(Y-nd)}\cos[kX\sqrt{(u^2-2ui)}]}{\sqrt{u^2-2ui}}du \\ &= \frac{-2ie^{-ikY}}{\pi}\int_0^{\infty}\frac{e^{iM(\beta+k)d}e^{ku(Y-(M-1)d)}}{(e^{kdu}-e^{i(\beta+k)d})}\frac{\cos[kX\sqrt{(u^2-2iu)}]}{\sqrt{u^2-2iu}}du. \end{aligned} \tag{3.98}$$

Now, using the result from [6], Equation 5.14 (16),

$$e^{-ib}H_0^{(1)}(\sqrt{a^2+b^2}) = \frac{-2i}{\pi}\int_0^{\infty}\frac{e^{-bu}\cos[a\sqrt{u^2-2ui}]}{\sqrt{u^2-2ui}}du, \tag{3.99}$$

for $a \in \mathbb{R}$, $b \geq 0$. Using this result with $a = kX$ and $b = k(nd - Y)$, we see that

$$H_0^{(1)}(kr_n) = \frac{-2ie^{-ikY}}{\pi}\int_0^{\infty}\frac{e^{ku(Y-nd)}e^{inkd}\cos[kX\sqrt{(u^2-2iu)}]}{\sqrt{u^2-2iu}}du, \quad k(nd-Y) \geq 0, \tag{3.100}$$

as $kr_n = \sqrt{(kX)^2 + (k(nd-Y))^2}$. Thus, reversing the order of integration and summation in (3.98), we see that

$$\begin{aligned} J &= \sum_{n=M}^{\infty} \frac{-2ie^{-ikY}}{\pi} \int_0^{\infty} \frac{e^{in(\beta+k)d} e^{ku(Y-nd)} \cos[kX\sqrt{(u^2-2ui)}]}{\sqrt{u^2-2ui}} du \\ &= \sum_{n=M}^{\infty} H_0^{(1)}(kr_n) e^{in\beta d}. \end{aligned} \tag{3.101}$$

Also

$$J = \frac{-2ie^{-ikY}}{\pi} \int_0^{\infty} \frac{e^{iM(\beta+k)d} e^{ku(Y-(M-1)d)}}{e^{kdu} - e^{i(\beta+k)d}} \frac{\cos[kX\sqrt{(u^2-2iu)}]}{\sqrt{u^2-2iu}} du \tag{3.102}$$

$$= \frac{-2ie^{-ikY}}{\pi} \int_0^{\infty} \frac{e^{(M-1)i(\beta+k)d+ku(Y-Md)} \cos[kX\sqrt{(u^2-2iu)}]}{(e^{-i(\beta+k)d} - e^{-kdu})\sqrt{u^2-2iu}} du. \tag{3.103}$$

Thus

$$\sum_{n=M}^{\infty} H_0^{(1)}(kr_n) e^{in\beta d} = \frac{-2ie^{-ikY}}{\pi} \int_0^{\infty} \frac{e^{(M-1)i(\beta+k)d+ku(Y-Md)} \cos[kX\sqrt{(u^2-2iu)}]}{(e^{-i(\beta+k)d} - e^{-kdu})\sqrt{u^2-2iu}} du. \tag{3.104}$$

In particular, when $M = 1$, the formula (3.104) is

$$\sum_{n=1}^{\infty} H_0^{(1)}(kr_n) e^{in\beta d} = \frac{-2ie^{-ikY}}{\pi} \int_0^{\infty} \frac{e^{ku(Y-d)} \cos[kX\sqrt{(u^2-2iu)}]}{(e^{-i(\beta+k)d} - e^{-kdu})\sqrt{u^2-2iu}} du, \tag{3.105}$$

and this agrees with Linton's (Equation 2.36, [28]). Arguing similarly we deduce that

$$\begin{aligned} \sum_{n=-\infty}^{-M} H_0^{(1)}(kr_n) e^{in\beta d} &= \sum_{n=M}^{\infty} H_0^{(1)}(kr_{-n}) e^{-in\beta d} \\ &= \frac{-2ie^{ikY}}{\pi} \int_0^{\infty} \frac{e^{(1-M)i(\beta-k)d} e^{-ku(Y+Md)} \cos[kX\sqrt{(u^2-2iu)}]}{(e^{i(\beta-k)d} - e^{-kdu})\sqrt{u^2-2iu}} du. \end{aligned} \tag{3.106}$$

Thus we conclude that

$$
\begin{aligned}
G^d_\beta(X,Y) &= \frac{-i}{4}\sum_{n=-\infty}^{\infty} H_0^{(1)}(kr_n)e^{in\beta d} \\
&= \frac{-i}{4}\left\{\sum_{n=1-M}^{M-1} H_0^{(1)}(kr_n)e^{in\beta d} + \sum_{n=M}^{\infty} H_0^{(1)}(kr_n)e^{in\beta d} \quad + \sum_{n=-\infty}^{-M} H_0^{(1)}(kr_n)e^{in\beta d}\right\}
\end{aligned} \tag{3.107}
$$

i.e.,

$$
\begin{aligned}
G^d_\beta(X,Y) = {} & \frac{-i}{4}\sum_{n=1-M}^{M-1} H_0^{(1)}(kr_n)e^{in\beta d} \\
& - \frac{e^{-ikY}}{2\pi}\int_0^\infty \frac{e^{(M-1)i(\beta+k)d}e^{ku(Y-Md)}\cos[kX\sqrt{(u^2-2iu)}]}{(e^{-i(\beta+k)d}-e^{-kdu})\sqrt{u^2-2iu}}du \\
& - \frac{e^{ikY}}{2\pi}\int_0^\infty \frac{e^{(1-M)i(\beta-k)d}e^{-ku(Y+Md)}\cos[kX\sqrt{(u^2-2iu)}]}{(e^{i(\beta-k)d}-e^{-kdu})\sqrt{u^2-2iu}}du.
\end{aligned} \tag{3.108}
$$

In order to apply the standard and modified midpoint rule approximation to (3.108), we express the Green's function formula (3.108) in two forms.

3.4.3.1 Form 1

We try to write the integrals in (3.108) in the form

$$
I = \int_{-\infty}^{\infty} e^{-\rho v^2}F(v)dv. \tag{3.109}
$$

Substituting $u = v^2$ into (3.108), we have

$$
\begin{aligned}
G^d_\beta(X,Y) = {} & \frac{-i}{4}\sum_{n=1-M}^{M-1} H_0^{(1)}(kr_n)e^{in\beta d} \\
& - \frac{e^{-ikY}}{2\pi}\int_{-\infty}^\infty \frac{e^{(M-1)i(\beta+k)d}e^{k(Y-Md)v^2}\cos[kXv\sqrt{(v^2-2i)}]}{(e^{-i(\beta+k)d}-e^{-kdv^2})\sqrt{v^2-2i}}dv \\
& - \frac{e^{ikY}}{2\pi}\int_{-\infty}^\infty \frac{e^{(1-M)i(\beta-k)d}e^{-k(Y+Md)v^2}\cos[kXv\sqrt{(v^2-2i)}]}{(e^{i(\beta-k)d}-e^{-kdv^2})\sqrt{v^2-2i}}dv.
\end{aligned} \tag{3.110}
$$

These integrals have the form (3.109) with $\rho = \rho_-$ and ρ_+ and $F = F_-$ and F_+, respectively, where

$$F_-(v) := \frac{e^{(M-1)i(\beta+k)d}\cos[kXv\sqrt{(v^2-2i)}]}{(e^{-i(\beta+k)d} - e^{-kdv^2})\sqrt{v^2-2i}}, \tag{3.111}$$

$$F_+(v) := \frac{e^{(1-M)i(\beta-k)d}\cos[kXv\sqrt{(v^2-2i)}]}{(e^{i(\beta-k)d} - e^{-kdv^2})\sqrt{v^2-2i}}, \tag{3.112}$$

and $\rho_\pm := k(Y \pm Md) > 0$. The truncated midpoint rule approximation to I is given by

$$I^{\pm}_{N,h} = h\sum_{n=-N}^{N+1} e^{-\rho v_n^2} F_\pm(v_n), \tag{3.113}$$

where $h = \sqrt{\frac{\pi}{\rho(N+1)}}$ and $v_n = (n-1/2)h$. The proposed approximation to $G^d_\beta(X,Y)$ is

$$G^d_\beta(X,Y) \approx G^N_h(X,Y) = \frac{-i}{4}\sum_{n=1-M}^{M-1} H^{(1)}_0(kr_n)e^{in\beta d} - \frac{he^{-ikY}}{2\pi}\sum_{n=-N}^{N+1} e^{-\rho_- v_n^2}F_-(v_n)$$
$$- \frac{he^{ikY}}{2\pi}\sum_{n=-N}^{N+1} e^{-\rho_+ v_n^2}F_+(v_n). \tag{3.114}$$

A modification of the truncated midpoint rule that takes into account the poles of $F = F_\pm$ which lie nearest to the real axis, is given by

$$I^{*\pm}_{N,h} = h\sum_{n=-N}^{N+1} e^{-\rho v_n^2} F_\pm(v_n) + G^{\pm,*}_{F_{m,m+1}} \tag{3.115}$$

where the correction factors $G^{-,*}_{F_{m,m+1}}$ are obtained following the same steps as (3.59), so that

$$G^{-,*}_{F_{m,m+1}} = 2\pi i e^{(M-1)i(\beta+k)d}\left(R^-_{+,m}\frac{e^{2i(\pi s_0/h+\frac{\pi}{2})}}{1-e^{2i(\pi s_0/h+\frac{\pi}{2})}} + R^-_{+,m+1}\frac{e^{2i(\pi s_1/h+\frac{\pi}{2})}}{1-e^{2i(\pi s_1/h+\frac{\pi}{2})}}\right). \tag{3.116}$$

Since

$$G^{-}_{F_{m,m+1}} = 2\pi i \left(R^{-}_{+,m} \frac{e^{2i(\pi s_0/h+\frac{\pi}{2})}}{1-e^{2i(\pi s_0/h+\frac{\pi}{2})}} + R^{-}_{+,m+1} \frac{e^{2i(\pi s_1/h+\frac{\pi}{2})}}{1-e^{2i(\pi s_1/h+\frac{\pi}{2})}} \right) \tag{3.117}$$

it follows that

$$G^{-,*}_{F_{m,m+1}} = e^{(M-1)i(\beta+k)d} G^{-}_{F_{m,m+1}}.$$

Similarly,

$$G^{+,*}_{F_{m,m+1}} = e^{(1-M)i(\beta-k)d} G^{+}_{F_{m,m+1}},$$

where $G^{-}_{F_{m,m+1}}$ and $G^{+}_{F_{m,m+1}}$ are defined in (3.70) and (3.71). Similarly to (3.73) and (3.74), we adjust these definitions to include only poles in the strip S_1, obtaining

$$\begin{aligned} G^{-,*}_{F_{m,m+1}} = A_- \Bigg(& \frac{\mathbf{H}(1-|\mathrm{Im} v^{-}_{+,m}|)e^{-iw^{-}_m\rho_-}(i(w^{-}_m-2))^{-1/2}\cos(kX\sqrt{iw^{-}_m}\sqrt{i(w^{-}_m-2)})}{e^{-ikdw^{-}_m}\sqrt{w^{-}_m}} \frac{e^{2i(\pi s_0/h+\frac{\pi}{2})}}{1-e^{2i(\pi s_0/h+\frac{\pi}{2})}} \\ & + \frac{\mathbf{H}(1-|\mathrm{Im} v^{-}_{+,m+1}|)e^{-iw^{-}_{m+1}\rho_-}(i(w^{-}_{m+1}-2))^{-1/2}\cos(kX\sqrt{iw^{-}_{m+1}}\sqrt{i(w^{-}_{m+1}-2)})}{e^{-ikdw^{-}_{m+1}}\sqrt{w^{-}_{m+1}}} \\ & \frac{e^{2i(\pi s_1/h+\frac{\pi}{2})}}{1-e^{2i(\pi s_1/h+\frac{\pi}{2})}} \Bigg). \end{aligned} \tag{3.118}$$

and

$$\begin{aligned} G^{+,*}_{F_{m,m+1}} = A_+ \Bigg(& \frac{\mathbf{H}(1-|\mathrm{Im} v^{+}_{+,m}|)e^{-iw^{+}_m\rho_+}(i(w^{+}_m-2))^{-1/2}\cos(kX\sqrt{iw^{+}_m}\sqrt{i(w^{+}_m-2)})}{e^{-ikdw^{+}_m}\sqrt{w^{+}_m}} \frac{e^{2i(\pi s^{+}_0/h+\pi/2)}}{1-e^{2i(\pi s^{+}_0/h+\pi/2)}} \\ & + \frac{\mathbf{H}(1-|\mathrm{Im} v^{+}_{+,m+1}|)e^{-iw^{+}_{m+1}\rho_+}(i(w^{+}_{m+1}-2))^{-1/2}\cos(kX\sqrt{iw^{+}_{m+1}}\sqrt{i(w^{+}_{m+1}-2)})}{e^{-ikdw^{+}_{m+1}}\sqrt{w^{+}_{m+1}}} \\ & \frac{e^{2i(\pi s^{+}_1/h+\pi/2)}}{1-e^{2i(\pi s^{+}_1/h+\pi/2)}} \Bigg), \end{aligned} \tag{3.119}$$

where $A_\pm := \frac{-2\pi i e^{\pm(1-M)i(\beta\mp k)d}}{kde^{i\pi/4}}$, and $|\mathrm{Im}(v^{-}_{+}, m)| = \sqrt{\frac{|w^{-}_m}{2}}$, $|\mathrm{Im}(v^{-}_{+,m+1})| = \sqrt{\frac{|w^{-}_{m+1}|}{2}}$ and $|\mathrm{Im}(v^{+}_{+}, m)| = \sqrt{\frac{|w^{+}_m}{2}}$, $|\mathrm{Im}(v^{+}_{+,m+1})| = \sqrt{\frac{|w^{+}_{m+1}|}{2}}$, also s_0, s_1, s^{+}_0, and s^{+}_1 are defined in (3.45) and (3.49), respectively. Thus our approximation is

$$G_h^{*N}(X,Y) = \frac{-i}{4}\sum_{n=1-M}^{M-1} H_0^{(1)}(kr_n)e^{in\beta d} - \frac{he^{-ikY}}{2\pi}\sum_{n=-N}^{N+1} e^{-\rho - v_n^2}F_-(v_n) + G^{-,*}_{F_{m,m+1}} - \frac{he^{ikY}}{2\pi}\sum_{n=-N}^{N+1} e^{-\rho + v_n^2}F_+(v_n) + G^{+,*}_{F_{m,m+1}}. \tag{3.120}$$

Numerical results are shown in Table 3.9 below with $h = \sqrt{\pi/\rho(N+1)}$. The modified truncated midpoint approximation (M.M.R) gives more accurate results than the standard midpoint rule (M.R) for the selected parameter values, and the accuracy increases as M is increased.

