Efficient Representation of Nonreflecting Boundary Conditions for the Time-Dependent Schrödinger Equation in Two Dimensions

SHIDONG JIANG
New Jersey Institute of Technology

AND

LESLIE GREENGARD
Courant Institute

Abstract
We present a fast algorithm for the evaluation of exact, nonreflecting boundary conditions for the time-dependent Schrödinger equation in two dimensions on the unit circle. After separation of variables, the exact outgoing condition for each Fourier mode contains a nonlocal term that is a convolution integral in time. The kernel for that convolution is the inverse Laplace transform of the logarithmic derivative of a modified Bessel function, and the convolution integral can be split into two parts: a local part and a history part, which can be treated separately. The local part is easily handled by an appropriate quadrature. For the history part, we show that the convolution kernel can be well approximated by a sum of exponentials. Once such a representation is available, the convolution integrals can be evaluated recursively, reducing the cost from $O(N^2)$ work to $O(N)$, where $N$ is the number of time steps. The main technical development lies in the uniform rational approximation of the logarithmic derivative of the modified Bessel function $K_\nu(\sqrt{t}x)$.

1 Introduction
The initial-value problem for the Schrödinger equation in unbounded domains arises in several areas, including quantum scattering, waveguide modeling, and underwater acoustics. In this paper, we consider the numerical solution of such problems in two dimensions. More precisely, we consider equations of the form

\[
\begin{align*}
    iu_t(x, t) &= \Delta u(x, t) + V(x, t)u(x, t), \quad x \in \mathbb{R}^2, \quad t > 0, \\
    u(x, 0) &= u_0(x),
\end{align*}
\]

where $V(x, t)$ and $u_0(x)$ are compactly supported. Since the solution at later times propagates in space, standard time-marching schemes require the imposition of an artificial boundary condition on a finite region $\Omega$.

In broad terms, there are two different approaches to constructing such boundary conditions. One class of methods modifies the potential function $V(x, t)$ on a
region exterior to the boundary $\partial \Omega$ so that the wave is absorbed or dampened as it passes through and the corresponding reflection is small. These boundary conditions are often referred to as “absorbing layers” or “perfectly matched layers” (see, e.g., [15, 21]). The method of “exterior complex scaling” also falls into this class. While originally designed for time-independent problems, it has recently been extended to the time-dependent case [19]. The methods in this class are often very effective. They are, however, difficult to put into a rigorous mathematical foundation in terms of accuracy, convergence rate, and computational costs. It should be noted that the Schrödinger equation is particularly unforgiving—unlike the scalar wave equation, errors at one point in space propagate with infinite speed in every direction. This is clear from inspection of the free-space Green’s function:

$$G(r, t) = \frac{e^{i r^2 / 4 t}}{\sqrt{4 \pi i t}}.$$ 

The second class of methods is to establish a nonreflecting boundary condition for which the resulting initial boundary value problem is equivalent to the original initial-value problem (restricted to the bounded domain). For an excellent review article, see [12]. Unfortunately, the exact nonreflecting boundary conditions are generally nonlocal in both space and time, so that direct implementation is highly inefficient in terms of both computation and storage cost. Hence most research has been devoted to approximations of the exact nonreflecting boundary conditions, particularly for the one-dimensional case (see, e.g., [3, 4, 8, 17, 23, 24, 25, 26]). A few papers in the literature consider the two-dimensional setting [5, 7, 22]. Of these, only the last [22] addresses the full problem discussed here. The methods considered in references [5, 7] are for the two-dimensional equation (1.1) but with periodic boundary conditions in one direction.

In this paper, we describe a fast algorithm for the imposition of the exact nonreflecting boundary conditions (ENRBC) on a unit disk. The one-dimensional case was treated in [14]. The scheme is a natural extension of the work on the scalar wave equation developed in [2]. Our analytic approach is classical, using the Fourier transform in space and the Laplace transform in time [12]. Here we concentrate on the ENRBC for each Fourier mode, which is nonlocal in time and will be shown to involve a convolution integral of the form

$$\int_0^t \mathcal{C}_\nu(t - \tau) \sigma(\tau) d\tau,$$

where $\mathcal{C}_\nu(t)$ is the inverse Laplace transform of the function

$$\hat{\mathcal{C}}_\nu(s) = \frac{\sqrt{i s} K'_\nu(\sqrt{i s})}{(s - s_\nu) K_\nu(\sqrt{i s})}.$$ 

In the preceding expression, $K_\nu(s)$ denotes the modified Bessel function of order $\nu$, $s_\nu$ is a complex constant depending on $\nu$, to be discussed below, and $\sigma$ is a density that depends on the computed solution.
Asymptotic analysis reveals that the convolution kernel \( C_\nu(t) \), sometimes called the “nonreflecting boundary kernel,” is singular at the origin. Thus, we proceed by splitting the convolution into two parts: the local part \((t - \delta \leq \tau \leq t)\) and the history part \(0 \leq \tau \leq t - \delta\). (Fast algorithms for the evaluation of heat potentials [9, 11] use an analogous decomposition.) The local part is computed by a suitable quadrature. For the history part, we approximate the kernel by the sum of a small number of exponentials, with the number of exponentials depending on the prescribed precision \( \epsilon \) and the mode number \( n \). Since convolution with an exponential function can be evaluated recursively, this approximation allows us to reduce the computational and storage costs dramatically. More specifically, if we let \( N_T \) denote the number of time steps in the simulation, and \( N(\epsilon, \nu) \) the number of exponentials needed for the approximation of the convolution kernel \( C_\nu \), then the direct implementation of the ENRBC for each Fourier mode requires \( O(N_T^2) \) work and \( O(N_T) \) storage, whereas the algorithm in this paper requires only \( O(N(\epsilon, \nu) \cdot N_T) \) work and \( O(N(\epsilon, \nu)) \) storage.

The central problem we face is that the convolution kernel \( C_\nu(t) \) is not available analytically. Only its Laplace transform \( \hat{C}_\nu(s) \) is explicitly known. In order to be able to invert the Laplace transform, it is convenient to approximate \( \hat{C}_\nu(s) \) by a sum of poles. This has two advantages. First, the inverse Laplace transform of a pole is a simple exponential function,

\[
\mathcal{L}^{-1}\left(\frac{1}{s - s_j}\right) = e^{s_j t}(s).
\]

Second, as mentioned earlier, once a function is expressed as a sum of exponentials, convolution in time can be carried out recursively.

The principal analytical result of this paper is that \( \hat{C}_\nu \) can be approximated in the right half-plane with an absolute error \( \epsilon \) by a sum of poles with the number of poles \( N(\epsilon, \nu) \sim O(\log(1/\epsilon) \cdot \log \nu + \log(1/\epsilon)) \) as \( \nu \to \infty \) and \( \epsilon \to 0 \). We apply an improved version of the nonlinear least-squares procedure developed in [2] to numerically compute such an approximation and show that the convolution kernel \( C_\nu \) in the physical (time) domain can be approximated by a sum of exponentials with the average number of exponentials \( \bar{N} \leq 80 \) to achieve a relative error \( \epsilon = 10^{-12} \) for \( 10^{-8} \leq t \leq 10^8 \) and \( 0 \leq \nu \leq 1024 \).

The paper is organized as follows. In Section 2, we derive the nonreflecting boundary conditions that are exact, nonlocal in time and space, and easily expressed in terms of a convolution operator. In Section 3, we develop a sum-of-exponentials approximation for the convolution kernel. Section 4 discusses the computation of the local part of the convolution, and Section 5 presents a discretization scheme for the resulting initial boundary problem. The performance of the scheme is illustrated in Section 6.
2 Exact Nonreflecting Boundary Conditions

In this section, we derive the exact nonreflecting boundary conditions for the two-dimensional Schrödinger equation on the unit circle. We use the general method based on the Fourier-Laplace transform laid out in [12]. We assume that both the initial data and the potential vanish outside the unit disk $D^2 = \{(x, y) \in \mathbb{R}^2 : x^2 + y^2 < 1\}$ and that the solution is bounded at infinity.