N	M	M.R approximation to $G^d_\beta(X,Y)$	M.M.R approximation to $G^d_\beta(X,Y)$
20	1	**-0.4595**858507315276 -**0.3509**9941195444506 i	**-0.4595298794**951679 - **0.3509130869**1452977 i
30	1	**-0.4595**1495074046667 - **0.35091**68421969744 i	**-0.459529879477**247- **0.350913086938**063 i
40	1	**-0.459529**2485922545 - **0.350910**077265403 i	**-0.45952987947737**3 - **0.35091308693821**976 i
20	2	**-0.459529**63961026716- **0.35091**036653857255 i	**-0.4595298794773**731 - **0.35091308693821**827 i
30	2	**-0.459529**97736545376 - **0.350913**2466351009 i	**-0.4595298794773**739- **0.3509130869382171** i
40	2	**-0.4595298**603878907- **0.35091308**40252365i	**-0.45952987947737**395 - **0.3509130869382171 i**
20	3	**-0.459529**95116241235- **0.350913**2388442773 i	**-0.4595298794773740** - **0.35091308693821716** i
30	3	**-0.4595298**7758771896- **0.35091308**09012767 i	**-0.459529879477374**0 - **0.3509130869382171**6 i
40	3	**-0.45952987**971926484 - **0.35091308**724701836 i	**-0.459529879477374**1- **0.3509130869382171** 6 i
20	4	**-0.4595298**644133187- **0.35091308**159931256 i	**-0.45952987947737**417 - **0.350913086938217**2 i
30	4	**-0.45952987**967839276 - **0.35091308**724045633 i	**-0.45952987947737**417- **0.350913086938217**27 i
40	4	**-0.4595298794**7009977- **0.3509130869**2548984 i	**-0.45952987947737**417- **0.350913086938217**2 i

Table 3.9: Comparison between the efficiency of the truncated midpoint approximation and the modified truncated midpoint rule approximation for $X = 0$, $Y = 0.04$, $\beta = \sqrt{2}/4$, $k = 0.5$ and $d = 4$.

3.4.3.2 Form 2

Now we show another useful form for numerical calculation for equation (3.108) which is equivalent to form 1, by substituting $u = (\frac{v}{\sqrt{\rho}})^2$ in (3.108), so the formula

(3.108) becomes

$$G^d_\beta(X,Y) = \frac{-i}{4}\sum_{n=1-M}^{M-1} H_0^{(1)}(kr_n)e^{in\beta d}$$
$$-\frac{e^{-ikY}}{2\pi\sqrt{\rho_-}}\int_{-\infty}^{\infty}\frac{e^{(M-1)i(\beta+k)d}e^{k(Y-Md)(\frac{v}{\sqrt{\rho_-}})^2}\cos[kX(\frac{v}{\sqrt{\rho_-}})\sqrt{((\frac{v}{\sqrt{\rho_-}})^2-2i)}]}{\left(e^{-i(\beta+k)d}-e^{-kd(\frac{v}{\sqrt{\rho_-}})^2}\right)\sqrt{(\frac{v}{\sqrt{\rho_-}})^2-2i}}dv$$
$$-\frac{e^{ikY}}{2\pi\sqrt{\rho_+}}\int_{-\infty}^{\infty}\frac{e^{(1-M)i(\beta-k)d}e^{-k(Y+Md)(\frac{v}{\sqrt{\rho_+}})^2}\cos[kX(\frac{v}{\sqrt{\rho_+}})\sqrt{((\frac{v}{\sqrt{\rho_+}})^2-2i)}]}{\left(e^{i(\beta-k)d}-e^{-kd(\frac{v}{\sqrt{\rho_+}})^2}\right)\sqrt{(\frac{v}{\sqrt{\rho_+}})^2-2i}}dv, \tag{3.121}$$

where $\rho_- = k(Md-Y) > 0$, $\rho_+ = k(Md+Y) > 0$. In order to evaluate the integrals in (3.121), we follow the same steps we have done for Form 1. We first write (3.121) in the form (3.124); we have

$$G^d_\beta(X,Y) = \frac{-i}{4}\sum_{n=1-M}^{M-1} H_0^{(1)}(kr_n)e^{in\beta d}$$
$$-\frac{e^{-ikY}}{2\pi\sqrt{\rho_-}}\int_{-\infty}^{\infty}\frac{e^{(M-1)i(\beta+k)d}e^{-v^2}\cos[kX(\frac{v}{\sqrt{\rho_-}})\sqrt{((\frac{v}{\sqrt{\rho_-}})^2-2i)}]}{(e^{-i(\beta+k)d}-e^{-kd(\frac{v}{\sqrt{\rho_-}})^2})\sqrt{(\frac{v}{\sqrt{\rho_-}})^2-2i}}dv$$
$$-\frac{e^{ikY}}{2\pi\sqrt{\rho_+}}\int_{-\infty}^{\infty}\frac{e^{(1-M)i(\beta-k)d}e^{-v^2}\cos[kX(\frac{v}{\sqrt{\rho_+}})\sqrt{((\frac{v}{\sqrt{\rho_+}})^2-2i)}]}{\left(e^{i(\beta-k)d}-e^{-kd(\frac{v}{\sqrt{\rho_+}})^2}\right)\sqrt{(\frac{v}{\sqrt{\rho_+}})^2-2i}}dv, \tag{3.122}$$

where $\mathrm{Re}\sqrt{(\frac{v}{\sqrt{\rho}})^2-2i} \geq 0$. Thus

$$G^d_\beta(X,Y) = \frac{-i}{4}\sum_{n=1-M}^{M-1} H_0^{(1)}(kr_n)e^{in\beta d} - \frac{e^{-ikY}}{2\pi\sqrt{\rho_-}}\widetilde{I}^- - \frac{e^{ikY}}{2\pi\sqrt{\rho_+}}\widetilde{I}^+ \tag{3.123}$$

where

$$\widetilde{I}^{\pm} = \int_{-\infty}^{\infty}\widetilde{f}_\pm(v)dv = \int_{-\infty}^{\infty}e^{-v^2}F_\pm(\frac{v}{\sqrt{\rho_\pm}})dv, \tag{3.124}$$

and

$$\widetilde{F}_\pm(v) := F_\pm(\frac{v}{\sqrt{\rho_\pm}}).$$

Explicitly,

$$\widetilde{F}_-(v) := F_-(\frac{v}{\sqrt{\rho_-}}) = \frac{e^{(M-1)i(\beta+k)d}\cos[kX(\frac{v}{\sqrt{\rho_-}})\sqrt{((\frac{v}{\sqrt{\rho_-}})^2-2i)}]}{(e^{-i(\beta+k)d}-e^{-kd(\frac{v}{\sqrt{\rho_-}})^2})\sqrt{(\frac{v}{\sqrt{\rho_-}})^2-2i}} \tag{3.125}$$

and

$$\widetilde{F}_+(v) := F_+(\frac{v}{\sqrt{\rho_+}}) = \frac{e^{(1-M)i(\beta-k)d}\cos[kX(\frac{v}{\sqrt{\rho_+}})\sqrt{((\frac{v}{\sqrt{\rho_+}})^2-2i)}]}{(e^{i(\beta-k)d}-e^{-kd(\frac{v}{\sqrt{\rho_+}})^2})\sqrt{(\frac{v}{\sqrt{\rho_+}})^2-2i}}. \tag{3.126}$$

Further, let

$$\widetilde{f}_\pm(v) := e^{-v^2}\widetilde{F}_\pm(v) = e^{-v^2}F_\pm(\frac{v}{\sqrt{\rho_\pm}}). \tag{3.127}$$

Let $\widetilde{I}^{\pm}_{N,h}$ be the truncated midpoint rule approximation to $\widetilde{I}^{\pm}$, given by

$$\widetilde{I}^{\pm}_{N,h} = h\sum_{n=-N}^{N+1} e^{-t_n^2}F_\pm(\frac{t_n}{\sqrt{\rho_\pm}}) \tag{3.128}$$

where $h = \sqrt{\pi/(N+1)}$ as recommended in [2], and $t_n = (n-0.5)h$. Then our approximation is

$$\widetilde{G}^N_h(X,Y) \approx \frac{-i}{4}\sum_{n=1-M}^{M-1} H_0^{(1)}(kr_n)e^{in\beta d} - \frac{e^{-ikY}}{2\pi\sqrt{\rho_-}}\widetilde{I}^{-}_{N,h} - \frac{e^{ikY}}{2\pi\sqrt{\rho_+}}\widetilde{I}^{+}_{N,h} \tag{3.129}$$

$$= \frac{-i}{4}\sum_{n=1-M}^{M-1} H_0^{(1)}(kr_n)e^{in\beta d} - \frac{he^{-ikY}}{2\pi\sqrt{\rho_-}}\sum_{n=-N}^{N+1} e^{-t_n^2}F_-(\frac{t_n}{\sqrt{\rho_-}}) - \frac{he^{ikY}}{2\pi\sqrt{\rho_+}}\sum_{n=-N}^{N+1} e^{-t_n^2}F_+(\frac{t_n}{\sqrt{\rho_+}}). \tag{3.130}$$

We implement (3.130) in Python with the same values of X, Y, k, d and β as in Part A. Since our approximation depends on the values of h and N, we choose an appropriate value of h as recommended in [2], which is $h = \sqrt{\pi/(N+1)}$, with different values of N. In order to obtain a high accuracy approximation, it is desirable to apply the modified truncated midpoint approximation to the formula (3.124). Let $\widetilde{I}^{*\pm}_{N,h}$ be the truncated modified midpoint rule approximation to $\widetilde{I}^{\pm}$, given by

$$\widetilde{I}^{*\pm}_{N,h} := \widetilde{I}^{\pm}_{N,h} + \widetilde{G}^{\pm}_{F_{m,m+1}}, \tag{3.131}$$

where $\widetilde{G}^{\pm}_{F_{m,m+1}}$ is the appropriate correction factor. Then the truncated modified midpoint rule approximation to (3.124) is

$$\widetilde{G}^{*N}_{\beta}(X,Y) \approx \frac{-i}{4}\sum_{n=1-M}^{M-1} H_0^{(1)}(kr_n)e^{in\beta d} - \frac{e^{-ikY}}{2\pi\sqrt{\rho_-}}\widetilde{I}^{*-}_{N,h} - \frac{e^{ikY}}{2\pi\sqrt{\rho_+}}\widetilde{I}^{*+}_{N,h}. \tag{3.132}$$

To calculate the correction factors $\widetilde{G}^{-}_{F_{m,m+1}}$ and $\widetilde{G}^{+}_{F_{m,m+1}}$, we first find the residues of $\widetilde{f}_{\pm}(v)$ at their poles. Since $F_-(v)$ has simple poles at

$$v^-_{\pm},_n := \pm e^{i\pi/4}\sqrt{w^-_n}$$

it follows that the function $\widetilde{F}_-(v) = F_-(\frac{v}{\sqrt{\rho_-}})$ has poles at

$$\widetilde{v}^-_{\pm},_n := \sqrt{\rho_-}v^-_{\pm},_n = \pm e^{i\pi/4}\sqrt{\rho_-}\sqrt{w^-_n}. \tag{3.133}$$

Similarly $\widetilde{F}_+(v) = F_+(\frac{v}{\sqrt{\rho_+}})$ has poles at

$$\widetilde{v}^+_{\pm},_n := \sqrt{\rho_+}v^+_{\pm},_n = \pm e^{i\pi/4}\sqrt{\rho_+}\sqrt{w^+_n}, \tag{3.134}$$

where w^-_n and w^+_n are defined in (3.36) and (3.38), respectively. The functions $\widetilde{F}_-(v)$ and $\widetilde{F}_+(v)$ have residues, denoted by $\widetilde{R}^-_{\pm,n}$ and $\widetilde{R}^+_{\pm,n}$, at the poles (3.133) and (3.134). Calculating these residues, repeating the procedure of (3.51 - 3.54), we see that, where

$$\widetilde{f}_{\pm}(v) := e^{-v^2}\widetilde{F}_{\pm}(v), \tag{3.135}$$

the residues of $\widetilde{f}_-(v)$ and $\widetilde{f}_+(v)$ are

$$Res(\widetilde{f}_-, \widetilde{v}^-_{\pm,n}) = \widetilde{R}^-_{\pm},_n \tag{3.136}$$

and

$$Res(\widetilde{f}_+, \widetilde{v}^+_{\pm,n}) = \widetilde{R}^+_{\pm,n}\,, \tag{3.137}$$

where

$$\widetilde{R}^-_{\pm,n} = \pm\sqrt{\rho_-}e^{(M-1)i(\beta+k)d}R^-_{\pm,n}\,, \tag{3.138}$$

and

$$\widetilde{R}^+_{\pm,n} = \pm\sqrt{\rho_+}e^{(1-M)i(\beta-k)d}R^+_{\pm,n}\,, \tag{3.139}$$

where $R^-_{\pm,n}$, and $R^+_{\pm,n}$, are defined by (3.53) and (3.54), respectively. Thus the residues of the functions $\widetilde{f}_\pm(v)$ are

$$\widetilde{R}^-_{\pm,n} = \pm\frac{\sqrt{\rho_-}e^{(M-1)i(\beta+k)d}(i(w_n^- - 2))^{-1/2}\cos(kX\sqrt{iw_n^-}\sqrt{i(w_n^- - 2)})e^{-iw_n^-\rho_-}}{2kde^{i\pi/4}\sqrt{w_n^-}e^{-ikdw_n^-}} \tag{3.140}$$

and

$$\widetilde{R}^+_{\pm,n} = \pm\frac{e^{(1-M)i(\beta-k)d}\sqrt{\rho_+}(i(w_n^+ - 2))^{-1/2}\cos(kX\sqrt{iw_n^+}\sqrt{i(w_n^+ - 2)})e^{-iw_n^+\rho_+}}{2kde^{i\pi/4}\sqrt{w_n^+}e^{-ikdw_n^+}}. \tag{3.141}$$

By the definition of the correction factor in Chapter 2, given by (2.31), for $F = \widetilde{F}_\pm(v)$, and repeating the steps from (3.59)- (3.63), we obtain

$$\widetilde{G}^-_{F_{m,m+1}} = 2\pi i\left(\widetilde{R}^-_{+,m}\frac{e^{2i(\pi\widetilde{s}_0/h+\frac{\pi}{2})}}{1-e^{2i(\pi\widetilde{s}_0/h+\frac{\pi}{2})}} + \widetilde{R}^-_{+,m+1}\frac{e^{2i(\pi\widetilde{s}_1/h+\frac{\pi}{2})}}{1-e^{2i(\pi\widetilde{s}_1/h+\frac{\pi}{2})}}\right) \tag{3.142}$$

and

$$\widetilde{G}^+_{F_{m,m+1}} = 2\pi i\left(\widetilde{R}^+_{+,m}\frac{e^{2i(\pi\widetilde{s^+_0}/h+\frac{\pi}{2})}}{1-e^{2i(\pi\widetilde{s^+_0}/h+\frac{\pi}{2})}} + \widetilde{R}^+_{+,m+1}\frac{e^{2i(\pi\widetilde{s^+_1}/h+\frac{\pi}{2})}}{1-e^{2i(\pi\widetilde{s^+_1}/h+\frac{\pi}{2})}}\right), \tag{3.143}$$

where

$$\widetilde{s}_0 := \widetilde{v}^-_{+,m} = e^{i\pi/4}\sqrt{\rho_-}\sqrt{w^-_m}, \tag{3.144}$$

$$\widetilde{s}_1 := \widetilde{v}^-_{+,m+1} = e^{i\pi/4}\sqrt{\rho_-}\sqrt{w^-_{m+1}}, \tag{3.145}$$

and $\widetilde{s}_2 := -\widetilde{s}_0$ and $\widetilde{s}_3 = -\widetilde{s}_1$ where m is defined in (3.44). Also,

$$\widetilde{s}_0^+ := \widetilde{v}_{+,m}^+ = e^{i\pi/4}\sqrt{\rho_+}\sqrt{w_m^+}, \tag{3.146}$$

$$\widetilde{s}_1^+ := \widetilde{v}_{+,m+1}^+ = e^{i\pi/4}\sqrt{\rho_+}\sqrt{w_{m+1}^+}, \tag{3.147}$$

$\widetilde{s}_2^+ := -\widetilde{s}_0^+$ and $\widetilde{s}_3^+ := -\widetilde{s}_1^+$, where m is defined in (3.50). Thus

$$\widetilde{G}_{F_{m,m+1}}^- := e^{(M-1)i(\beta+k)d}\sqrt{\rho_-}G_{F_{m,m+1}}^- \tag{3.148}$$

and

$$\widetilde{G}_{F_{m,m+1}}^+ := e^{(1-M)i(\beta-k)d}\sqrt{\rho_+}G_{F_{m,m+1}}^+, \tag{3.149}$$

where $G_{F_{m,m+1}}^-$ and $G_{F_{m,m+1}}^+$ are given by (3.70) and (3.71).

Similarly to (3.73) and (3.74), we adjust these definitions to include only poles in S_1, obtaining

$$\begin{aligned}\widetilde{G}_{F_{m,m+1}}^- = A_-\Bigg(&\frac{\mathbf{H}(1-|\mathrm{Im}v_{+,m}^-|)e^{-iw_m^-\rho_-}(i(w_m^- -2))^{-1/2}\cos(kX\sqrt{iw_m^-}\sqrt{i(w_m^- -2)})}{e^{-ikdw_m^-}\sqrt{w_m^-}}\frac{e^{2i(\pi\widetilde{s}_0/h+\frac{\pi}{2})}}{1-e^{2i(\pi\widetilde{s}_0/h+\frac{\pi}{2})}}\\ &+\frac{\mathbf{H}(1-|\mathrm{Im}v_{+,m+1}^-|)e^{-iw_{m+1}^-\rho_-}(i(w_{m+1}^- -2))^{-1/2}\cos(kX\sqrt{iw_{m+1}^-}\sqrt{i(w_{m+1}^- -2)})}{e^{-ikdw_{m+1}^-}\sqrt{w_{m+1}^-}}\\ &\frac{e^{2i(\pi\widetilde{s}_1/h+\frac{\pi}{2})}}{1-e^{2i(\pi\widetilde{s}_1/h+\frac{\pi}{2})}}\Bigg)\end{aligned} \tag{3.150}$$

and

$$\begin{aligned}\widetilde{G}_{F_{m,m+1}}^+ = A_+\Bigg(&\frac{\mathbf{H}(1-|\mathrm{Im}v_{+,m}^+|)e^{-iw_m^+\rho_+}(i(w_m^+ -2))^{-1/2}\cos(kX\sqrt{iw_m^+}\sqrt{i(w_m^+ -2)})}{e^{-ikdw_m^+}\sqrt{w_m^+}}\frac{e^{2i(\pi\widetilde{s}_2/h+\pi/2)}}{1-e^{2(i\pi\widetilde{s}_2/h+\pi/2)}}\\ &+\frac{\mathbf{H}(1-|\mathrm{Im}v_{+,m+1}^+|)e^{-iw_{m+1}^+\rho_+}(i(w_{m+1}^+ -2))^{-1/2}\cos(kX\sqrt{iw_{m+1}^+}\sqrt{i(w_{m+1}^+ -2)})}{e^{-ikdw_{m+1}^+}\sqrt{w_{m+1}^+}}\\ &\frac{e^{2i(\pi\widetilde{s}_3/h+\pi/2)}}{1-e^{2i(\pi\widetilde{s}_3/h+\pi/2)}}\Bigg),\end{aligned} \tag{3.151}$$

where $A_{\pm} = \frac{-2\pi i \sqrt{\rho_{\pm}} e^{\pm(1-M)i(\beta \mp k)d}}{kde^{i\pi/4}}$, and $\mathbf{H}$ is defined in (3.72). Hence our approximation is

$$\widetilde{G}_h^{*N}(X,Y) = \frac{-i}{4} \sum_{n=1-M}^{M-1} H_0^1(kr_n)e^{in\beta d} - \frac{e^{-ikY}}{2\pi\sqrt{\rho_-}} \left(h \sum_{n=-N}^{N+1} e^{-t_n^2} F_-(\frac{t_n}{\sqrt{\rho_-}}) + \widetilde{G}^-_{F_{m,m+1}} \right)$$
$$- \frac{e^{ikY}}{2\pi\sqrt{\rho_+}} \left(h \sum_{n=-N}^{N+1} e^{-t_n^2} F_+(\frac{t_n}{\sqrt{\rho_+}}) + \widetilde{G}^+_{F_{m,m+1}} \right), \tag{3.152}$$

where $t_n = (n - 1/2)h$ and $h = \sqrt{\pi/N + 1}$.

We perform a similar test to Form 1, but now we approximate $\widetilde{I}^{\pm}$, given by (3.124), by the modified truncated midpoint rule approximation, given by (3.152), with the same set of input values that we used for Table 3.9. The results are shown in Table 3.10. The numerical results for evaluating (3.110) and (3.122)

N	M	the truncated midpoint rule approximation	the modified truncated midpoint rule approximation
20	1	**-0.4595**8585073152763-**0.3509**9941195444506 i	**-0.459529879**4951679-**0.350913086**9145297 i
30	1	**-0.4595**1495074046667-**0.35091**684219697433 i	**-0.459529879477**247-**0.3509130869380**6295 i
40	1	**-0.459529**2485922545-**0.35091**0077265403 i	**-0.45952987947737** 3-**0.3509130869382**199 i
20	2	**-0.459529**63961026716-**0.35091**036653857255 i	**-0.45952987947737**306 -**0.3509130869382**183 i
30	2	**-0.459529**97736545376 -**0.350913**2466351009 i	**-0.4595298794773**739 -**0.3509130869382171 i**
40	2	**-0.4595298**603878907 -**0.35091308**40252366 i	**-0.45952987947737**395 -**0.35091308693821716**i
20	3	**-0.459529**95116241235-**0.350913**2388442773 i	**-0.459529879477374 - 0.3509130869382171 i**
30	3	**-0.45952987**758771896-**0.35091308**09012767 i	**-0.45952987947737**41 -**0.35091308693821716** i
40	3	**-0.45952987**971926484- **0.35091308**72470183 i	**-0.459529879477374- 0.3509130869382171 i**
20	4	**-0.4595298**644133188 -**0.35091308**159931256 i	**-0.45952987947737**417- **0.3509130869382172** i
30	4	**-0.45952987**967839276- **0.35091308**72404562 i	**-0.45952987947737**417- **0.3509130869382172** i
40	4	**-0.4595298794**700997-**0.3509130869**2548984 i	**-0.45952987947737**417- **0.35091308693821716** i

Table 3.10: Comparison between the efficiency of the truncated midpoint approximation and the modified truncated midpoint approximation when $N = 20, 30, 40$ with $M = 1, 2, 3, 4$ for $X = 0, Y = 0.04, k = 0.5$ and $\beta = \sqrt{2}/4$.

using the modified truncated midpoint approximation formula and the truncated midpoint approximation with the same inputs, taken from (Table 2, [28]), with $M = 1, 2, 3, 4$, are shown in Tables 3.9 and 3.10. We obtain the same results from both forms. From Tables 3.9 and 3.10 we see that the accuracy achieved by the modified truncated midpoint rule approximation is dramatically increased, achieving 10, 12, 14 digits accuracy for $N = 20, 30, 40$ with $M = 1$, compared to the accuracy of the approximation by the standard midpoint rule which achieves only $4, 4, 6$ digits accuracy, respectively, for the same numbers of quadrature points. For $N = 20, 30, 40$ with $M = 4$, we see that the modified truncated midpoint rule obtains 15 digits accuracy, whereas the truncated midpoint rule achieves only $7, 9, 11$ correct digits for $N = 20, 30, 40$ respectively. Thus for both forms, we achieve faster convergence using the modification, and significantly higher accuracy with larger values of M.

3.5 Comparison with other methods

Now, as promised at the beginning of the chapter, we compare results from our modified midpoint rule approximation with Ewald's method (E.M.), recommended as the most efficient computational method in the review paper [28], and with the recent asymptotic correction terms method (A.C.T.) of [30]. The modified truncated midpoint rule (M.M.R.) shows perfect agreement with these state-of-the-art methods. We first state the approximation formulas for these methods which have been applied to evaluate the quasi-periodic Green's function. The first formula is Ewald's, given in [28, Eq.(2.65)] as

$$G_\beta^d(X,Y) \approx \frac{-1}{4} \sum_{m=-M_1}^{M_1} \frac{e^{i\beta_m Y}}{\gamma_m d} \left[e^{\gamma_m Y} \mathrm{erfc}\left(\frac{\gamma_m d}{2a} + \frac{2X}{d}\right) + e^{-\gamma_m X} \mathrm{erfc}\left(\frac{\gamma_m d}{2a} - \frac{2X}{d}\right)\right] - \frac{1}{4\pi} \sum_{m=-M_2}^{M_2} e^{im\beta d} \sum_{n=0}^{N} \frac{1}{n!} \left(\frac{kd}{2a}\right)^{2n} E_{n+1}\left(\frac{a^2 r_m^2}{d^2}\right), \tag{3.153}$$

where β_m and γ_m are given in and above (3.21), and M_1, M_2, $N \in \mathbb{N}$ and $a > 0$ are parameters to be chosen that determine the accuracy of this approximation. The second is the asymptotic correction terms formula, proposed in [30, Eq.(3.6)], given by

$$G_\beta^d(X,Y) \approx \sigma_+(M) + \sigma_-(M) - \frac{i}{4} \sum_{n=1-M}^{M-1} H_0^{(1)}(kr_n) e^{idn\beta}, \tag{3.154}$$

where

$$\sigma_\pm(M) := \frac{-i}{4}\sqrt{\frac{2}{\pi kd}}e^{i(\pm kY-\pi/4)}\frac{e^{iM\alpha\pm}}{\sqrt{M}(1-e^{i\alpha_\pm})}\left(1+C_\pm/M+D_\pm/M^2\right),$$

$$C_\pm := A_\pm/kd \mp \frac{e^{i\alpha_\pm}}{2(1-e^{i\alpha_\pm})},$$

$$A_\pm := \frac{-i\pm 4kY}{8}, \quad \alpha_\pm = d(k\pm\beta),$$

$$B_\pm := \frac{-9+16k^2(3Y^2-2X^2)\pm 24kY}{128},$$

and

$$D_\pm := \frac{B_\pm}{k^2d^2} - \frac{3A_\pm e^{i\alpha\pm}}{2kd(1-e^{i\alpha_\pm})} \pm \frac{3e^{i\alpha_\pm}(1+e^{i\alpha_\pm})}{8(1-e^{i\alpha_\pm})^2}.$$

The third is our approximation, given by

$$G_h^d(X,Y) \approx G_h^{*N}(X,Y) = \frac{-i}{4}\sum_{n=1-M}^{M-1} H_0^{(1)}(kr_n)e^{in\beta d} - \frac{he^{-ikY}}{2\pi}\sum_{n=-N}^{N+1} e^{-\rho_- v_n^2}F_-(v) + G^{-,*}_{F_{m,m+1}}$$
$$- \frac{he^{ikY}}{2\pi}\sum_{n=-N}^{N+1} e^{-\rho_+ v_n^2}F_+(v) + G^{+,*}_{F_{m,m+1}}, \tag{3.155}$$

where $G^{-,*}_{F_{m,m+1}}$ and $G^{+,*}_{F_{m,m+1}}$ are given by (3.118) and (3.119), respectively. Ewald's formula involves the complementary error function erfc and an exponential integral E_n, defined in (7.2.1) and (5.1.4) in [1], respectively, as

$$\text{erfc}(z) = \frac{2}{\sqrt{\pi}}\int_z^\infty e^{-t^2}dt = 1-\text{erf}(z)$$

and

$$E_n(z) = \int_1^\infty \frac{e^{-zt}}{t^n}dt.$$

To evaluate (3.153) requires the evaluation of a sum with $2M_1+1$ terms, each term requiring two evaluations of erfc, plus evaluations of a double sum with $(2M_2+1)(N+1)$ terms, each term requiring evaluations of an exponential integral.