**Theorem 2.1** Suppose that the functions $V, u_0 : \mathbb{R}^2 \to \mathbb{C}$ vanish outside the unit disk $D^2$. Suppose further that the solution of the pure initial-value problem (1.1) is expanded into the Fourier series

\[ u(r, \theta, t) = \sum_{\nu = -\infty}^{\infty} e^{i\nu \theta} R_\nu(r, t). \]

Then, at $r = 1$, each Fourier mode satisfies the exact nonreflecting boundary condition

\[ \frac{\partial}{\partial r} R_\nu(1, t) = R_\nu(1, t) * L^{-1}\left[ \sqrt{i s} K'_\nu(\sqrt{i s}) \right](t), \]

where $*$ denotes Laplace convolution

\[ (f * g)(t) = \int_0^t f(\tau) g(t - \tau) d\tau, \]

and $L^{-1}$ denotes the inverse Laplace transform

\[ L^{-1}[g](t) = \frac{1}{2\pi i} \int_{i\infty}^{i\infty} e^{st} g(s) ds. \]

**Proof:** Substituting (2.1) into (1.1) and applying the condition that $V(r, \theta) = 0$ for $r \geq 1$, we obtain

\[ i \frac{\partial R_\nu(r, t)}{\partial t} = \left( \frac{\partial^2}{\partial r^2} + \frac{1}{r} \frac{\partial}{\partial r} - \frac{\nu^2}{r^2} \right) R_\nu(r, t) \quad \text{for } t > 0, r \geq 1. \]

Furthermore, by the condition that $u_0(r, \theta) = 0$ for $r \geq 1$, we have

\[ R_\nu(r, 0) = 0 \quad \text{for } r \geq 1. \]

Applying the Laplace transform in time to (2.5) under the condition (2.6), we obtain

\[ \left( \frac{\partial^2}{\partial r^2} + \frac{1}{r} \frac{\partial}{\partial r} - \left( is + \frac{\nu^2}{r^2} \right) \right) \hat{R}_\nu(r, s) = 0, \]

where $\hat{R}_\nu$ is the Laplace transform of $R_\nu$ defined by the formula

\[ \hat{R}_\nu(r, s) = \int_0^{\infty} e^{-st} R_\nu(r, t) dt. \]
Now, a comparison of (A.8) and (2.7) shows that the general solution of (2.7) is given by the formula
\[ \hat{R}_v(r, s) = a_v(s) K_v(\sqrt{i s} r) + b_v(s) I_v(\sqrt{i s} r), \quad r \geq 1, \]
where \( K_v \) and \( I_v \) are modified Bessel functions, the coefficients \( a_v \) and \( b_v \) are arbitrary functions analytic in the right half-plane, and the branch of the square root is determined by
\[ \sqrt{z} = e^{(\log |z| + i \arg z)/2}, \quad -\pi < \arg z \leq \pi. \]
Obviously, since the solution \( u \) is bounded at infinity, \( \hat{R}_v(r, s) (s > 0) \) cannot grow exponentially as \( r \to \infty \). By the asymptotic expansions of \( K_v, I_v \) (see, for example, (A.9) and (A.10) in the Appendix), we must have \( b_v(s) = 0 \), i.e.,
\[ \hat{R}_v(r, s) = a_v(s) K_v(\sqrt{i s} r), \quad r \geq 1. \]
Combining (2.11) and (2.12), we have
\[ \frac{\partial}{\partial r} \hat{R}_v(r, s) = a_v(s) \sqrt{i s} K_v'(\sqrt{i s} r), \quad r \geq 1. \]
Finally, (2.2) follows from substituting \( r = 1 \) into (2.13) and applying the inverse Laplace transform.\[ \square \]

From the asymptotic expansions of \( K_v \) and \( K_v' \) (see, for example, (A.10) and (A.12) in the Appendix), we have
\[ \frac{\sqrt{i s} K_v'(\sqrt{i s})}{K_v(\sqrt{i s})} \sim -\sqrt{i s} - \frac{1}{2} + O(s^{-1/2}), \quad s \to \infty. \]
Thus, the convolution kernel in (2.2) is a generalized function and inconvenient for computation. Therefore, we remove the singular behavior by following the treatment in [13]. For this, we simply divide the kernel by a factor \( (s - s_v) \) where \( s_v \) lies close to the turning point \( i v^2 \) in the left half of the complex plane. (It has to be on the left half of the complex plane to preserve causality.) That is to say, we rewrite (2.13) with \( r = 1 \) as follows:
\[ \frac{\partial}{\partial r} \hat{R}_v(1, s) = (s - s_v) \hat{R}_v(1, s) \cdot \left( \frac{\sqrt{i s} K_v'(\sqrt{i s})}{(s - s_v) K_v(\sqrt{i s})} \right). \]
From the assumption \( R_v(1, t) = 0 \) for \( t \leq 0 \) and standard properties of the Laplace transform, we obtain the exact nonreflecting boundary conditions in the following form:
\[ \frac{\partial}{\partial r} R_v(1, t) = \int_0^t C_v(t - \tau) \left( \frac{\partial}{\partial \tau} - s_v \right) R_v(1, \tau) d\tau, \]
where the function \( C_\nu : [0, \infty) \rightarrow \mathbb{C} \) is defined by the formula

\[
C_\nu(t) = \mathcal{L}^{-1} \left[ \frac{\sqrt{is} K'_\nu(\sqrt{is})}{(s - s_\nu) K_\nu(\sqrt{is})} \right](t)
\]

and is now a proper function.

**Remark 2.2.** The exact value of \( s_\nu \) does not have great significance so long as it does not coincide with one of the zeros of \( K_\nu(\sqrt{is}) \). To be precise, we set \( s_\nu = (i \nu^2 - i k_{\nu,1}^2)/2 \), where \(-i k_{\nu,1}^2\) (defined by (A.19) in Lemma A.3) is the closest zero of \( K_\nu(\sqrt{is}) \) to the point \( i \nu^2 \).

### 3 Approximation of the Convolution Kernel

In this section, we will show that the convolution kernel \( \hat{C}_\nu(t) \) defined by (2.17) can be uniformly approximated by a sum of decaying exponential functions for \( t \geq \delta > 0 \). We accomplish this by rational approximation of

\[
\hat{C}_\nu(s) = \frac{\sqrt{is} K'_\nu(\sqrt{is})}{(s - s_\nu) K_\nu(\sqrt{is})}.
\]

Our principal result is Theorem 3.4, which states that in the right half-plane the function \( \hat{C}_\nu \) can be approximated by a sum of poles with the number of poles \( d = O(\log(1/\epsilon) \cdot (\log \nu + \log(1/\epsilon))) \) within any prescribed precision \( \epsilon \). Although the proof is somewhat technical, the underlying ideas are rather simple. That is, we first represent \( \hat{C}_\nu(s) \) as a sum of poles (discrete and continuous) by using the residue theorem with a properly chosen contour. Then we approximate it by a far fewer number of poles with an exponential convergence rate in a region that is well separated from the locations of the poles, using ideas related to the fast multipole method [10].

We begin with a rather complicated representation of \( \hat{C}_\nu(z) \) that happens to be most suitable for the analysis of its rational approximation (following the common practice in complex analysis, from now on we will use \( z \) instead of \( s \) to denote the argument of the function \( \hat{C}_\nu \)).

**Theorem 3.1** Let \( \theta_\nu \) be specified as in Lemma A.6 for \( \nu \geq \frac{1}{2} \) and \( \theta_0 = \pi \). Let \( k_{\nu,1}, \ldots, k_{\nu,P} \) be the zeros of \( K_\nu(z) \) with \( \pi/2 < \arg k_{\nu,i} < \theta_\nu/2 + \pi/4 \), \( i = 1, \ldots, P \). Then the function \( \hat{C}_\nu(z) \) admits a representation

\[
\hat{C}_\nu(z) = \frac{w_\nu(s_\nu)}{z - s_\nu} + \sum_{n=1}^{P} \frac{2k_{\nu,n}^2/(k_{\nu,n}^2 - i s_\nu)}{z + i k_{\nu,n}^2} - \frac{1}{2\pi i} \int_0^\infty \frac{w_\nu(re^{-\pi i}) + \nu}{(r + s_\nu)(r + z)} dr \\
- \frac{e^{-i\theta_\nu}}{2\pi i} \int_0^\infty \frac{w_\nu(re^{i\theta_\nu}) + \nu}{(r - s_\nu e^{-i\theta_\nu})(r - z e^{-i\theta_\nu})} dr
\]
for \( z \in \{ z : z \in \mathbb{C}, -\pi < \arg z < \theta_v \} \setminus \{ 0, s_v, -ik_n^2, \ldots, -ik_P^2 \} \), where \( w_v \) is defined by the formula

\[
(3.3) \quad w_v(z) = \frac{\sqrt{iz} K'_v(\sqrt{iz})}{K_v(\sqrt{iz})}.
\]