To evaluate the asymptotic correction terms formula (3.154) requires the evaluation of the same sum with $2M-1$ terms, each term requiring evaluation of the Hankel function, plus computation of $\sigma_{\pm}(M)$. Our approximation formula (3.155) requires the evaluation of a sum with $2M-1$ terms, each term requiring an evaluation of a Hankel function, plus two $N+1$ term sums to evaluate the two midpoint rule approximations. Table 3.11 summarises these computational requirements.

Method	Computations needed to evaluate the approximations	Numbers of terms for data of Table 3.13
M.M.R	A $2M-1$ term sum, with a Hankel function to evaluate in each term, plus	$2M-1=5$
	two $N+1$ term sums to evaluate the two midpoint rule approximations	$2(N+1)=14$
A.C.T.	A $2M-1$ term sum, with a Hankel function to evaluate in each term	$2M-1=513$
E.M.	A $2M_1+1$ term sum, each term requiring 2 evaluations of erfc, plus a	$2M_1+1=9$
	$(2M_2+1)(N+1)$ term sum, each term needing evaluation of an exponential integral	$(2M_2+1)(N+1)=145$

Table 3.11: Computational requirements of the modified truncated midpoint rule method (M.M.R), the asymptotic correction terms formula (A.C.T) and Ewald's method (E.M).

Tables 3.12 and 3.13 compare our method with E.M. and A.C.T, using the same parameter values previously selected in [28] and [30]. Table 3.12 shows the results for $X=0$, $Y=0.04$, $k=0.5$ and $\beta=\sqrt{2}/4$, which corresponds to an incident wave of wavelength 4π at 45° to a grating, and Table 3.13 shows the results for $X=0$, $Y=0.04$, $k=10/4=5/2$ (a higher frequency), and $\beta=5\sqrt{2}/4$, which corresponds to an incident wavelength $4\pi/5$ at 45° to a grating. The use of Ewald's method accelerates the convergence of the series (3.19) significantly; according to Linton [28] the optimal values of the parameters M_1, M_2, N and a are $N=7$, $M_1=3$, $M_2=2$ and $a=2$ (see [28, Table 2]) for the parameter values of Table 3.12, and $N=28$, $M_1=4$, $M_2=2$ and $a=1$ ([28, Table 3]) for the parameter values of Table 3.13, to achieve 10-figures accuracy in both the real and imaginary parts, as sought by Linton. The asymptotic correction terms method requires $M=936$ (see [30, Table 1]) and $M=257$ in (see [30, Table 2]) to reach the same accuracy for the same parameter values. In Tables 3.12 and 3.13 we compare these results with our approximation. We obtain the same 10-figure accuracy with $M=3$ and $N=6$ in both tables.

Method	N	M	M_1	M_2	a	$G^d_\beta(X,Y)$
E.M.	7	N/A	3	2	2	**-0.4595298794 - 0.3509130869i**
A.C.T.	N/A	936	N/A	N/A	N/A	**-0.4595298794 - 0.3509130869i**
M.M.R.	6	3	N/A	N/A	N/A	**-0.4595298794 - 0.3509130869i**

Table 3.12: Comparison between our method and Ewald's method (3.153) from [28] and the asymptotic correction terms method (3.154) from [30]

Method	N	M	M_1	M_2	a	$G^d_\beta(X,Y)$
E.M	28	N/A	4	2	1	**-0.3538172307 - 0.1769332383i**
A.C.T.	N/A	257	N/A	N/A	N/A	**-0.3538172307 - 0.1769332383i**
M.M.R.	6	3	N/A	N/A	N/A	**-0.3538172307 - 0.17693323825i**

Table 3.13: Comparison between our method and Ewald's method (3.153) from [28] and the asymptotic correction terms method (3.154) from [30]

.

The modified truncated midpoint rule approximation for these two test cases taken from [28] and [30] shows good agreement with both Ewald's method and the asymptotic correction term method. For these specific test cases, used in [28], [30], our method does not require such a large number of terms to be calculated in order to reach 10 significant figures as the other methods, we are comparing with, taken from [28] [30](see Tables 3.11, 3.12 and 3.13), so that our computational method appears to be more efficient. Also, our method has only two truncation parameters M and N to adjust, unlike Ewald's method, which requires four parameters to be chosen. On the other hand, the A.C.T. method only has the parameter M; to achieve a specific accuracy it is a matter simply of increasing M until this accuracy is reached. It is unclear for our method, except by trial and error in a specific case, how to choose M and N optimally. (The same comment applies to the four parameters of Ewald's method.) Having said this, in Section 4.2 (see Tables 41-44) we will establish choices of M and N which provide high accuracy over wide ranges of the parameters X, Y, k, d, and β.

Chapter 4

Error Analysis

In this chapter we provide a bound on the actual error in the modified truncated midpoint rule based on our new Theorem 2.9, for $F = F_{-}$, given by (3.33). This function is analytic in the strip $S_H = \{v \in \mathbb{C} : |\mathrm{Im}(v)| < H\}$. We will apply our new Theorem 2.9, showing how the theoretical bound on the actual error is obtained. In Section 4.1 we first provide a bound on the actual error $|E_h^{*N}|$, choosing an appropriate values of H (in the definition of S_H) and an appropriate value of h. Then we turn our attention to find the upper bounds of $F_{-}(v)$, denoted by $M^{(1)}, M^{(2)}$ and $M^{(3)}$, and we show a completely explicit error bound in Theorem 4.10. In section 4.2, we test the standard truncated midpoint rule approximation and the modified truncated midpoint rule more systematically throughout the possible range of parameter values (see tests A and B). For these two tests, we see that the modified truncated midpoint rule is more accurate and efficient, provided X is not too large and d in not too small.

4.1 Bound on the actual error E_h^{*N}

Here we demonstrate a bound on $|E_h^{*N}| = |I - I_h^{*N}|$, when $I^{\pm}$ is approximated by the truncated modified midpoint method, this approximation denoted by $I_{N,h}^{*\pm}$. By

Theorem 2.9, we have

$$
\begin{aligned}
|E_h^{*N}| \leq & \frac{2\sqrt{\pi} M_3(H,(N+1)h) e^{\rho H^2 - 2\pi H/h}}{\sqrt{\rho}(1-e^{-2\pi H/h})} \\
& + e^{-\rho(N+1)^2 h^2} \left(\frac{M_1((N+1)h)}{\rho(N+1)h} + 2H M_2(H,(N+1)h) \right)
\end{aligned}
\tag{4.1}
$$

provided $h < 2\pi/\rho H$. We choose a fixed $H \in (0,1)$, close to 1 (e.g.$H = 0.9$) and choose h to equalise the exponents in $e^{-\rho(N+1)^2h^2}$ and $e^{\rho H^2 - 2\pi H/h}$ (i.e choose h so that $\rho H^2 - 2\pi H/h = -\rho(N+1)^2h^2$). Precisely, let

$$
p(h) := \rho(N+1)^2 h^3 + \rho H^2 h - 2\pi H, \qquad h > 0.
$$

Then $\rho H^2 - 2\pi H/h = -\rho(N+1)^2h^2) \iff p(h) = 0$. Further since $p(0) = -2\pi H < 0$, $p^{'}(h) = 3\rho(N+1)^2h^2 + \rho H^2 > 0$, for $h > 0$. The equation $p(h) = 0$ has a unique positive solution of that, we will denote it by h^*. Let $\phi := \frac{h^*}{h^+}$, where $h^+ := (\frac{2\pi H}{\rho(N+1)^2})^{1/3}$. Then We can express the $p(h^*) = 0$ as

$$
\phi^3 + 3b\phi - 1 = 0 \tag{4.2}
$$

where

$$
b := \frac{H^2}{3(N+1)^2(h^+)^2}. \tag{4.3}
$$

Clearly (4.2) has a unique real solution ϕ with $\phi \in (0,1)$. From the standard formula for solutions of cubic equations

$$
\begin{aligned}
\phi &= \sqrt[3]{\frac{1}{2} + \sqrt{\frac{1}{4} + b^3}} + \sqrt[3]{\frac{1}{2} - \sqrt{\frac{1}{4} + b^3}}, \\
&= \frac{1}{\left(\sqrt{\frac{1}{4} + b^3} + \frac{1}{2}\right)^{2/3} + b + \left(\sqrt{\frac{1}{4} + b^3} - \frac{1}{2}\right)^{2/3}}.
\end{aligned}
\tag{4.4}
$$

so $\phi \sim \frac{1}{3b}$, as $b \to \infty$, and $\phi \to 1$, as $b \to 0$. We will require the following Lemma for bounding ϕ in terms of b (see [26], Proposition 2.3.17).

Lemma 4.1. *If $b > 0$ and ϕ is given by (4.4), then*

$$\frac{1}{1+3b} \leq \phi \leq \frac{1}{1+b}. \tag{4.5}$$

By setting $h = h^* = h^+\phi \geq c := \left(\frac{2\pi H}{\rho(N+1)^2}\right)^{1/3} \frac{1}{1+3b}$ and $A := (N+1)h^*$ in (4.1) we have

$$\begin{aligned} |E_{h^*}^{*N}| &\leq e^{-\rho(N+1)^2 h^{*2}} \left(\frac{2\sqrt{\pi} M_{H,A}}{\sqrt{\rho}(1-e^{-2\pi H/h^*})} + \frac{M_A}{\rho(N+1)h^*} + 2HM^{H,A} \right) \\ &= e^{-\rho(N+1)^2(h^+\phi)^2} \left(\frac{2\sqrt{\pi} M_{H,A}}{\sqrt{\rho}(1-e^{-2\pi H/(h^+\phi)})} + \frac{M_A}{\rho(N+1)h^+\phi} + 2HM^{H,A} \right). \end{aligned} \tag{4.6}$$

Let $a = \rho(N+1)^2$ so that $-\rho(N+1)^2(h^+\phi)^2 = -a(h^+\phi)^2$. Since $h^+\phi \geq c > 0$, it follows that

$$a(h^+\phi)^2 \geq ac^2$$

$$\implies -a(h^+\phi)^2 \leq -ac^2$$

$$\implies e^{-a(h^+\phi)^2} \leq e^{-ac^2}$$

where

$$ac^2 = \frac{\rho^{1/3}(2\pi)^2(H)^{2/3}(N+1)^2}{[(N+1)^{2/3}(2\pi)^{2/3} + H^{4/3}\rho^{2/3}]^2}. \tag{4.7}$$

Also, $\rho(N+1)h^+\phi \geq \frac{\rho(N+1)h^+}{1+3b} =: \hat{s} > 0$,

$$\implies \frac{1}{\rho(N+1)h^+\phi} \leq \frac{1}{\hat{s}},$$

where

$$\hat{s} = \frac{\rho^{2/3} 2\pi(N+1)H^{1/3}}{(2\pi)^{2/3}(N+1)^{2/3} + \rho^{2/3}H^{4/3}}. \tag{4.8}$$

Using (4.5), further, where $s := \frac{2\pi H(1+b)}{h^+}$

$$h^+\phi \leq \frac{h^+}{1+b} \implies \frac{1}{h^+\phi} \geq \frac{1+b}{h^+}$$

$$\Longrightarrow \frac{-2\pi H}{h^+\phi} \le \frac{-2\pi H(1+b)}{h^+} = -s \Longrightarrow e^{\frac{-2\pi H}{h^+\phi}} \le e^{-s}$$

$$\Longrightarrow 1 - e^{\frac{-2\pi H}{h^+\phi}} \ge 1 - e^{-s} \Longrightarrow \frac{1}{1 - e^{\frac{-2\pi H}{h^+\phi}}} \le \frac{1}{1 - e^{-s}},$$

where

$$s = (2\pi H)^{2/3}(N+1)^{2/3}\rho^{1/3} + \frac{H^2\rho}{3}. \tag{4.9}$$

Hence

$$|E_{h^*}^{*N}| \le e^{-ac^2}\left(\frac{2\sqrt{\pi}M_{H,A}}{\sqrt{\rho}(1-e^{-s})} + \frac{M_A}{\hat{s}} + 2HM^{H,A}\right). \tag{4.10}$$

Next, we concern ourselves with deriving formulas for the terms $M_{(N+1)h}$, $M_{H,(N+1)h}$ and $M^{H,(N+1)h}$, we denote them respectively as $M^{(1)}, M^{(2)}$, and $M^{(3)}$.