**Proof:** We consider the following contour integral:

\[
(3.4) \quad I = \oint_{\gamma} \frac{w_v(\zeta) + v}{(\zeta - s_v)(\zeta - z)} d\zeta,
\]

where \( \gamma \) is chosen to be the simple closed curve shown in Figure 3.1, which proceeds counterclockwise along the circle \( C_R \) of radius \( R \) centered at the origin from \( \arg z = -\pi \) to \( \theta_v \), to the segment \( z = \rho e^{i\theta_v}, \rho \in [r, R] \), to the circle \( C_r \) of radius \( r \) centered at the origin from \( \arg z = \theta_v \) to \( -\pi \), to the segment \( z = \rho e^{-\pi}, \rho \in [r, R] \), and back to the first circle. Then (3.2) follows from an application of the residue theorem, Lemma A.4, and the following facts:

\[
(3.5) \quad \hat{C}_v(z) = \frac{w_v(z)}{z - s_v},
\]

\[
(3.6) \quad \lim_{r \to 0} \int_{C_r} \frac{w_v(\zeta) + v}{(\zeta - s_v)(\zeta - z)} d\zeta = 0,
\]

\[
(3.7) \quad \lim_{R \to \infty} \int_{C_R} \frac{w_v(\zeta) + v}{(\zeta - s_v)(\zeta - z)} d\zeta = 0,
\]

\[
(3.8) \quad \oint_{\gamma} \frac{v}{(\zeta - s_v)(\zeta - z)} d\zeta = 0.
\]

\[\square\]
The representation (3.2) already expresses $\hat{C}_ν(z)$ as a sum (discrete and continuous) of poles where all the poles lie in the left half-plane of $C$. To find an effective rational approximation of $\hat{C}_ν(z)$ with far fewer poles when $z$ lies in the right half-plane, we invoke Lemma A.1 for the second term of (3.2) and Lemma A.2 for the last two terms of (3.2).

**LEMMA 3.2** For any sufficiently small $\epsilon > 0$ and $ν ≥ \frac{1}{2}$, the function

$$p_ν(z) = \sum_{n=1}^{p_ν} \frac{2k_{ν,n}^2/(k_{ν,n}^2 - is_ν)}{z + ik_{ν,n}^2}$$

admits an approximation $g(z)$ that is a sum of $d = O(\log ν \cdot \log (1/ε))$ poles, with

$$|p_ν(z) - g(z)| ≤ \epsilon$$

provided $\text{Re}(z) ≥ 0$.

**PROOF:** By Lemma A.3, we clearly can cover all the poles $-ik_{ν,1}^2, \ldots, -ik_{ν,p_ν}^2$ by $n = O(\log ν)$ disks, where each is well separated from the imaginary axis by its radius.

Then, by Lemma A.1, the function $p_ν(z)$ admits an approximation $g(z)$ for $\text{Re}(z) ≥ 0$ that is a sum of $m \cdot n$ poles with the error bounded by

$$|p_ν(z) - g(z)| ≤ \frac{10}{2^n - 1} |F_ν(z)|,$$

where

$$F_ν(z) = \sum_{n=1}^{p_ν} \frac{|2k_{ν,n}^2/(k_{ν,n}^2 - is_ν)|}{z + ik_{ν,n}^2}.$$
Using Lemma A.3 again, we have the following estimates:

\begin{align}
|k_{v,n}| & \leq c v, \\
|k_{v,n}^2 - i s_v| & \geq cn^{2/3} v^{4/3}, \\
|z + i k_{v,n}^2| & \geq cn^{2/3} v^{4/3},
\end{align}

for \( \text{Re}(z) \geq 0 \) and \( n = 1, \ldots, P_v \). Then

\begin{align}
|F_v(z)| & \leq c \sum_{n=1}^{P_v} v^{-2/3} n^{-4/3} \leq \frac{c'}{v}.
\end{align}

Therefore, a choice of

\begin{equation}
m = O \left( \log \left( \frac{1}{\epsilon} \right) \right),
\end{equation}

suffices to give (3.10).

\begin{proof}
Let \( I_0 = (0, 2^{-m}) \), \( I_j = (2^j, 2^{j+1}) \) for \( j = -m, \ldots, n - 1 \), and \( I_\infty = (2^n, \infty) \). We split the integral into three parts accordingly:

\begin{equation}
q_v(z) = q_v^0(z) + q_v^1(z) + q_v^2(z),
\end{equation}

where \( q_v^0, q_v^1, \) and \( q_v^2 \) are defined by the formulae

\begin{align}
q_v^0(z) &= \int_{I_0} \omega_v(z)(r)dr, \\
q_v^1(z) &= \sum_{j=-m}^{n-1} \int_{I_j} \omega_v(z)(r)dr, \\
q_v^2(z) &= \int_{I_\infty} \omega_v(z)(r)dr.
\end{align}

\end{proof}

**Lemma 3.3** For any sufficiently small \( \epsilon > 0 \) and \( v \) a positive integer or half an odd integer, the functions

\begin{align}
q_v(z) &= \int_{0}^{\infty} \frac{w_v(re^{-\pi i}) + v}{(r + s_v)(r + z)} dr = \int_{0}^{\infty} \omega_v(z)(r)dr \\
r_v(z) &= \int_{0}^{\infty} \frac{w_v(re^{i\theta_v}) + v}{(r - s_v e^{-i\theta_v})(r -ze^{-i\theta_v})} dr
\end{align}

admit approximations \( g_1(z) \) and \( g_2(z) \), respectively, which are a sum of \( d = O \left( \log \left( \frac{1}{\epsilon} \right) \cdot (\log v + \log \left( \frac{1}{\epsilon} \right)) \right) \) poles, with

\begin{align}
|q_v(z) - g_1(z)| &\leq \epsilon \\
|r_v(z) - g_2(z)| &\leq \epsilon
\end{align}

provided \( \text{Re}(z) \geq 0 \).

**Proof:** Let \( I_0 = (0, 2^{-m}) \), \( I_j = (2^j, 2^{j+1}) \) for \( j = -m, \ldots, n - 1 \), and \( I_\infty = (2^n, \infty) \). We split the integral into three parts accordingly:

\begin{equation}
q_v(z) = q_v^0(z) + q_v^1(z) + q_v^2(z),
\end{equation}

where \( q_v^0, q_v^1, \) and \( q_v^2 \) are defined by the formulae

\begin{align}
q_v^0(z) &= \int_{I_0} \omega_v(z)(r)dr, \\
q_v^1(z) &= \sum_{j=-m}^{n-1} \int_{I_j} \omega_v(z)(r)dr, \\
q_v^2(z) &= \int_{I_\infty} \omega_v(z)(r)dr.
\end{align}
We now choose $m$ and $n$ so that $q^0_\nu$ and $q^n_\nu$ can be ignored and then use Lemma A.2 to approximate $q^1_\nu$. From (A.27) and the fact that $\nu$ is positive, we have

\begin{align}
\nu < 1, \quad O(z^\nu), \\
\nu = 1, \quad O(z \log z), \\
\nu > 1, \quad O(z),
\end{align}

Let us now write $q^0_\nu(z)$ explicitly as

\begin{align}
q^0_\nu(z) = \int_{2^{-m}}^{2^m} \frac{w_\nu(re^{-\pi i}) + \nu}{(r + s_\nu)(r + z)} dr.
\end{align}

By Lemma A.3 and Remark 2.2, $s_\nu$ is very close to the point $i\nu^2$. Hence

\begin{align}
|r + s_\nu| \geq \text{Im}(r + s_\nu) = \text{Im}(s_\nu) \geq \frac{|s_\nu|}{C}
\end{align}

for some constant $C$. Also, since we assume that $\text{Re}(z) \geq 0$, we have

\begin{align}
|r + z| \geq \text{Re}(r + z) \geq r.
\end{align}

Combining (3.24), (3.25), (3.26), and (3.27), we obtain

\begin{align}
|q^0_\nu(z)| &\leq \frac{C}{|s_\nu|} \int_{2^{-m}}^{2^m} \frac{|w_\nu(re^{-\pi i}) + \nu|}{r} dr \\
&\approx \frac{C}{|s_\nu|} \left\{ \begin{array}{ll}
\int_{2^{-m}} f^{2^{-m}} dr = O\left(\frac{1}{2^{2m}}\right), & \frac{1}{2} < \nu < 1, \\
\int_{2^{-m}} f^{2^{-m}} d\nu = O\left(\frac{m}{2^m}\right), & \nu = 1, \\
\int_{2^{-m}} f^{2^{-m}} \frac{1}{2} dr = O\left(\frac{1}{2^{2m}}\right), & \nu > 1.
\end{array} \right.
\end{align}

Hence a choice of

\begin{align}
m = O(\log (1/\epsilon))
\end{align}

suffices to guarantee

\begin{align}
|q^0_\nu(z)| \leq \epsilon.
\end{align}

Using (A.28) and assuming $n$ is sufficiently large, we have

\begin{align}
|q^n_\nu(z)| \leq c \int_{2^n}^{\infty} \frac{\sqrt{r} + \nu}{r^2} dr = c \left(\frac{\nu}{2^n} + \frac{1}{2^{(n-2)/2}}\right).
\end{align}

Hence a choice of

\begin{align}
n = O(\log (1/\epsilon) + \log \nu),
\end{align}

suffices to guarantee

\begin{align}
|q^n_\nu(z)| \leq \epsilon.
\end{align}
Now by Lemma A.2, $q^1_\nu(z)$ admits an approximation $g(z)$ for $\Re(z) \geq 0$ that is a sum of $p \cdot (m + n)$ poles with the error bounded by

\begin{equation}
|q^1_\nu(z) - g(z)| \leq \frac{10}{2^p - 1} \int_{2^{-m}}^{2^n} |\omega_{\nu,z}(r)| dr.
\end{equation}

Using Lemmas A.4, A.5, and A.6 we have

\begin{equation}
\int_{2^{-m}}^{2^n} |\omega_{\nu,z}(r)| dr \leq c \int_{2^{-m}}^{2^n} \frac{\sqrt{r + \nu}}{r + \nu} dr + c \int_{2^{-m}}^{2^n} \frac{\nu}{r + \nu} dr
\end{equation}

\begin{equation}
\leq c \int_{2^{-m}}^{1} \frac{1}{\nu^2 r} dr + c \int_{1}^{2^n} \frac{1}{r^2} dr + c \int_{2^{-m}}^{1} \frac{\nu}{\nu^2 r^2} dr + c \int_{1}^{2^n} \frac{1}{2\nu r^2} dr
\end{equation}

\begin{equation}
\leq c \left( \frac{1}{\nu^2} + c_1 + \frac{m}{\nu} + c_2 \right) \leq C_1 + C_2 \frac{m}{\nu}
\end{equation}

for some constants $C_1$ and $C_2$. Hence a choice of

\begin{equation}
p = O(\log(1/\epsilon)), \quad \epsilon \to 0,
\end{equation}

suffices to guarantee

\begin{equation}
|q^1_\nu(z) - g(z)| \leq \epsilon.
\end{equation}

The conclusion for $q_\nu(z)$ follows. The proof for $r_\nu(z)$ is almost identical to the above, except that we now have $|r - ze^{-i\theta}| \geq \frac{\epsilon}{2}$ instead of $|r + z| \geq r$. This has no effect on our conclusion. \square

Combining Theorem 3.1 and Lemmas 3.2 and 3.3, we obtain a pole approximation for $\hat{C}_\nu(z)$.

**Theorem 3.4** Let $\nu$ be a positive integer or half a positive odd integer. Let $\epsilon > 0$ be the desired precision. Then there exists a positive integer $d$ with

\begin{equation}
d = O(\log(1/\epsilon) \cdot (\log \nu + \log(1/\epsilon))),
\end{equation}

and complex numbers $w_1, \ldots, w_d$ and $z_1, \ldots, z_d$, depending on $\nu$ and $\epsilon$, such that the function

\begin{equation}
g_{\nu,\epsilon}(z) = \sum_{n=1}^{d} \frac{w_n}{z - z_n}
\end{equation}

approximates the function $\hat{C}_\nu(z)$ with the bound

\begin{equation}
|\hat{C}_\nu(z) - g_{\nu,\epsilon}(z)| \leq \epsilon
\end{equation}

provided that $\Re(z) \geq 0$. 

Due to its special asymptotic behavior at the origin, the case \( \nu = 0 \) requires a somewhat different treatment. In principle, we could still find a pole approximation of \( \hat{C}_0(z) \) for \( \text{Re}(z) \geq 0 \). But a similar derivation shows that an exceedingly large number of poles is needed. Hence we relax the condition \( \text{Re}(z) \geq 0 \) to \( \text{Re}(z) \geq \eta > 0 \). By the same argument as in [2], this will lead to accurate approximations of the convolution for time \( T \leq \eta^{-1} \).

**Theorem 3.5** For any sufficiently small \( \epsilon > 0 \) and \( \eta > 0 \), there exists a positive integer \( d \) with

\[
d = O((\log (1/\epsilon) + \log (1/\eta)) \cdot \log (1/\epsilon)),
\]

and complex numbers \( w_1, \ldots, w_d \) and \( z_1, \ldots, z_d \), depending on \( \eta \) and \( \epsilon \), such that the function

\[
g_{\eta, \epsilon}(z) = \sum_{n=1}^{d} \frac{w_n}{z - z_n}
\]

approximates the function \( \hat{C}_0(z) \) with the bound

\[
|\hat{C}_0(z) - g_{\eta, \epsilon}(z)| \leq \epsilon
\]

provided that \( \text{Re}(z) \geq \eta \).

**Proof:** By (3.2), we only need to consider the approximation of the following integral:

\[
s(z) = \int_{0}^{\infty} \frac{w_0(re^{\pi i}) - w_0(re^{-\pi i})}{(r + s_0)(r + z)} \, dr = \int_{0}^{\infty} \omega_z(r) \, dr.
\]

We split the integral into two parts

\[
s(z) = s_1(z) + s_2(z),
\]

where

\[
s_1(z) = \int_{0}^{2m\eta} \omega_z(r) \, dr, \quad s_2(z) = \int_{2m\eta}^{\infty} \omega_z(r) \, dr.
\]

Using (A.28) and assuming \( m \) is sufficiently large, we have

\[
|s_2(z)| \leq c \int_{2m\eta}^{\infty} \frac{\sqrt{r}}{r^2} \, dr = \frac{2c}{\sqrt{2m\eta}}.
\]

Hence a choice of

\[
m = O((\log (1/\epsilon) + \log (1/\eta))
\]

suffices to guarantee

\[
|s_2(z)| \leq \epsilon.
\]
Now an application of Lemma A.2 shows there is a function \( g(z) \) which is a sum of \( p \cdot m \) poles such that

\[
|s_1(z) - g(z)| \leq \frac{10}{2^p - 1} \int_0^{2^n} |\omega_z(r)| dr \leq \frac{c}{2^p - 1}.
\]

A choice of

\[
p = O(\log (1/\epsilon))
\]

suffices to guarantee

\[
|s_1(z) - g(z)| \leq \epsilon,
\]

and the theorem follows. □

We are now in a position to present our principal analytical result.

**Theorem 3.6** Let \( \nu \) be a positive integer or half of a positive odd integer. For any sufficiently small \( \epsilon > 0 \) and \( \delta > 0 \), there exists a positive integer \( d \) with

\[
d = O((\log (1/\epsilon) + \log (1/\delta)) \cdot (\log \nu + \log (1/\epsilon) + \log (1/\delta))),
\]

and complex numbers \( w_1, \ldots, w_d \) and \( z_1, \ldots, z_d \), depending on \( \nu, \epsilon, \) and \( \delta \), such that the function

\[
G_{\nu, \epsilon, \delta}(t) = \sum_{n=1}^{d} w_ne^{zn t}
\]

approximates the convolution kernel \( C_{\nu}(t) \) defined by (2.17) with the bound

\[
|C_{\nu}(t) - G_{\nu, \epsilon, \delta}(t)| \leq \epsilon
\]

provided that \( t \geq \delta \).