4.1.1 A bound for $M^{(1)}, M^{(2)}, M^{(3)}$

From the definition of these three upper bounds in Chapter 2,Theorem 2.9, given by (2.41), (2.42), and (2.43), let $F = F_-$. We will find these upper bounds of the function F_- which is given by (3.33)

$$F_-(v) = \frac{\cos[kXv\sqrt{v^2-2i}]}{(e^{-kdv^2} - e^{i(\beta+k)d})\sqrt{v^2-2i}} \tag{4.11}$$

where suprema of $F_-(v)$ are given respectively by

$$M^{(1)} := \sup_{v\ge A}|F(v)| \quad \text{for} \quad A > 0, \tag{4.12}$$

$$M^{(2)} := \sup_{-A\le t\le A}|F(t+iH)| \quad \text{for} \quad 0 < H < 1, \tag{4.13}$$

and

$$M^{(3)} := \max_{0\le y\le H}|F(A+iy) + F(-A+iy)| \quad \text{for} \quad 0 < H < 1. \tag{4.14}$$

4.1.1.1 A bound for $M^{(1)}$

First , let us bound $M^{(1)}$

$$M^{(1)} := \sup_{v \geq A} |F(v)| \tag{4.15}$$

where

$$|F(v)| = \frac{|\cos(kXv\sqrt{v^2 - 2i})|}{|e^{-kdv^2} - e^{i(\beta+k)d}\sqrt{v - 2i}|}. \tag{4.16}$$

For $A > 0$ and $v \geq A$, we have

$$\begin{aligned} |e^{-kdv^2} - e^{i(\beta+k)d}| &\geq |e^{-kdv^2}| - |e^{i(\beta+k)d}| \\ &= 1 - e^{-kdv^2}. \end{aligned} \tag{4.17}$$

For $v \geq A > 0$, $e^{-kdv^2} < e^{-kdA^2} < 1$, so

$$|e^{-kdv^2} - e^{i(\beta+k)d}| \geq 1 - e^{-kdA^2} > 0,$$

so

$$\frac{1}{|e^{-kdv^2} - e^{i(\beta+k)d}|} \leq \frac{1}{1 - e^{-kdA^2}}, \tag{4.18}$$

$v \geq A > 0$. Also,

$$|v^2 - 2i|^{1/2} = (v^4 + 4)^{1/4} \geq 4^{1/4} = \sqrt{2}, \tag{4.19}$$

$v \in \mathbb{R}$. Now, for $x, y \in \mathbb{R}$,

$$\begin{aligned} |\cos(x + iy)| &= \sqrt{\cos^2(x)\cosh^2(y) + \sin^2(x)\sinh^2(y)} \\ &= \sqrt{(1 - \sin^2(x))\cosh^2(y) + \sin^2(x)\sinh^2(y)} \\ &= \sqrt{\cosh^2(y) - \sin^2(x)\cosh^2(y) + \sin^2(x)\sinh^2(y)} \\ &= \sqrt{\cosh^2(y) - \sin^2(x)(\cosh^2(y) - \sinh^2(y))}. \end{aligned}$$

Since $\cosh^2(y) - \sinh^2(y) = 1$, it follows that

$$|\cos(x+iy)| = \sqrt{\cosh^2(y) - \sin^2(x)} \leq \sqrt{\cosh^2(y)} = \cosh(y). \tag{4.20}$$

We have shown (also see [1] equation[4.3.84, p 75]),that, for $z = x + iy \in \mathbb{C}$,

$$|\cos(z)| = |\cos(x+iy)| \leq \cosh(y) = \cosh(\mathrm{Im}(z)).$$

Thus for $v \in \mathbb{R}$,

$$\begin{aligned} |\cos(kXv\sqrt{v^2-2i})| &\leq \cosh(\mathrm{Im}(kXv\sqrt{v^2-2i})) \\ &= \cosh(kXv\mathrm{Im}(\sqrt{v^2-2i})). \end{aligned} \tag{4.21}$$

Now $\sqrt{v^2-2i} = x + yi$, with

$$x = \pm\sqrt{\frac{v^2+\sqrt{v^4+4}}{2}}$$

and

$$y = \pm\frac{-\sqrt{2}}{\sqrt{v^2+\sqrt{v^4+4}}}.$$

Since cosh is even function (4.21) becomes

$$|\cos(kXv\sqrt{v^2-2i})| \leq \cosh(kXv\frac{\sqrt{2}}{\sqrt{v^2+\sqrt{v^4+4}}}), \tag{4.22}$$

since $v^4 + 4 > v^4$, this implies that,

$$|\cos(kXv\sqrt{v^2-2i})| < \cosh(kX), \tag{4.23}$$

for all $v \in \mathbb{R}$. By (4.18), (4.19) and (4.23) we have

$$|F(v)| \leq \frac{\cosh(kX)}{\sqrt{2}(1-e^{-kdA^2})}. \tag{4.24}$$

Hence

$$M^{(1)} := \sup_{v \geq A} |F(v)| \leq \frac{\cosh(kX)}{\sqrt{2}(1 - e^{-kdA^2})}. \tag{4.25}$$

4.1.1.2 A bound for $M^{(2)}$

Now, let us bound $M^{(2)}$ in the case when $F = F_{-}$. From the formula (3.33), we have that

$$|F(t + iH)| = \frac{|\cos[kX(t + iH)((t + iH)^2 - 2i)^{1/2}]|}{|e^{-kd(t+iH)^2} - e^{i(\beta+k)d}||(t + iH)^2 - 2i|^{1/2}} \tag{4.26}$$

Lemma 4.2. *Given $H \in (0, 1)$, and $t \in \mathbb{R}$, if $v = t + iH$, then*

$$|v^2 - 2i| \geq 1 - H^2. \tag{4.27}$$

Proof. Notting that $|v^2 - 2i| = |v - (1 + i)||v + (1 + i)|$, we have

$$\begin{aligned} |v^2 - 2i| &= |t + iH - (1 + i)||t + iH + (1 + i)| \\ &= |(t - 1) + i(H - 1)||(t + 1) + i(H + 1)| \\ &= \sqrt{(t - 1)^2 + (H - 1)^2}\sqrt{(t + 1)^2 + (H + 1)^2} \\ &\geq |H - 1||H + 1| = |H^2 - 1| = 1 - H^2. \end{aligned} \tag{4.28}$$

□

It is useful to note that, if $-A \leq t \leq A$, $H \in (0, 1)$, and $v = t + iH$, then

$$|e^{-kdv^2} - e^{i(\beta+k)d}| \geq |e^{-kd(t+iH)^2}| - |e^{i(\beta+k)d}| \geq e^{kd(H^2-t^2)} - 1. \tag{4.29}$$

Note also that with $t = \pm H$, the $e^{kd(H^2-t^2)} - 1$ will be zero. It means when $t = H$, there is a pole located on the line $\text{Im}(v) = H$, if the distance between this pole and other poles is zero the bound on $|e^{-kdv^2} - e^{i(\beta+k)d}| = 0$. So for this reason, it is a sensible to choose H which does not pass through the points, that make $|e^{-kdv^2} - e^{i(\beta+k)d}| \neq 0$.

We have two cases

Case 1 $|H^2 - t^2| \geq \epsilon$

- For $t^2 \geq H^2 + \epsilon$, and $v = t + iH$, then

$$\begin{aligned} |e^{-kdv} - e^{i(\beta+k)d}| &\geq |e^{i(\beta+k)d}| - |e^{-kdv^2}| \\ &\geq 1 - e^{kd(H^2-t^2)}, \\ &\geq 1 - e^{-kd\epsilon} = e^{-kd\epsilon}(e^{kd\epsilon} - 1) \quad \geq kd\epsilon e^{-kd\epsilon}. \end{aligned} \tag{4.30}$$

- For $t^2 \leq H^2 - \epsilon$, and $v = t + iH$, then

$$\begin{aligned} |e^{-kdv^2} - e^{i(\beta+k)d}| &\geq |e^{-kdv^2}| - |e^{i(\beta+k)d}|, \\ &\geq e^{kd(H^2-t^2)} - 1 \\ &\geq e^{kd\epsilon} - 1 \\ &\geq kd\epsilon \geq kd\epsilon e^{-kd\epsilon}. \end{aligned} \tag{4.31}$$

So, for $|H^2 - t^2| \geq \epsilon$, we have

$$\frac{1}{|e^{-kdv^2} - e^{i(\beta+k)d}|} \leq \frac{e^{kd\epsilon}}{kd\epsilon}. \tag{4.32}$$

Case 2 $|H^2 - t^2| < \epsilon$

We now consider the case $|H^2 - t^2| < \epsilon$. In this case we can not obtain a positive lower bound on $|e^{-kdv^2} - e^{i(\beta+k)d}|$, where $v = t + iH$ and $0 < H < 1$. We use another way to find a positive lower bound, so

$$\begin{aligned} e^{-kdv^2} - e^{i(\beta+k)d} &= e^{-kd(t^2-H^2)}e^{-2iHtkd} - e^{i(\beta+k)d} \\ &= e^{-2iHtkd}\left(e^{kd(H^2-t^2)} - e^{i((\beta+k)d+2tHkd)}\right) \\ &= e^{-2iHtkd}(r - e^{i\alpha t}) \end{aligned} \tag{4.33}$$

where $r = e^{kd(H^2-t^2)}$ and

$$\alpha(t) = (\beta + k)d + 2tHkd. \tag{4.34}$$

Taking absolute values we have

$$|e^{-kdv^2} - e^{i(\beta+k)d}| = |r - e^{i\alpha}| = |r - \cos\alpha - i\sin\alpha| \tag{4.35}$$

so

$$|e^{-kdv^2} - e^{i(\beta+k)d}| = \sqrt{(r - \ \cos\alpha)^2 + \sin^2\alpha} \geq |\sin\alpha(t)| \tag{4.36}$$

Note that $|\sin\alpha(t)|$ is not bounded below by a positive constant on the whole real line, since $|\sin\alpha(t)| = 0$ if $t = \frac{n\pi-(\beta+k)d}{2kdH}$, for some $n \in \mathbb{Z}$. So it can be useful to obtain a lower bound if we choose t close to $+H$ or $-H$. Let

$$\alpha^{\pm} := (\beta + k)d \pm 2H^2kd \tag{4.37}$$

i.e,

$$\alpha^{\pm} = \alpha(\pm H).$$

If we choose $t = \pm H$ or t close to $\pm H$, then $\alpha(t)$ will be close to the corresponding value $\alpha^{\pm}$, and, if $\sin\alpha^{\pm} \neq 0$, then $|\sin\alpha(t)| > 0$ for t close to $\pm H$. So, assuming that we choose $H \in (0, 1)$ so that $\sin\alpha^{\pm} \neq 0$, to show that $|\sin\alpha(t)| > 0$ for t close to $\pm H$, we have two cases, case A and case B.

Case A Suppose $|t-H| < \delta$, for some $\delta > 0$ small enough. The difference between $\alpha(t)$ and $\alpha(H)$ is

$$\alpha(t) - \alpha(H) = -2kdH(H - t) = 2kdH(t - H)$$

so that

$$
\begin{aligned}
\sin(\alpha(t)) &= \sin(\alpha(H) + (\alpha(t) - \alpha(H))) \\
&= \sin(\alpha^+ - 2kdH(H-t)) \\
&= \sin(\alpha^+)\cos(2kdH(H-t)) - \cos(\alpha^+)\sin(2kdH(H-t))
\end{aligned}
\tag{4.38}
$$

Taking absolute values and applying the reverse triangle inequality, we have

$$
|\sin(\alpha(t))| \geq |\sin(\alpha^+)||\cos(2kdH(H-t))| - |\cos(\alpha^+)||\sin(2kdH(H-t))|.
\tag{4.39}
$$

Now, simplifying by using $|\cos\alpha^+| \leq 1$, and $|\sin x| \leq |x|$, for $x \in \mathbb{R}$,

$$
|\cos(\alpha^+)||\sin(2kdH(H-t))| \leq 2kdH|H-t|
$$

and

$$
\begin{aligned}
|\sin(\alpha(t))| &\geq |\sin(\alpha^+)||\cos(2kdH(H-t))| - 2kdH|H-t|, \\
&= |\sin(\alpha^+)|\sqrt{1-\sin^2(2kdH(H-t))} - 2kdH|H-t|.
\end{aligned}
\tag{4.40}
$$

Since $\sin^2(2kdH(H-t)) \leq 4H^2k^2d^2(H-t)^2$, it follows that

$$
\sqrt{1-\sin^2(2kdH(H-t))} \geq \sqrt{1-4H^2k^2d^2(H-t)^2},
$$

so

$$
|\sin(\alpha(t))| \geq |\sin(\alpha^+)|\sqrt{1-4H^2k^2d^2(H-t)^2} - 2kdH|H-t|,
\tag{4.41}
$$

provided $2kdH|H-t| \leq 1$. Hence, provided $2kdH|H-t| \leq 1$,

$$
|e^{-kdv^2} - e^{i(\beta+k)d}| \geq |\sin(\alpha(t))| \geq |\sin(\alpha^+)|\sqrt{1-4H^2k^2d^2(H-t)^2} - 2kdH|H-t|.
\tag{4.42}
$$

Now suppose that $|\sin(\alpha^+)| > 0$, and let $\theta = 2kdH|(H-t)|$ and $p = |\sin(\alpha^+)| \in$

$(0, 1]$, so that (4.42) is

$$|e^{-kdv^2} - e^{i(\beta+k)d}| \geq p\sqrt{1-\theta^2} - \theta. \tag{4.43}$$

If $\theta \leq p/2$, then $-\theta \geq -p/2$, and

$$\begin{aligned} |e^{-kdv^2} - e^{i(\beta+k)d}| &\geq p\sqrt{1-p^2/4} - p/2 \\ &= \frac{p}{2}\left(\sqrt{4-p^2} - 1\right) \\ &= \frac{p(3-p^2)}{2(1+\sqrt{4-p^2})}, \end{aligned} \tag{4.44}$$

since $3 - p^2 \geq 2$ and $4 - p^2 \leq 4$ it follows that

$$|e^{-kdv^2} - e^{i(\beta+k)d}| \geq \frac{p}{3}. \tag{4.45}$$

So if $|\ \mathrm{sin}\alpha^+| > 0$, and $\theta = 2kdH|H-t| \leq \frac{|\mathrm{sin}\alpha^+|}{2}$, then

$$|e^{-kdv^2} - e^{i(\beta+k)d}| \geq \frac{|\mathrm{sin}\alpha^+|}{3}. \tag{4.46}$$

Recall as case 2 condition that $|H^2 - t^2| = |H+t||H-t| \leq \epsilon$. If t is close to $+H$, then $|H+t|$ is close to $2H$, so this condition is quite similar to $\theta = 2kdH|H-t| \leq \frac{|\mathrm{sin}\alpha^+|}{2}$, if we take $\epsilon = \frac{|\ \mathrm{sin}\alpha^+|}{2}$.