**Proof:** By Theorem 3.4, given \( \epsilon' > 0 \) there exists a function \( g_{\nu, \epsilon'}(z) = \sum_{n=1}^{d'} \frac{w_n}{z - z_n} \), which is a sum of \( d' = O(\log (1/\epsilon') \cdot (\log \nu + \log (1/\epsilon'))) \) poles such that

\[
|\hat{C}_\nu(z) - g_{\nu, \epsilon'}(z)| \leq \epsilon'
\]

for \( \text{Re}(z) \geq 0 \). Now define the function \( G_{\nu, \epsilon'}(t) \) by

\[
G_{\nu, \epsilon'}(t) = \mathcal{L}^{-1}[g_{\nu, \epsilon'}](t) = \sum_{n=1}^{d'} w_ne^{zn t}.
\]

Using (2.4) and (2.17) we have

\[
|C_{\nu}(t) - G_{\nu, \epsilon'}(t)| = \left| \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{ity} (\hat{C}_\nu(iy) - g_{\nu, \epsilon'}(iy)) dy \right| \leq I_1 + I_2 + I_3,
\]
where \(I_1, I_2,\) and \(I_3\) are defined by the formulae

\[
I_1 = \frac{1}{2\pi} \left| \int_{-L}^{L} e^{iyt} (\hat{C}_v(iy) - g_{v,e}(iy)) dy \right|,
\]

\[
I_2 = \frac{1}{2\pi} \left| \int_{-\infty}^{-L} e^{iyt} (\hat{C}_v(iy) - g_{v,e}(iy)) dy \right|,
\]

\[
I_3 = \frac{1}{2\pi} \left| \int_{L}^{\infty} e^{iyt} (\hat{C}_v(iy) - g_{v,e}(iy)) dy \right|.
\]

The estimate for \(I_1\) follows immediately from (3.56),

\[
I_1 \leq \frac{1}{\pi} L \epsilon'.
\]

From the asymptotic behavior of \(\hat{C}_v,\) we have

\[
I_2, I_3 \sim \frac{1}{2\pi} \frac{1}{t \sqrt{L}}, \quad L \to \infty,
\]

and

\[
|C_v(t) - G_{v,e'}(t)| \leq c \left( Le' + \frac{1}{t \sqrt{L}} \right) \leq c \left( Le' + \frac{1}{\delta \sqrt{L}} \right).
\]

The minimum of the right-hand side is achieved when

\[
L = (\delta \epsilon')^{-2/3}.
\]

Hence

\[
|\hat{C}_v(t) - G_{v,e'}(t)| \leq c \frac{e^{1/3}}{\delta^{2/3}},
\]

and the theorem follows from setting \(\epsilon' = \epsilon^3 \delta^2.\)

\[\Box\]

Remark 3.7. The above error estimate is rather pessimistic. Since \(L \gg \frac{1}{\tau},\) the integration interval \([-L, L]\) contains many periods of the function \(e^{iyt}.\) Thus the integral will usually be much smaller than \(Le'\) because of cancellation caused by the highly oscillatory integrand. (It is very unlikely that the phase of the function \(\hat{C}_v(iy) - g_{v,e}(iy)\) will match that of \(e^{iyt}.\) Hence we expect that \(\epsilon'\) should be of the order \(\epsilon \delta\) instead of \(\epsilon^3 \delta^2,\) which is much better from a practical viewpoint.

Second, the above estimate does suggest a numerical method to find a good sum-of-exponentials approximation for the kernel \(C_v(t).\) Namely, one could try to find a rational approximation for \(\hat{C}_v(z)\) over a very large interval \([-iL, iL]\) along the imaginary axis. Here \(L\) should satisfy the condition \(L \gg \max(v^2, \frac{1}{\tau})\) so that both \(\hat{C}_v(z)\) and its rational approximation are smooth outside the interval \([-iL, iL]\) and the resulting exponential approximation will be good for \(t \geq \delta.\)

Theorem 3.5 leads also to the following result for \(\nu = 0:\)
Theorem 3.8 Let $0 < \delta \leq t \leq T$, and let $\epsilon > 0$ be the desired precision. Then there exists a positive integer $d$ with

$$d = O((\log(1/\epsilon) + \log(T/\delta)) \cdot (\log(1/\epsilon) + \log(1/\delta)))$$

and complex numbers $w_1, \ldots, w_d$ and $z_1, \ldots, z_d$, depending on $\epsilon, \delta,$ and $T$, such that the function

$$G_{\epsilon, \delta, T}(t) = \sum_{n=1}^{d} w_n e^{z_n t}$$

approximates the convolution kernel $C_0(t)$ with the bound

$$|C_0(t) - G_{\epsilon, \delta, T}(t)| \leq \epsilon.$$

We have designed a rather robust numerical method for computing sum-of-poles representations (see [13] for details). Obviously, finding an optimal sum-of-poles representation is a very ill-conditioned problem. To cope with this ill conditioning, we first extract the nearby poles that are close to the imaginary axis in the complex plane and close to the singular point of the kernel by applying the least-squares algorithm in [2] on a small interval centered around the singular point of the kernel. We then form a new function that is simply the difference of the original kernel with the sum of poles we just found. This new function is less singular than the original kernel, and we can then apply the least-squares algorithm to find its sum-of-poles representation on a larger interval. By repeating this procedure successively, we will be able to find the sum-of-poles representation of the original kernel on a much larger interval.

Figure 3.3 plots the number of poles versus the kernel index $\nu$. Here we choose the interval discussed in Remark 3.7 to be $[-10^8 i, 10^8 i]$ and set the $L^2$ norm relative precision to be $\epsilon = 10^{-12}$. The resulting sum-of-exponential approximations
achieve 12-digit accuracy for $10^{-8} \leq t \leq 10^8$ and $0 \leq \nu \leq 1024$, which is sufficient for most practical purposes. The sum-of-poles representation obtained from our algorithm is by no means optimal. However, from Figure 3.3, we see that the average number of poles needed is less than 80, and it is quite satisfactory considering the highly ill-conditioned nature of the problem. (The weights and pole locations are publicly available for download; see [13].)

The reader will note that the plot of the required number of poles in Figure 3.3 is rather noisy. This is due to the fact that our numerical algorithm for finding the pole approximation treats each $\nu$ separately. A more global algorithm would likely be better at producing a more efficient set of poles and a smoother curve in Figure 3.3.

Finally, Figure 3.4 shows the locations of poles used for approximating $\hat{C}_{200}(z)$, which is rather typical for $0 \leq \nu \leq 1024$.

Remark 3.9. The extreme size of the pole locations shown in Figure 3.4 is due to the fact that our numerical algorithm for the pole approximation is not optimal. However, it will not lead to artificial time step restrictions or unnecessary stiffness. The poles $z_i$ with very large negative real parts correspond in physical space to exponential functions $e^{z_i t}$ that decay very rapidly and thus contribute very little to the summation process. They are not “numerical modes” being integrated by a finite difference approximation. Thus, they lead to some inefficiency, but not instability. One can, in fact, delete these poles if $|e^{z_i \Delta t}|$ is below the desired precision for a time step $\Delta t$.

4 The Local Part of the Convolution

The computation of the local part, i.e., $\int_{t-\delta}^t C_\nu(t - \tau) R_\nu(1, \tau) d\tau$, consists of two steps. First, we have to compute $C_\nu(t)$ for $0 < t \leq \delta$ directly from the formula $C_\nu(t) = L^{-1}(\hat{C}_\nu)(t)$. Then we need to replace the integral by a quadrature rule. By
(2.4), the inverse Laplace transform can be viewed as the Fourier transform for the function $\hat{C}_\nu(iy)$, i.e.,

$$C_\nu(t) = \frac{1}{2\pi} \int_{-\infty}^{\infty} \hat{C}_\nu(iy) e^{iyt} \, dy.$$  

We split the above integral into three parts:

$$C_\nu(t) = \frac{1}{2\pi} \int_{-L_\nu}^{L_\nu} \hat{C}_\nu(iy) e^{iyt} \, dy + \frac{-e^{iL_\nu t}}{2\pi i} \int_{0}^{\infty} \hat{C}_\nu(iL_\nu - x) e^{-xt} \, dx + \frac{e^{-iL_\nu t}}{2\pi i} \int_{0}^{\infty} \hat{C}_\nu(-iL_\nu - x) e^{-xt} \, dx,$$

where $L_\nu$ is some large number, say $2\nu^2$, such that no poles of $\hat{C}_\nu$ lie in the region \{z \in \mathbb{C} : \text{Re}(z) < 0, |\text{Im}(z)| > L_\nu\}.

Since $t$ is very small, $e^{iyt}$ is slowly oscillatory and the first integral can be computed by standard adaptive integration very accurately. We use Laguerre quadrature [6] to compute the last two integrals since their integrands are exponentially decaying.

**Remark 4.1.** Because the evaluation of $C_\nu(t)$ by the above method is very accurate, we can use it as a reference to check the accuracy of the sum-of-exponentials approximation.

To discretize the local part of the convolution, we first note that the asymptotic expansion of $C_\nu(t)$ as $t \to 0$ is of the form $c_1/\sqrt{t} + c_2 + c_3\sqrt{t} + \cdots$. This can easily be deduced from the asymptotic behavior of $\hat{C}_\nu(z)$ as $z \to \infty$. Since $R_\nu(t)$ is differentiable with respect to $t$, we will obtain an accuracy of order $2.5$ if the quadrature rule can integrate functions $f$ of the form $c_1/\sqrt{t} + c_2 + c_3\sqrt{t} + c_4 t$ exactly. The difficulty here is that the coefficients $c_i$ are not available and the function $f$ can only be evaluated in toto. Fortunately, the generalized Gaussian quadrature rules for systems of arbitrary functions developed by Ma, Rokhlin, and Wandzura [18] are ideal for our problem. A simple application of the algorithm in [18] gives us the following two-point quadrature rule:

$$\int_{0}^{1} f_k(x) dx = \sum_{i=1}^{2} w_i f_k(x_i) \quad \text{for } k = 1, 2, 3, 4,$$

where $\{f_k\} = \{1, 1/\sqrt{x}, x, \sqrt{x}\}$, $w_{1,2} = (1 \pm \sqrt{1/3})/2$, and $x_i = w_i^2$ for $i = 1, 2$. We will use this rule (after scaling) to evaluate the local part of the convolution.

**5 Discretization**

For ease of implementation, we use a variant of the splitting method as the basic marching scheme. The semidiscretization in time is done using Strang splitting

$$u(t + dt) = e^{-\frac{1}{2}V dt} e^{-i\Delta t} e^{-\frac{1}{2}V dt} u(t)$$
which is of second-order accuracy. In other words, for each time step, we carry out the following three steps:

1. \( u_1 = e^{-\left(i/2\right)Vd t} u(t) \),
2. \( u_2 = e^{-i \Delta t} u_1 \), and
3. \( u(t + dt) = e^{-\left(i/2\right)Vd t} u_2 \).

The first and third steps can be carried out inside the unit disk without any difficulty since the operator \( e^{-\left(i/2\right)Vd t} \) is simply a multiplication operator in physical space. For the second step, we note that since \( V \) has compact support in the unit disk, \( u(t + dt) = u_2 \) on the unit circle. Hence \( u_2 \) satisfies exactly the same nonreflecting boundary condition as \( u(t + dt) \). Thus, when solving for \( u_2 \), a full description of the problem to be solved is

\[
\begin{cases}
    i \frac{\partial}{\partial t} u_2(x, t) = \Delta u_2(x, t) & \text{for } t > 0, x \in D^2, \\
    u_2(x, 0) = u_1(x, t) & \text{for } x \in D^2, \\
    Bu_2 = 0 & \text{for } x \in S^1,
\end{cases}
\]

where \( B \) is the nonreflecting boundary condition operator. We use the trapezoidal rule in time. For spatial discretization, we use an \( M_0 \times N_r \) polar grid. By expanding \( u_2 \) in a Fourier series

\[
\sum_{k=-M_0/2}^{M_0/2} R_k(r, t) e^{ik \theta},
\]

the partial differential equation (5.1) is converted into a set of ordinary differential equations for each radial function \( R_k \). We solve these stiff two-point boundary value problems using the fast integral equation-based method developed by Lee and Greengard [16].

The asymptotic CPU and storage requirements of the complete algorithm are now straightforward to analyze. For each time step, \( O(M_0 N_r) \) work is required for the multiplication operator \( e^{-\left(i/2\right)Vd t} \). By using the fast Fourier transform, we calculate that \( O(M_0 \log M_0 N_r) \) work is required to convert \( u_2 \) into its Fourier coefficients (and vice versa). \( O(M_0 N_r) \) work is required to solve the necessary two-point boundary value problems using the solver of [16]. Finally, \( O(C_k) \) work is required to evaluate the convolution term in the nonreflecting boundary condition for each Fourier coefficient \( R_k \), where \( C_k \) is the number of exponentials needed for approximating the convolution kernel \( C_k \). Thus the total cost of the evaluation of the nonreflecting boundary conditions is of the order \( O(C M_0) \) where

\[
C = \frac{2}{M_0} \sum_{k \leq M_0/2} C_k.
\]

Since \( C < 80 \) for \( M_0 \leq 2048 \), which is sufficient for most applications, it is clear that the cost of imposing the exact boundary condition is negligible compared to that of the interior domain solver. As for storage, we note that \( O(C M_0) \) values are
required to keep track of the locations and weights of the poles and the history part of the convolution.

6 A Numerical Example

To test the quality of the ENRBC, we consider the homogeneous Schrödinger equation with initial data

\begin{equation}
\frac{1}{\sqrt{\alpha_x \alpha_y}} e^{ik_x x - \frac{x^2}{2\alpha_x}} e^{ik_y y - \frac{y^2}{2\alpha_y}},
\end{equation}

i.e., the product of two one-dimensional Gaussian wave packets. The exact solution is readily obtained:

\begin{equation}
\frac{1}{\sqrt{(\alpha_x - it)(\alpha_y - it)}} e^{ik_x (x+kt) - \frac{(x+kt)^2}{4(\alpha_x - it)}} e^{ik_y (y+kt) - \frac{(y+kt)^2}{4(\alpha_y - it)}}.
\end{equation}

We set \(\alpha_x = 0.01\), \(\alpha_y = 0.01\), \(k_x = 5\), and \(k_y = -5\) and evolve the solution from time \(t = 0\) to \(T = 0.5\) (the wave goes almost completely out of the computational domain at \(T\)).

We take \(M_\theta = 41\) and \(N_r = 70\). Figure 6.1 shows the time evolution of the \(L^2\) norm relative errors for \(\Delta t = 0.002\). A similar pattern was seen in the one-dimensional case [14]. For our scheme, the computational error is dominated by the time discretization. Figure 6.2 shows the maximum \(L^2\) norm relative error as a function of time step \(\Delta t\), from which we see that our scheme is second-order accurate in time. In other words, the nonreflecting boundary condition is working as expected to the precision tested.

7 Conclusions

We have proven that the nonreflecting boundary kernel for the two-dimensional Schrödinger equation can be approximated by a small sum of exponentials to high
precision. We believe that our approach will be of value in several areas of applied physics, including semiconductor device simulation, which consists in part of quantum scattering of a single particle from a given potential, and fiber optics, for which a nonlinear Schrödinger equation is often used to describe transmission over long distances.

Some open mathematical issues remain, including a rigorous analysis of the well-posedness of coupling the exact nonreflecting boundary conditions to spatial discretization schemes. We intend to address this question, as well as some of the applications mentioned above, at a later date.

Appendix

In this appendix, we summarize several results from classical analysis to be used in the paper.

A.1 Two Lemmas from Alpert, Greengard, and Hagstrom [2]

In Section 3, we have frequently used lemmas 3.4 and 3.5 in [2]. For the sake of completeness, we include these two lemmas below.