Case B

Similarly for case B, suppose $|t + H| < \delta$ for some small δ, so the difference between $\alpha(t)$ and $\alpha^- = \alpha(-H)$ is

$$\alpha(t) - \alpha(-H) = 2Hkd(t+H). \tag{4.47}$$

Then

$$\begin{aligned} \sin(\alpha(t)) &= \sin(\alpha(-H) + (\alpha(t) - \alpha(-H))) \\ &= \sin(\alpha^- + 2kdH(H+t)) \\ &= \sin(\alpha^-)\cos(2kdH(H+t)) + \cos(\alpha^-)\sin(2kdH(H+t)). \end{aligned} \tag{4.48}$$

Taking absolute values, applying the reverse triangle inequality, also simplifying by using $|\cos\alpha^-| \leq 1$, and $|\sin x| \leq |x|$, for $x \in \mathbb{R}$, we have

$$\begin{aligned} |\sin(\alpha(t))| &\geq |\sin(\alpha^-)||\cos(2kdH(H+t))| - |\cos(\alpha^-)||\sin(2kdH(H+t))| \\ &\geq |\sin(\alpha^-)||\cos(2kdH(H+t))| - 2kdH|H+t| \\ &\geq |\sin(\alpha^-)|\sqrt{1-4H^2k^2d^2(H+t)^2} - 2k^2d^2H|H+t|. \end{aligned} \tag{4.49}$$

provided $2kdH|H+t| < 1$. Hence, provided $2kdH|H+t| < 1$,

$$|e^{-kdv^2} - e^{i(\beta+k)d}| \geq |\sin(\alpha(t))| \geq |\sin(\alpha^-)|\sqrt{1-4H^2k^2d^2(H+t)^2} - 2kdH|H+t|. \tag{4.50}$$

Now suppose that $|\sin(\alpha^-)| > 0$, and let $\theta = 2kdH|(H+t)|$ and $p = |\sin(\alpha^-)| \leq 1$, so that

$$|e^{-kdv^2} - e^{i(\beta+k)d}| \geq p\sqrt{1-\theta^2} - \theta. \tag{4.51}$$

If $\theta \leq p/2$, then $-\theta \geq -p/2$,

$$\begin{aligned} |e^{-kdv^2} - e^{i(\beta+k)d}| &\geq p\sqrt{1-p^2/4} - p/2 \\ &= \frac{p}{2}\left(\sqrt{4-p^2} - 1\right) \\ &= \frac{p(3-p^2)}{2(1+\sqrt{4-p^2})} \end{aligned} \tag{4.52}$$

since $3 - p^2 \geq 2$ and $4 - p^2 \leq 4$ it follows that

$$|e^{-kdv^2} - e^{i(\beta+k)d}| \geq \frac{p}{3}. \tag{4.53}$$

So if $|\sin\alpha^-| > 0$, and $\theta = 2kdH|H+t| \leq \frac{|\sin\alpha^-|}{2}$, then

$$|e^{-kdv^2} - e^{i(\beta+k)d}| \geq \frac{|\sin\alpha^-|}{3}. \tag{4.54}$$

Recall as case 2 condition that $|H^2 - t^2| = |H+t||H-t| \leq \epsilon$. If t is close to $-H$, then $|H-t|$ is close to $2H$, so this condition is quite similar to $\theta = 2Hkd|H+t| \leq \frac{|\sin\alpha^-|}{2}$, if we take $\epsilon = \frac{|\sin\alpha^-|}{2}$. Clearly, in case A, when t is close to $+H$, specifically $2kdH|H-t| \leq \frac{|\sin\alpha^+|}{2}$, then

$$|e^{-kdv^2} - e^{i(\beta+k)d}| \geq \frac{|\sin\alpha^+|}{3}.$$

Also,in case B , when t is close to $-H$, specifically $2Hkd|H+t| \leq \frac{|\sin\alpha^-|}{2}$, then

$$|e^{-kdv^2} - e^{i(\beta+k)d}| \geq \frac{|\sin\alpha^-|}{3}.$$

Case C

For t is not close to $\pm H$,(i.e, the other values of t is not covered by Cases A and B), for which

$$2kdH|H-t| > \frac{|\sin\alpha^+|}{2} \tag{4.55}$$

and

$$2kdH|H+t| > \frac{|\sin\alpha^-|}{2}. \tag{4.56}$$

then

$$\begin{aligned} 4H^2k^2d^2|H^2-t^2| &> \frac{|\sin\alpha^+||\sin\alpha^-|}{4} \\ \iff |H^2-t^2| &> \epsilon := \frac{|\sin\alpha^+||\sin\alpha^-|}{16H^2k^2d^2}. \end{aligned} \tag{4.57}$$

So , if we are not in case A or case B, then we are in case C and that tells us $|H^2 - t^2| > \epsilon$, we are in case 1 with

$$\epsilon = \frac{|\sin\alpha^+||\sin\alpha^-|}{16H^2k^2d^2}. \tag{4.58}$$

Hence

$$|e^{-kdv^2} - e^{i(\beta+k)d}| \geq m_H := \min\left(\frac{|\sin\alpha^+|}{3}, \frac{|\sin\alpha^-|}{3}, kd\epsilon e^{-kd\epsilon}\right), \tag{4.59}$$

with ϵ which is defined in (4.58). It is convent to recall the following standard calculation as a lemma.

Lemma 4.3. *For $a, b \in \mathbb{R}$, $\sqrt{a+ib} = \pm(x+iy)$, where*

$$x = \sqrt{\frac{a+\sqrt{a^2+b^2}}{2}},$$

$$y = \frac{|b|}{\sqrt{2a+2\sqrt{a^2+b^2}}}.$$

Now we find the supremum of $F(v)$ on $\Gamma_{H,N}$, for $H \in (0,1)$, i.e. for $v = t+iH$ with $-A \leq t \leq A$. For $v = t+iH$ with $-A \leq t \leq A$, $v^2 - 2i = (t^2 - H^2) + 2i(Ht-1)$, so that by Lemma 4.3, we have $\sqrt{v^2-2i} = x+iy$, with

$$x = \sqrt{\frac{t^2 - H^2 + \sqrt{(H^2+t^2)^2 + 4(1-2Ht)}}{2}}$$

and

$$y = \frac{|(Ht-1)|\sqrt{2}}{\sqrt{t^2 - H^2 + \sqrt{(H^2+t^2)^2 + 4(1-2tH)}}}.$$

Thus $\mathrm{Im}(v\sqrt{v^2-2i}) = \mathrm{Im}[(t+iH)(x+iy)]$, i.e.

$$\mathrm{Im}(v\sqrt{v^2-2i}) = xH + yt = f(t),$$

where, for $t \in \mathbb{R}$,

$$f(t) := H\sqrt{\frac{t^2 - H^2 + \sqrt{(H^2+t^2)^2 + 4(1-2Ht)}}{2}} + \frac{|(Ht-1)|t\sqrt{2}}{\sqrt{t^2 - H^2 + \sqrt{(H^2+t^2)^2 + 4(1-2tH)}}}$$

$$= \frac{H(t^2 - H^2) + H\sqrt{(H^2 + t^2)^2 + 4(1 - 2Ht)} + 2t|(Ht - 1)|}{\sqrt{2}\sqrt{t^2 - H^2 + \sqrt{(H^2 + t^2)^2 + 4(1 - 2tH)}}}. \tag{4.60}$$

Thus

$$\begin{aligned} \sup_{v \in \Gamma_{H,N}} |\cos(kXv\sqrt{v^2 - 2i})| &\le \sup_{v \in \Gamma_{H,N}} \cosh(kX\mathrm{Im}(v\sqrt{v^2 - 2i})) \\ &= \sup_{-A \le t \le A} \cosh(kXf(t)). \end{aligned} \tag{4.61}$$

Lemma 4.4. *For $|t| \le A$,*

$$|2t(Ht - 1)| \le 2A(AH + 1) \tag{4.62}$$

Proof.

$$\begin{aligned} |2t(Ht - 1)| &= |2t||Ht - 1| \\ &\le 2|t|(H|t| + 1) \le 2A(AH + 1). \end{aligned}$$

□

Lemma 4.5. *Suppose that $A \ge 1$. Then, for $|t| \le A$, we have*

$$|t^2 - H^2| \le A^2. \tag{4.63}$$

Proof. If $|t| \le H$, then

$$|t^2 - H^2| = H^2 - t^2 \le H^2 < 1 \le A^2.$$

If $H < |t| \le A$, then

$$|t^2 - H^2| = t^2 - H^2 \le t^2 \le A^2.$$

Hence

$$|t^2 - H^2| \le A^2, \quad |t| \le A.$$

□

Lemma 4.6. *For $0 < H < 1$ and $|t| \leq A$ we have*

$$t^2 - H^2 + \sqrt{(H^2 + t^2)^2 + 4(1 - 2tH)} \geq 2(1 - H^2) \tag{4.64}$$

Proof. consider $|t| \geq H$ and let

$$g(h) = (H^2 + t^2)^2 + (4 - 8Ht)$$

so

$$\begin{aligned} |(H^2 + t^2)^2 + (4 - 8Ht)| &\geq |(H^2 + t^2)|^2 - |4 - 8Ht| \\ &\geq (H^2 + |t|^2)^2 - 8H|t| - 4 \\ &\geq (2H^2)^2 - 8H^2 - 4 \geq 4H^4 - 8H^2 - 4. \end{aligned} \tag{4.65}$$

We can write the L.H.S of (4.64) as

$$J(t, H) := t^2 - H^2 + \sqrt{(H^2 + t^2)^2 + 4(1 - 2tH)} = t^2 - H^2 + \sqrt{(H^2 - t^2)^2 + 4(Ht - 1)^2} \tag{4.66}$$

since $(H^2 - t^2)^2 + 4(Ht - 1)^2 \geq (H^2 - t^2)^2$, it follows that

$$\begin{aligned} t^2 - H^2 + \sqrt{(H^2 - t^2)^2 + 4(tH - 1)^2} &\geq t^2 - H^2 + \sqrt{(H^2 - t^2)^2} \\ &\geq t^2 - H^2 + |H^2 - t^2|, \end{aligned} \tag{4.67}$$

where

$$t^2 - H^2 + |H^2 - t^2| = \begin{cases} 0, \quad if & H^2 - t^2 > 0 \\ 2(t^2 - H^2) \quad if & t^2 - H^2 > 0. \end{cases} \tag{4.68}$$

If $t = H$, then (4.66) becomes

$$J(H, H) = 0 + \sqrt{0 + 4(H^2 - 1)^2} = 2(1 - H^2). \tag{4.69}$$

We use $t^2 - H^2 + \sqrt{(H^2 - t^2)^2 + 4(Ht-1)^2}$ in two different cases to obtain the same lower bound, so

- $$\begin{aligned} t^2 - H^2 + \sqrt{(H^2 - t^2)^2 + 4(Ht-1)^2} &\geq t^2 - H^2 + \sqrt{(H^2 - t^2)^2} \\ &= t^2 - H^2 + |H^2 - t^2|. \end{aligned} \tag{4.70}$$

  If $t^2 \geq 1$, i.e $|t| \geq 1$, then

  $$t^2 - H^2 + \sqrt{(H^2 - t^2)^2 + 4(Ht-1)^2} \geq 2(1 - H^2). \tag{4.71}$$

- $t^2 - H^2 + \sqrt{(H^2 - t^2)^2 + 4(Ht-1)^2} \geq t^2 - H^2 + 2|Ht - 1|$. If $|t| < 1$ and $0 < H < 1$, then

  $$\begin{aligned} t^2 - H^2 + 2|Ht - 1| &= t^2 - H^2 + 2(1 - Ht) \\ &= (t - H)^2 - 2H^2 + 2 \\ &\geq 2 - 2H^2 = 2(1 - H^2). \end{aligned} \tag{4.72}$$

Hence

$$t^2 - H^2 + \sqrt{(H^2 + t^2)^2 + 4(1 - 2tH)} \geq 2(1 - H^2). \tag{4.73}$$

□

Lemma 4.7. *Suppose $A \geq 1$, Then, for $|t| \leq A$, we have*

$$|(H^2 + t^2)^2 + 4(1 - 2tH)| \leq A^4 + 4(1 + A)^2 \tag{4.74}$$

Proof. If $A \geq 1$ then, for $|t| \leq A$, using Lemma 5

$$|(H^2 + t^2)^2 + 4(1 - 2tH)| = (H^2 - t^2)^2 + 4(Ht - 1)^2,$$

$$\begin{aligned} &\leq A^4 + 4(1 + HA)^2 \\ &\leq A^4 + 4(1 + A)^2 \end{aligned} \tag{4.75}$$

for $H < 1$. □

So our upper bound on $|\cos(kXv\sqrt{v^2 - 2i})|$ is

$$|\cos(kXv\sqrt{v^2 - 2i})| \leq \cosh(kXf(t)), \tag{4.76}$$

where

$$|f(t)| \leq \frac{HA^2 + H(A^2 + 2A + 2) + 2A(HA + 1)}{2\sqrt{1 - H^2}} = \frac{H(2A^2 + A + 1) + A}{\sqrt{1 - H^2}} \tag{4.77}$$

for $0 < H < 1$. Thus, for all $t \in \mathbb{R}$, $H \in (0, 1)$, $A \geq 1$,

$$\begin{aligned} M^{(2)} &= \sup_{-A \leq t \leq A} |F(t + iH)| \\ &\leq \frac{\cosh(kX(H(2A^2 + A + 1) + A)/(\sqrt{1 - H^2}))}{m_H\sqrt{1 - H^2}}. \end{aligned} \tag{4.78}$$

4.1.1.3 A bound for $M^{(3)}$

For the third maximum of F_- , that is

$$M^{(3)} := \max_{0 \leq y \leq H} |F(A + iy) + F(-A + iy)| \quad \text{for} \quad 0 < H < 1. \tag{4.79}$$

We have

$$|F(A + iy)| = \frac{|\cos[kX(A + iy)((A + iy)^2 - 2i)^{1/2}]|}{|e^{-kd(A+iy)^2} - e^{i(\beta+k)d}||(A + iy)^2 - 2i|^{1/2}} \tag{4.80}$$

and

$$|F(-A + iy)| = \frac{|\cos[kX(-A + iy)((-A + iy)^2 - 2i)^{1/2}]|}{|e^{-kd(-A+iy)^2} - e^{i(\beta+k)d}||(-A + iy)^2 - 2i|^{1/2}} \tag{4.81}$$

Now, we will find the bound on $|F(A+iy)|$, we will start with the numerator of (4.80), we assume throughout that $A > 1$. Let $r = A + iy$, we have

$$\begin{aligned}\max_{0\le y\le H}|\cos(kXr\sqrt{r^2-2i})| &\le \max_{0\le y\le H}\cosh(kX\mathrm{Im}(r\sqrt{r^2-2i}))\\ &= \max_{0\le y\le H}\cosh(kX\frac{y(A^2-y^2)+y\sqrt{(y^2+A^2)^2+4(1-2yA)}+2t|(Ay-1)|}{\sqrt{2}\sqrt{A^2-y^2+\sqrt{(y^2+A^2)^2+4(1-2Ay)}}}),\\ &= \max_{0\le y\le H}\cosh(kXf(y)),\end{aligned} \tag{4.82}$$

for $A \in \mathbb{R}$,

$$f(y) := \frac{y(A^2-y^2)+y\sqrt{(y^2+A^2)^2+4(1-2Ay)}+2A|(Ay-1)|}{\sqrt{2}\sqrt{A^2-y^2+\sqrt{(y^2+A^2)^2+4(1-2Ay)}}}. \tag{4.83}$$

Now, we find the bound on $|f(y)|$, we begin by finding the bound on the expressions in numerator. So, for $A \ge 1$, and $0 \le y \le H < 1$, we have

$$A^2 - y^2 \le A^2. \tag{4.84}$$

Also, for $A \ge 1$, and $0 \le y \le H$, we have

$$2A|Ay-1| \le 2A(HA+1). \tag{4.85}$$

Lemma 4.8. *For $A \ge 1$, and $0 \le y \le H < 1$*

$$|(y^2+A^2)^2 + 4(1-2Ay)| \le A^4 + 4(1+A)^2 \tag{4.86}$$

Proof. Since

$$(y^2+A^2)^2 + 4(1-2Ay) = (y^2-A^2)^2 + 4(1-Ay)^2,$$

it follows that,

$$|(y^2 - A^2)^2 + 4(1 - Ay)^2| = |y^2 - A^2|^2 + 4|1 - Ay|^2, \tag{4.87}$$

by Lemma 4.8, for $|y| \leq A$, we have

$$|(y^2 - A^2)^2 + 4(1 - Ay)^2| \leq A^4 + 4(1 + A)^2. \tag{4.88}$$

□

Lemma 4.9. *For $A \geq 1$, and $0 \leq y \leq H < 1$, then*

$$A^2 - y^2 + \sqrt{(y^2 + A^2)^2 + 4(1 - 2Ay)} \geq 2(A^2 - 1) \tag{4.89}$$

Proof.

$$\begin{aligned} A^2 - y^2 + \sqrt{(y^2 + A^2)^2 + 4(1 - 2Ay)} &= A^2 - y^2 + \sqrt{(y^2 - A^2)^2 + 4(1 + Ay)^2} \\ &\geq A^2 - y^2 + A^2 - y^2 = 2(A^2 - y^2) \geq 2(A^2 - 1), \end{aligned} \tag{4.90}$$

for $A \geq 1$. □

Thus,

$$|f(y)| \leq \frac{\cosh(kX(HA^2 + H\sqrt{A^4 + 4(1 + A)^2} + 2A(HA + 1)))}{2\sqrt{A^2 - 1}} \tag{4.91}$$

Now

$$\begin{aligned} |(A + iy)^2 - 2i| &= |(A - 1) + i(y - 1)||(A + 1) + i(y + 1)| \\ &= \sqrt{(A - 1)^2 + (y - 1)^2}\sqrt{(A + 1)^2 + (y + 1)^2} \\ &\geq (A - 1)(A + 1) = A^2 - 1 \end{aligned} \tag{4.92}$$

for $A > 1$. For $A \geq 1$ and $0 \leq y \leq H < 1$, then

$$\begin{aligned} |e^{-kd(A+iy)^2} - e^{i(\beta+k)d}| &\geq |e^{i(\beta+k)d}| - |e^{-kd(A+iy)^2}| \\ &\geq 1 - e^{kd(y^2-A^2)} \\ &\geq 1 - e^{-kdA^2} > 0. \end{aligned} \tag{4.93}$$

Then, for $0 \leq y \leq H$, and $A \geq 1$,

$$\begin{aligned} M^{(3)} :&= \max_{0\leq y\leq H} |F(A+iy) + F(-A+iy)| \\ &\leq \frac{2\cosh(kX(HA^2 + H\sqrt{A^4+4(1+A)^2} + 2A(HA+1)/(2\sqrt{A^2-1})))}{(1-e^{-kdA^2})\sqrt{A^2-1}} \\ &= \frac{2\cosh(kX(H(2A^2+A+1)+A)/(\sqrt{A^2-1})))}{(1-e^{-kdA^2})\sqrt{A^2-1}}. \end{aligned} \tag{4.94}$$

Thus, by $M^{(1)}, M^{(2)}$,and $M^{(3)}$, our bound on $|E_{h^*}^{*N}|$ is

$$|E_{h^*}^{*N}| \leq e^{-ac^2}\left(\frac{2\sqrt{\pi}M^{(2)}}{\sqrt{\rho}(1-e^{-s})} + \frac{M^{(1)}}{\hat{s}} + 2HM^{(3)}\right) \tag{4.95}$$

where ac^2, $\hat{s}$, and s, are defined in (4.7), (4.8), and (4.9) respectively. We see that we have shown the following result.

Theorem 4.10. *For $N \in \mathbb{N}$, then for every $H \in (0,1)$ such that $(\beta+k)d \pm 2H^2kd \neq \pi\mathbb{Z}$, if we choose the step size $h = h^*$, where $h^* = h^+\theta$, and if $A = (N+1)h^* = \frac{(N+1)^{2/3}(2\pi H)^{1/3}}{\rho^{1/3}(1+3b)} \geq 1$, then*

$$|E_{h}^{*N}| \leq e^{-ac^2}\left(\frac{2\sqrt{\pi}M^{(2)}}{\sqrt{\rho}(1-e^{-s})} + \frac{M^{(1)}}{\hat{s}} + 2HM^{(3)}\right) \tag{4.96}$$

where

$$ac^2 = \frac{\rho^{1/3}(2\pi)^2(H)^{2/3}(N+1)^2}{[(N+1)^{2/3}(2\pi)^{2/3} + H^{4/3}\rho^{2/3}]^2},$$

$$s = (2\pi H)^{2/3}(N+1)^{2/3}\rho^{1/3} + \frac{H^2\rho}{3},$$

$$\hat{s} = \frac{\rho^{2/3} 2\pi (N+1) H^{1/3}}{(2\pi)^{2/3}(N+1)^{2/3} + \rho^{2/3} H^{4/3}},$$

where M^1, M^2, and M^3 are defined in (4.25), (4.78), and (4.94) respectively. Linton in (p.394, [28]) suggests that accurate computation in the case when $X = 0$ is particularly challenging. The above theorem reduces to the following simpler statement in that case.

Corollary 4.11. *For $N \in \mathbb{N}$, then for every $H \in (0,1)$ such that $(\beta+k)d \pm 2H^2 kd \neq \pi\mathbb{Z}$, if we choose the step size $h = h^*$, where $h^* = h^+\theta$, and if $A = (N+1)h^* = \frac{(N+1)^{2/3}(2\pi H)^{1/3}}{\rho^{1/3}(1+3b)} \geq 1$ and $X = 0$, then*

$$|E_h^{*N}| \leq e^{-ac^2} \left(\frac{2\sqrt{\pi}}{m_H \sqrt{\rho}(1-e^{-s})(1-H^2)} + \frac{1}{\hat{s}\sqrt{2}(1-e^{-kdA^2})} + \frac{4H}{(1-e^{-kdA^2})\sqrt{A^2-1}} \right), \tag{4.97}$$

where ac^2, s and $\hat{s}$ are as defined in Theorem 4.10.

4.2 A more systematic testing

4.2.1 Systematic testing A

Recall that $G_\beta^d(X,Y)$ is given by equations (3.108)-(3.112). In this section, we carry out a more systematic testing of the accuracy of the approximations $G_h^N(X,Y)$ and $G_h^{*N}(X,Y)$ to $G_\beta^d(X,Y)$, investigating dependence of the accuracy on the various parameter values. Recall that $G_h^N(X,Y)$ is the approximation to $G_\beta^d(X,Y)$ given by replacing the integrals in (3.110) by truncated midpoint rule approximations, i.e., $G_h^N(X,Y)$ is given by (3.113). $G_h^{*N}(X,Y)$ is the approximation given by replacing the integrals in (3.110) by the modified truncated midpoint rule approximation.

Now we perform a more systematic testing of the accuracy of the approximation $G_h^{*N}(X,Y)$ defined in (3.120) over the full range of possible parameter values. It is enough (because the value of $G_\beta^d(X,Y)$ depends only on the values of $k\beta$, kd, kX, and kY) to fix $k = 1$. For various fixed choices of X we compute the maximum error as β varies over the interval $0 \leq \beta \leq p/2$, where $p = 2\pi/d$, d varies over the range $10^{-1} \leq d \leq 10$, and Y over the range $\epsilon d \leq Y \leq (1-\epsilon)d$, for some small $\epsilon > 0$ that we take as $\epsilon = 0.01$. The reason for choosing these restricted parameter ranges for Y and β is that:

- By (3.12) it is enough to consider Y in an interval of length d, $0 \leq Y \leq d$. But the quasi-periodic Green's function blows up when $X = 0$ with $Y = 0$ or $Y = d$. To avoid that we choose the range $\epsilon d \leq Y \leq (1-\epsilon)d$, for some small $\epsilon > 0$.

- As noted by Linton [28], it is enough to restrict consideration to β in an interval of length $p = 2\pi/d$, since

  $$G^d_{\beta+p}(X, Y) = G^d_\beta(X, Y), \quad \text{for} \quad \beta \in \mathbb{R}.$$

  E.g., considering β in the restricted range $-p/2 \leq \beta \leq p/2$ is enough. Further, from (3.11) it follows that

  $$G^d_{-\beta}(X, Y) = G^d_\beta(X, -Y),$$

  so it is enough to consider β in the restricted range $0 \leq \beta \leq p/2$.

We show in Table 4.1 the maximum values of the error $|G_h^{*500} - G_h^{*N}|$ over the ranges $0 \leq \beta \leq p/2$, $10^{-1} \leq d \leq 10$ and $0.01d \leq Y \leq 0.99d$, for $N = 20, 30, 40, 50$ with $M = 10, 15, 20, 25$, and for $X = 0, 1, 2, 3, 4, 10$. Note that we compute $G_h^{*500}(X, Y)$ with $M = 50$ to estimate the true value of $G^d_\beta(X, Y)$, and we replace the true maximum by a discrete maximum, replacing the intervals $[0, p/2]$ and $[0.01d, 0.99d]$ by $0(10)p/2$ and $0.01d(10)0.99d$, i.e., by 10 points equally spaced on the respective intervals and including the two end points. Similarly we replace the interval $d \in \{10^r : -1 \leq r \leq 1\}$ with the ten points $d \in \{10^r : r = -1(10)1\}$.

Similarly, we perform a more systematic testing of the standard midpoint rule

N	M	$\max\|G_h^{*500} - G_h^{*N}\|$
20	10	3.5×10^{-7}
30	15	1.0×10^{-10}
40	20	3.5×10^{-14}
50	25	7.6×10^{-15}

(a) with $X = 0$

N	M	$\max\|G_h^{*500} - G_h^{*N}\|$
20	10	5.7×10^{-7}
30	15	1.1×10^{-10}
40	20	3.8×10^{-14}
50	25	7.2×10^{-15}

(b) with $X = 1$

N	M	$\max\|G_h^{*500} - G_h^{N}\|$
20	10	1.4×10^{-5}
30	15	2.3×10^{-9}
40	20	3.3×10^{-13}
50	25	8.4×10^{-15}

(c) with $X = 2$

N	M	$\max\|G_h^{*500} - G_h^{N}\|$
20	10	7.2×10^{-3}
30	15	6.2×10^{-8}
40	20	9.3×10^{-12}
50	25	8.2×10^{-15}

(d) with $X = 3$

N	M	$\max\|G_h^{*500} - G_h^{N}\|$
20	10	0.25
30	15	7.4×10^{-5}
40	20	2.8×10^{-10}
50	25	3.9×10^{-14}

(e) with $X = 4$

N	M	$\max\|G_h^{*500} - G_h^{*N}\|$
20	10	1016.2
30	15	304.6
40	20	18.59
50	25	0.178

(f) with $X = 10$

Table 4.1: The maximum of $|G_h^{*500} - G_h^{*N}|$

$G_h^N(X, Y)$. In Table 4.2 we show the maximum value of the error $|G_h^{500} - G_h^N|$ over the same set of input parameters that we used in Table 4.1.

N	M	$\max\|G_h^{500} - G_h^{N}\|$
20	10	2.9×10^{-4}
30	15	3.4×10^{-6}
40	20	4.5×10^{-8}
50	25	5.8×10^{-10}

(a) with $X = 0$

N	M	$\max\|G_h^{500} - G_h^{N}\|$
20	10	3.8×10^{-4}
30	15	3.4×10^{-6}
40	20	4.4×10^{-8}
50	25	5.7×10^{-10}

(b) with $X = 1$

N	M	$\max\|G_h^{500} - G_h^{N}\|$
20	10	7.1×10^{-4}
30	15	6.3×10^{-6}
40	20	5.7×10^{-8}
50	25	5.2×10^{-10}

(c) with $X = 2$

N	M	$\max\|G_h^{500} - G_h^{N}\|$
20	10	1016.20
30	15	304.63
40	20	18.59
50	25	0.17

(d) with $X = 10$

Table 4.2: The maximum of $|G_h^{500} - G_h^N|$

4.2.2 Systematic testing B

We repeat the above testing with the difference that we restrict d to the range $1 \le d \le 10$, avoiding very small values of d. We replace the interval $d \in \{10^r : 0 \le r \le 1\}$ with the ten points $d \in \{10^r : r = 0(10)1\}$.

We show in Tables 4.3, and 4.4 the maximum values of the errors $|G_h^{*500} - G_h^{*N}|$ and $|G_h^{500} - G_h^N|$, for $N = 10, 20, 30, 40, 50$ with $M = 5, 10, 15, 20, 25$, and with $X = 0, 1, 2, 10$. Again we use $G_h^{*500}(X, Y)$ with $M = 50$ as the true value of $G_\beta^d(X, Y)$.