**Lemma A.1** (Lemma 3.4 in [2]) Suppose \( n \) and \( p \) are positive integers, \( q_1, \ldots, q_n \) are complex numbers, and \( z_1, \ldots, z_n \) are complex numbers contained in disks \( D_1, \ldots, D_p \) of radii \( r_1, \ldots, r_p \), centered at \( c_1, \ldots, c_p \), respectively. The function

\[
    f(z) = \sum_{j=1}^{n} \frac{q_j}{z - z_j}
\]
can be approximated for \( z \) satisfying \( \text{Re}(z - c_i) \geq ar_i > r_i \) for \( i = 1, \ldots, p \) by the \( m \cdot p \) pole expansion

\[
g_m(z) = \sum_{i=1}^{p} \sum_{j=0}^{m-1} \frac{\gamma_{ij}}{z - (c_i + r_i \omega^j)},
\]

where \( \gamma_{ij} \) is defined by

\[
\gamma_{ij} = \frac{1}{m} \sum_{l=0}^{m-1} \omega^{-jl} \sum_{\zeta_k \in D_i \setminus U_{i-1}} q_k \cdot \left( \frac{\zeta_k - c_i}{r_i} \right)^l,
\]

\( i = 1, \ldots, p, \ j = 0, \ldots, m - 1, \)

with \( U_i = \bigcup_{j \leq i} D_j. \) The error of the approximation is bounded by

\[
|f(z) - g_m(z)| \leq \frac{2(a^2 + 1)|F(z)|}{(am - 1)(a - 1)^2},
\]

where

\[
F(z) = \sum_{j=1}^{n} \frac{|q_j|}{z - z_j}.
\]

**Lemma A.2 (Lemma 3.5 in [2])** Suppose that the discrete poles of the above lemma are replaced with a density \( q \) defined on a curve \( C \) with \( C \subset U_p = D_1 \cup \cdots \cup D_p; \) specifically,

\[
f(z) = \int_C \frac{q(\xi)}{z - \xi} d\xi,
\]

which is finite for \( z \) outside \( U_p, \) and that \( g_m \) is defined by (A.2) with \( \gamma_{ij} \) defined by

\[
\gamma_{ij} = \frac{1}{m} \sum_{l=0}^{m-1} \omega^{-jl} \int_{C \cap (D_i \setminus U_{i-1})} q(\xi) \left( \frac{\xi - c_i}{r_i} \right)^l d\xi,
\]

\( i = 1, \ldots, p, \ j = 0, \ldots, m - 1, \)

with \( U_i = \bigcup_{j \leq i} D_j. \) Then the bound (A.4) holds as before.

**A.2 Modified Bessel Functions**

The modified Bessel functions \( K_\nu(z) \) and \( I_\nu(z) \) are two linearly independent solutions of the differential equation

\[
z^2 \frac{d^2 w}{dz^2} + z \frac{dw}{dz} - (z^2 + \nu^2) w = 0.
\]
Asymptotic expansions of the modified Bessel functions and their derivatives (see, for example, [1, §9.6]) are given by the formulae

\[
I_\nu(z) \sim \frac{e^z}{\sqrt{2\pi z}} \left(1 - \frac{\mu - 1}{8z} + \frac{(\mu - 1)(\mu - 9)}{2!(8z)^2} + \cdots\right), \quad |\arg z| < \frac{1}{2},
\]

\[\text{(A.9)}\]

\[
K_\nu(z) \sim \sqrt{\frac{\pi}{2z}} e^{-z} \left(1 + \frac{\mu - 1}{8z} + \frac{(\mu - 1)(\mu - 9)}{2!(8z)^2} + \cdots\right), \quad |\arg z| < \frac{3}{2},
\]

\[\text{(A.10)}\]

\[
I'_\nu(z) \sim \frac{e^z}{\sqrt{2\pi z}} \left(1 - \frac{\mu + 3}{8z} + \frac{(\mu - 1)(\mu + 15)}{2!(8z)^2} + \cdots\right), \quad |\arg z| < \frac{1}{2},
\]

\[\text{(A.11)}\]

\[
K'_\nu(z) \sim -\sqrt{\frac{\pi}{2z}} e^{-z} \left(1 + \frac{\mu + 3}{8z} + \frac{(\mu - 1)(\mu + 15)}{2!(8z)^2} + \cdots\right), \quad |\arg z| < \frac{3}{2},
\]

\[\text{(A.12)}\]

where \(\mu = 4\nu^2\).

The zeros of \(K_\nu\) have been studied in great detail in the literature; the following lemma summarizes several facts concerning their distribution to be used subsequently.

**Lemma A.3 (The Zeros of \(K_\nu(z)\), \(\nu \geq 0\), \(|\arg z| \leq \pi\))**

\(K_\nu(z)\) has no zeros for which \(|\arg z| \leq \frac{\pi}{2}\). If \(z\) is a zero of \(K_\nu(z)\), then \(\bar{z}\) is also a zero of \(K_\nu(z)\). If \(\nu - \frac{1}{2}\) is an integer, then the number of zeros is exactly \(\nu - \frac{1}{2}\). Otherwise, the number of zeros is the even integer nearest to \(\nu - \frac{1}{2}\) and there are no zeros on the lines \(\arg z = \pm \pi\).

Furthermore, the zeros of \(K_\nu(z)\) in the region \(\frac{\pi}{2} < |\arg z| \leq \pi\) are given by the asymptotic expansion

\[
k_{\nu,n} \sim \nu z(\zeta_n) + O(\nu^{-1}), \quad \nu \to \infty,
\]

\[\text{(A.13)}\]

uniformly in \(n\), where \(\zeta_n\) is defined by the equation

\[
\zeta_n = e^{-\frac{2\pi i}{\nu}} \nu^{-\frac{3}{2}} d_n,
\]

\[\text{(A.14)}\]
The scaled zeros \( k_{\nu, n}/\nu \) of \( K_{\nu}(z) \) lie near the curve whose parametric equation is

\[
z(t) = -(t^2 - t \tanh t)^{1/2} \pm i(t \coth t - t^2)^{1/2},
\]

for \( t \in [0, t_0] \), where \( t_0 = 1.19968 \ldots \) is the positive root of \( t = \coth t \). The zeros in the third quadrant satisfy the inequality

\[
|\text{Re}(k_{\nu, n})| \geq c n^{\frac{2}{3}} \nu^{\frac{1}{3}}.
\]

The distance between two adjacent zeros in each quadrant decreases towards the negative real axis for large \( \nu \). Finally, the zero nearest to the turning point \( i\nu \) is given by the equation

\[
k_{\nu, 1} \sim i\nu + e^{\pi i/6} \left( \frac{\nu}{2} \right)^{1/3} a_1,
\]

where \( a_1 \approx 2.338 \).

**PROOF:** All of these results can be found in the literature [1, 2, 20, 27], except the one concerning the distance between two adjacent zeros. To prove that claim, we substitute (A.16) and (A.14) into (A.15) and introduce a new variable

\[
x_n = \left( n - \frac{1}{4} \right)/\nu.
\]

We then obtain

\[
\pi i x_n \simeq \frac{i (1 + \sqrt{1 + z_n^2})}{z_n} - \sqrt{1 + z_n^2}
\]

with \( z_n = z(z_n) \). Differentiating the above equation gives us

\[
\pi i dx_n \simeq -\frac{\sqrt{1 + z_n^2}}{z_n} dz_n.
\]

For large \( \nu \), we may substitute \( dx_n \simeq x_n - x_{n-1} = 1/\nu \) and \( dz_n \simeq z_n - z_{n-1} \) into (A.21) to obtain

\[
|z_n - z_{n-1}| \simeq \left| \frac{\pi z_n}{\sqrt{1 + z_n^2}} \right| |x_n - x_{n-1}| \leq \left| \frac{\pi z_n}{\nu \sqrt{1 + z_n^2}} \right|.
\]
The claim now follows from the fact that $|z/\sqrt{1+z^2}|$ decreases along the curve (A.17) in each quadrant approaching the negative real axis. Finally, we observe that combining (A.17) and (A.22) leads to

(A.23) \[ |z_n - z_{n-1}| \geq \frac{c}{\nu} \]

with $c$ a positive number. \qed

A.3 Logarithmic Derivative of $K_\nu(e^{\pi i/4}\sqrt{z})$

We now define the functions $v_\nu, w_\nu: \mathbb{C} \to \mathbb{C}$ by the formulae

(A.24) \[ v_\nu(z) = \frac{zK'_\nu(z)}{K_\nu(z)}, \]

(A.25) \[ w_\nu(z) = v_\nu(e^{\pi i/4}\sqrt{z}), \]

with the branch cut chosen along the negative real axis and $-\pi < \arg z \leq \pi$. The properties of the function $v_\nu$ have been studied in detail in [2]. Here we will apply them to study the function $w_\nu$. The next lemma collects a few facts about $w_\nu$ to be used subsequently. It follows immediately from Lemma A.3 and [2, theorem 4.1].