N	M	max $\|G_h^{*500} - G_h^{*N}\|$
10	5	5.135 $\times 10^{-10}$
20	10	1.157 $\times 10^{-14}$
30	15	1. 043 $\times 10^{-14}$
40	20	9.103 $\times 10^{-15}$
50	25	7.850 $\times 10^{-15}$

(a) with $X = 0$

N	M	max $\|G_h^{*500} - G_h^{*N}\|$
10	5	3.833 $\times 10^{-10}$
20	10	1.230 $\times 10^{-14}$
30	15	1.09 $\times 10^{-14}$
40	20	9.693 $\times 10^{-15}$
50	25	9.09 $\times 10^{-15}$

(b) with $X = 1$

N	M	max $\|G_h^{*500} - G_h^{*N}\|$
10	5	1.713 $\times 10^{-9}$
20	10	1.285 $\times 10^{-14}$
30	15	1.158 $\times 10^{-14}$
40	20	9.912 $\times 10^{-15}$
50	25	8.427 $\times 10^{-15}$

(c) with $X = 2$

N	M	max $\|G_h^{*500} - G_h^{*N}\|$
10	5	0.985
20	10	2.05 $\times 10^{-10}$
30	15	1.12 $\times 10^{-14}$
40	20	8.98 $\times 10^{-15}$
50	25	7.54 $\times 10^{-15}$

(d) with $X = 10$

Table 4.3: The maximum of $|G_h^{*500} - G_h^{*N}|$

N	M	$\max\lvert G_h^{500} - G_h^N\rvert$
10	5	0.6840
20	10	0.1153
30	15	1.91 $\times 10^{-2}$
40	20	3.26 $\times 10^{-3}$
50	25	5.57 $\times 10^{-4}$

(a) with $X = 0$

N	M	$\max\lvert G_h^{500} - G_h^N\rvert$
10	5	0.6865
20	10	0.1157
30	15	1.92 $\times 10^{-2}$
40	20	3.28 $\times 10^{-3}$
50	25	5.592 $\times 10^{-4}$

(b) with $X = 1$

N	M	$\max\lvert G_h^{500} - G_h^N\rvert$
10	5	0.6939
20	10	0.1170
30	15	1.941 $\times 10^{-2}$
40	20	3.315 $\times 10^{-3}$
50	25	5.65 $\times 10^{-4}$

(c) with $X = 2$

N	M	$\max\lvert G_h^{500} - G_h^N\rvert$
10	5	0.9850
20	10	0.1593
30	15	2.64 $\times 10^{-2}$
40	20	4.51 $\times 10^{-3}$
50	25	7.69 $\times 10^{-4}$

(d) with $X = 10$

Table 4.4: The maximum of $|G_h^{500} - G_h^N|$

We have tested the accuracy of the modified truncated midpoint rule $G_h^{*N}(X,Y)$ and the standard truncated midpoint rule $G_h^N(X,Y)$ over a wide range of values Y, β, d with rather small values of $N = 10, 20, 30, 40, 50$, and $M = 5, 10, 15, 20, 25$, and the results are shown in Tables 4.1, 4.2, 4.3 and 4.4 above. From Tables 4.1 and 4.3 it is clear that, for the same values of N, the modified truncated midpoint rule provides more accurate results for smallest values of X than the results of the truncated midpoint rule shown in Tables 4.2 and 4.4. Also, from both Tables 4.1 and 4.2, we can see that the modified truncated midpoint rule when $X = 10$ has the same value as the standard truncated midpoint rule with $X = 10$; the correction factors in the modification are negligible when $X = 10$. Further from Tables 4.1 and 4.3 the modified truncated midpoint rule is more accurate in the range $1 \leq d \leq 10$ than in the range $0.1 \leq d \leq 10$. These observations are consistent with the theoretical bound in Theorem 4.10 in Section 4.1 which blows up as $X \to \infty$ and as $d \to 0$.

Chapter 5

Conclusion and Future Work

5.1 Conclusion

This thesis aimed to:

- develop numerical methods for efficient calculation of integrals of the form

$$I = \int_{-\infty}^{\infty} e^{-\rho v^2} F(v) dv, \quad \rho > 0, \tag{5.1}$$

  in the case when F is analytic near the real line except for simple poles, and provide new error estimates for such methods;

- implement these methods to treat the problem of computing the free space quasi-periodic Green's function in two dimensions.

In Chapter 2, building on the previous work of [17], [2], 26 and [3] - see Propositions 2.3 and 2.4 - we showed that the truncated midpoint rule can be improved in terms of efficiency, in particular when simple poles of F lie near the real line, by including a correction factor based on a calculation of the residues of F at its poles (which lie inside the specified domain S_H). The resulting numerical method was termed the modified truncated midpoint rule. Furthermore, Theorem 2.9, which is a new theorem, was proved, providing an error estimation when F is even and Assumption 2.1 is satisfied. This error estimate is given by

$$
\begin{aligned}
|E_h^{*N}| \leq & \frac{2\sqrt{\pi} M_3(H,(N+1)h) e^{\rho H^2 - 2\pi H/h}}{\sqrt{\rho}(1-e^{-2\pi H/h})} \\
& + e^{-\rho(N+1)^2 h^2} \left(\frac{M_1((N+1)h)}{\rho(N+1)h} + 2HM_2(H,(N+1)h) \right),
\end{aligned}
\tag{5.2}
$$

where the various notations are as defined in (2.42), (2.43), and (2.41) in Chapter 2.

In Chapter 3 we considered the problem of computing acoustic propagation from an infinite array of line sources in free space. We showed a new integral representation for the quasi-periodic Green's function, given by (3.108), of the form (5.1). We applied the numerical integration methods proposed in Chapter 2 to this integral. The accuracy of the method is discussed in Section 3.4 (numerical implementation) where we saw that 15-digit accuracy was achieved with a small number of quadrature points N and a small value of M (e.g $N = 20$ and $M = 4$, see Table 3.9). Also, for particular sets of test case parameter values suggested in the review paper [28], we compared our method with others such as the asymptotic correction terms method, proposed in [30], and Ewald's method, as discussed in [28]. The results showed, in particular, that the efficiency of our method far surpasses the asymptotic correction terms method's efficiency.

The first section of Chapter 4 is concerned with theoretical error estimates for the modified midpoint rule approximations to the quasi-periodic Green's function proposed in Chapter 3. Using the general Theorem 2.9, i.e., the inequality (5.2), we proved as Theorem 4.10 a rigorous bound on the actual error in our approximation. We also in Chapter 4 tested our approximations more systematically by numerical experiments over the full possible range of parameter values. It is clear from Tables 4.1 and 4.2 that the modified truncated midpoint rule approximation is more accurate and efficient than the standard truncated midpoint rule approximation.

Clearly, we have achieved our objectives, and we are delighted to present a new, robust, accurate, and efficient computation method for the 2D quasi-periodic Green's function.

5.2 Future work

There are many extensions that could be considered to the work that has been done in this thesis. Firstly, in Chapter 2, in considering the modified midpoint rule for integrals of the form (5.1), we have made the standing Assumption 2.1 that the only poles of the function F that lie near the real axis are simple poles. The extension of the methods of this thesis to higher order poles, while somewhat complicated, is relatively clear, as indicated in Remark 2.2. A useful piece of additional research would be to work this out in detail (cf. [7]). Much less clear, but important for many applications, is the possibility of extension to the case where there are singularities near the real axis that are not poles, notably branch point singularities (cf. the brief discussion in [21]).

In Chapters 3 and 4 we talked about computing the quasi-periodic Green's function, i.e., computing the acoustic field due to an infinite array of line sources in free space. This thesis showed that the quasi-periodic Green's function can be written as an integral of the form (5.1), where F is an analytic function except for simple poles in a strip around the real line. The truncated modified midpoint rule approximation (2.38) can be used to approximate this quasi-periodic Green's function, and we have demonstrated by computations that this can be an effective method. But it would be a useful extension to carry out further numerical investigations of the methods that we have proposed, and further comparisons with the other methods for computation of this Green's function that we have cited from the literature.

Notably, at the end of Section 3.4.2 we have made some comparisons between modified midpoint rule approximations that:

- Include a correction factor associated to just the nearest poles of F to the real axis;
- Include a correction factor associated to all the poles of the function F that lie within distance 0.9 of the real axis.

Based on limited examples our recommendation from these computations are that there is no particular advantage to including all the poles within distance 0.9, it is enough to construct the correction factor using just the (up to 4) nearest poles. But, as we discussed at the end of Section 3.4.2, it would be good to carry out a more thorough numerical investigation across a wider range of examples. Similarly, following computations in Chapter 3 for the particular parameter combinations used previously as test cases in the review paper [28], in Section 4.2 we have carried out more systematic testing over a wide range of parameter values, but it would be good to repeat these using a finer discretisation grid to obtain a better approximation to the true maximum error over the ranges of parameter values that we explored.

It would also be good, as further work, to apply the general methods and analysis of Chapter 2 to other examples. One example of this sort would be to apply the methods in Chapter 2 and Chapter 3 to the problem stated in [19], which is the problem of propagation from an infinite array of coherent line sources above an impedance plane. In particular [19, Eqs (20), (21)] provide a representation for this Green's function to which the methods and analysis of Chapters 2 and 3 may be applicable. Indeed, the poles of this integrand in [19] are the poles of the integrand in Chapter 3 plus a finite number of additional poles associated to the impedance boundary condition.

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Appendix A

A.1 Python code for spatial representation

```
from scipy.special import hankel1
from cmath import exp,sqrt
d=4
X=0
Y=0.01*d
k= 0.5
beta= sqrt(2)/d
N=5000
sum=0
for n in range(-N,N+1):
        kr = k*sqrt(X**2+(Y-n*d)**2)
        sum += hankel1(0, kr)*exp(1j*beta*n*d)
G= (-1j*0.25)*sum
print("G=",G)
```

A.2 Python code for spectral representation

```
from cmath import exp,sqrt,pi
d=4
X=0
Y=0.04
k=0.5
beta=sqrt(2)/4
N=5000
sum=0
p=(2*pi)/d
for n in range(-N,N+1):
    beta1=beta+n*p
    gamma=-1j*sqrt(k**2-beta1**2)
    sum += exp(-gamma*abs(X))*exp(1j*beta1*Y)/gamma
G=(-0.5*1/d)*sum
print("G=",G)
```

A.3 Python codes part C

```
from cmath import sqrt,cos,exp,pi
from math import floor
from numpy.lib.scimath import *
from scipy.special import hankel1
from MyFunctions import Hankelsum
d=4
k=0.5
beta=sqrt(2)/4
Y=0.04
X=0
N=10
M=3
#################
sumA=0
alpha=0.5
rho=k*(M*d-Y)
h=sqrt(pi/(rho*(N+1)))
for j in range(-N,N+2):
    v= ((j-alpha)*h)
    a=exp(1j*(M-1)*(beta+k)*d)*cos(k*v*X*sqrt(v**2-2*1j))
    b=(exp(-1j*d*(beta+k))-exp(-k*d*v**2))*sqrt(v**2-2*1j)
    sumA +=exp(-rho*v**2)*(a/b)
print("h*sumA=",h*sumA)
E=1+beta/k
m=floor(E*k*d/(2*pi))
print('m=',m)
n=m
w1=E-2*pi*n/(k*d)
print('w1=',w1)
s0=exp(1j*pi/4)*sqrt(w1)
print('s0=',s0)
n=m+1
w2=E-2*pi*n/(k*d)
print('w2=',w2)
s1=exp(1j*pi/4)*sqrt(w2)
print('s1=',s1)
# calculation G1
p1=cos(k*X*sqrt(1j*w1)*sqrt(1j*w1-1j*2))*exp(2*1j*(pi*s0/h+ pi/2))*exp(-rho*1j*w1)
f1=exp(-1j*k*d*w1)*sqrt(w1)*sqrt(1j*w1-1j*2)*(1-exp(2*1j*(pi*s0/h+pi/2)))
p2=cos(k*X*sqrt(1j*w2)*sqrt(1j*w2-1j*2))*exp(2*1j*(pi*s1/h+pi/2))*exp(-rho*1j*w2)
```

```
f2=exp(-1j*k*d*w2)*sqrt(w2)*sqrt(1j*w2-1j*2)*(1-exp(2*1j*(pi*s1/h+
G1=((-2*1j*pi*exp(1j*(M-1)*(beta+k)*d))/(k*d*exp(1j*pi/4)))*(p1/f1+p2/f2)
print('G1=',G1)
################################
sumB=0
rho1=k*(Y+M*d)
h1=sqrt(pi/(rho1*(N+1)))
for j in range(-N,N+2):
    v=((j-alpha)*h1)
    a1=exp(1j*(1-M)*(beta-k)*d)*cos(k*X*v*sqrt(v**2-2*1j))
    b1=(exp(1j*d*(beta-k))-exp(-k*d*(v**2)))*sqrt(v**2-2*1j)
    sumB +=exp(-rho1*v**2)*(a1/b1)
print("h*sumB=",h*sumB)
E1=1-beta/k
m1=floor(E1*k*d/(2*pi))
print("m1=",m1)
n=m1
wa=E1-2*pi*n/(k*d)
s3= exp(1j*pi/4)*sqrt(wa)
print('wa=',wa)
n=m1+1
wb=E1-2*pi*n/(k*d)
s4= exp(1j*pi/4)*sqrt(wb)
print('wb=', wb)
#calculate G2
p3=cos(k*X*sqrt(1j*wa)*sqrt(1j*wa-1j*2))*exp(2*1j*(pi*s3/h1+pi/2))*exp(-rho1*1j*wa)
f3=exp(-1j*k*d*wa)*sqrt(wa)*sqrt(1j*wa-1j*2)*(1-exp(2*1j*(pi*s3/h1+pi/2)))
p4=cos(k*X*sqrt(1j*wb)*sqrt(1j*wb-2*1j))*exp((2*1j*(pi*s4/h1+pi/2)))*exp(-rho1*1j*wb)
f4=exp(-1j*k*d*wb)*sqrt(wb)*sqrt(1j*wb-1j*2)*(1-exp(2*1j*(pi*s4/h1+pi/2)))
G2= (-2*1j*pi*exp(1j*(1-M)*(beta-k)*d)/(k*d*exp(1j*pi/4)))*(p3/f3+p4/f4)
print('G2=', G2)
H=(-1j*0.25)*Hankelsum(X,Y,k,beta,d,M-1)
Gappro =H-exp(-1j*k*Y)*(h*sumA+G1)/(2*pi)-exp(1j*k*Y)*(h1*sumB+G2)/(2*pi)
print("Gappro=",Gappro)
```