**Lemma A.4** Let $k_{\nu,1}, \ldots, k_{\nu,N_\nu}$ denote the zeros of $K_\nu(z)$. Let $k_{\nu,1}, \ldots, k_{\nu,M_\nu}$ be those zeros with $\frac{\nu}{2} < \arg k_{\nu,i} \leq \frac{3\nu}{2}, i = 1, \ldots, M_\nu$. Then the function $w_\nu(z)$ admits a representation

(A.26) \[ w_\nu(z) = -e^{\frac{\pi i}{4}\sqrt{z}} - \frac{1}{2} \sum_{n=1}^{N_\nu} \frac{k_{\nu,n}}{e^{\pi i/4}\sqrt{z} - k_{\nu,n}} + \frac{1}{\pi} \int_0^\infty \operatorname{Im}(v_\nu(re^{-\pi i})) \frac{dr}{r + e^{\pi i/4}\sqrt{z}} \]

for $z \in \mathbb{C} \setminus \{0, -i k_{\nu,1}^2, \ldots, -i k_{\nu,M_\nu}^2\}$. Furthermore, the limiting forms of $w_\nu$, as $z \to 0$, are

(A.27) \[ w_\nu(z) \sim \begin{cases} (\log (e^{\pi i/4}\sqrt{z}/2) + \gamma)^{-1} + O(z), & \nu = 0, \\ -|\nu| + O(z^{1/2}), & 0 < |\nu| < 1, \\ -|\nu| + O(z \log z), & |\nu| = 1, \\ -|\nu| + O(z), & |\nu| > 1, \end{cases} \]

where $\gamma$ is the Euler constant. As $z \to \infty$,

(A.28) \[ w_\nu(z) \sim -e^{\frac{\pi i}{4}\sqrt{z}} - \frac{1}{2} + O(z^{-\frac{3}{2}}). \]

Lastly, the function $w_\nu$ satisfies the recurrence relation

(A.29) \[ w_\nu(z) = \frac{-iz}{\nu - 1 - w_{\nu-1}(z)} - \nu. \]

Finally, we will need to have a more detailed analysis of the last two terms on the right-hand side of (A.26).
LEMMA A.5 Let

\[(A.30)\quad f_\nu(z) = \int_0^\infty \Im(v_\nu(re^{-\pi i})) \frac{1}{r + e^{\pi i/4}\sqrt{z}} dr.\]

Then if \(\nu = k + \frac{1}{2}\) for integral \(k\) (i.e., half of an odd integer), \(f_\nu(z) = 0\). If \(\nu\) is a nonnegative integer, then \(|f_\nu(z)| \leq c\), where \(c\) is independent of \(\nu\) and \(z\).

PROOF: If \(\nu = k + \frac{1}{2}\) for integral \(k\), then

\[(A.31)\quad v_\nu(z) = -z - \frac{1}{2} + \sum_{n=1}^{N_\nu} \frac{z}{n} - k_{\nu,n}.\]

Since the zeros of \(K_\nu\) always come into conjugate pairs in this case (Lemma A.3), we have \(\Im(v_\nu(re^{-\pi i})) = 0\). The first statement in the lemma follows.

For nonnegative integer \(\nu\), by lemma 4.2 in [2], we have

\[(A.32)\quad \Im(v_\nu(re^{-\pi i})) = \frac{(-1)^\nu \pi}{K_\nu^2(r) + \pi^2 I_\nu^2(r)},\]

\[(A.33)\quad \Im(v_\nu(re^{-\pi i})) \sim \begin{cases} \frac{-\pi}{4} + \pi \nu, & \nu = 0, \quad r \to 0, \\ \frac{-\pi}{4} + \pi \nu, & \nu \neq 0, \quad r \to 0, \end{cases}\]

\[(A.34)\quad \Im(v_\nu(re^{-\pi i})) \sim 2(-1)^\nu r e^{-r}, \quad r \to \infty,\]

\[(A.35)\quad \Im(v_\nu(re^{-\pi i})) \sim \frac{(1+e^{-\nu r})}{\cosh(2\phi(r))}, \quad \nu \to \infty,\]

where

\[(A.36)\quad \phi(r) = \sqrt{1 + r^2} + \ln \frac{r}{1 + \sqrt{1 + r^2}}.\]

For \(-\pi < \arg z \leq \pi\), we have \(-\frac{\pi}{4} < \arg e^{\pi i/4}\sqrt{z} \leq \frac{3\pi}{4}\), and a simple estimate gives us

\[(A.37)\quad |r + e^{\pi i/4}\sqrt{z}| \geq \frac{r}{2}.\]

Hence

\[(A.38)\quad |f_\nu(z)| \leq 2 \int_0^\infty \frac{1}{r} |\Im(v_\nu(re^{-\pi i}))| dr.\]

The right-hand side of the above inequality is finite according to (A.33) and (A.34). To see that this bound is independent of \(\nu\), we apply the change of variable \(r = \nu x\).
and substitute (A.35) into the integrand for large \( \nu \) to obtain
\[
\int_0^\infty \frac{2}{r} |\text{Im}(v_\nu(re^{-\pi i}))| \, dr
= \int_0^\infty \frac{2}{x} |\text{Im}(v_\nu(\nu xe^{-\pi i}))| \, dx
\sim \int_0^\infty \frac{2\nu \sqrt{1+x^2}}{x \cosh (2\nu \phi(x))} \, dx
\leq 4\nu \int_0^\infty \frac{\sqrt{1+x^2}}{x} e^{-2\nu |\phi(x)|} \, dx
= 4\left( \int_0^{x^*} e^{2\nu \phi(x)} \nu \phi'(x) \, dx + \int_{x^*}^\infty e^{-2\nu \phi(x)} \nu \phi'(x) \, dx \right)
= 4\left( \int_{-\infty}^0 e^{2\nu \phi(y)} \nu \phi'(y) \, dy + \int_0^\infty e^{-2\nu \phi(y)} \nu \phi'(y) \, dy \right), \quad y = \nu \phi(x),
\]
\[= 4\]
as \( \nu \to \infty \), where \( x^* \) is the only positive zero of \( \phi(x) \). The second statement follows. \( \square \)

**Lemma A.6** Let
\[
h_\nu(z) = \sum_{n=1}^{N_\nu} \frac{k_{\nu,n}}{e^{\pi i/4} \sqrt{z} - k_{\nu,n}}.
\]
Then \( h_0(z) = 0 \) and given \( \nu_0 > 0 \), \( h_\nu(z) \) satisfies the inequality
\[
|h_\nu(z)| \leq \frac{C \nu}{1 + |\sqrt{z}|/\nu}
\]
for \( \nu > \nu_0 \) and \( -\pi \leq \arg z \leq \frac{\pi}{2} \). Furthermore, there exists \( \theta_\nu \) with \( \frac{15\pi}{36} \leq \theta_\nu < \pi \) such that
\[
|h_\nu(z)| \leq \frac{C \nu^2}{1 + |\sqrt{z}|/\nu}
\]
for all \( \nu \) with \( \nu > \nu_0 \) and all \( z \) with \( \arg z = \theta_\nu \).

**Proof:** The claim that \( h_0(z) = 0 \) follows from the fact that \( K_0(z) \) has no zero along the branch we have chosen. (A.41) is taken from lemma 4.5 in [2].

To prove the last statement, let us choose \( \theta_\nu \) to be \( \arg k_{\nu,M_\nu} + \arg k_{\nu,M_\nu-1} - \frac{\pi}{2} \), where \( k_{\nu,M_\nu} \) is specified in Lemma A.4 as the zero nearest to the ray \( \arg z = \frac{5\pi}{4} \) from above. Then (A.42) is trivial except for \( |\sqrt{z}/\nu| \approx 1 \). But Lemma A.3 shows that
\[
\left| \frac{e^{\pi i/4} \sqrt{z}}{\nu} - \frac{k_{\nu,n}}{\nu} \right| \geq \frac{c}{\nu},
\]
since $z$ lies between two adjacent zeros of $K_{\nu}$ (see (A.23)). Hence, for $|\sqrt{z}/\nu| \approx 1,$

$$|h_{\nu}(z)| = \left| \sum_{n=1}^{N_{\nu}} \frac{k_{\nu,n}/\nu}{e^{\pi i/4}\sqrt{z}/\nu - k_{\nu,n}/\nu} \right| \leq \sum_{n=1}^{N_{\nu}} \frac{\nu}{c} \leq C\nu^2.$$ (A.44)

\[ \square \]

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