Finite Difference Schemes on unbounded Domains

Matthias Ehrhardt

ehrhardt@math.tu-berlin.de

Institut für Mathematik, Technische Universität Berlin, Straße des 17.Juni 136, D–10623 Berlin, Germany.

Abstract

We discuss the nonstandard problem of using the finite difference method to solve numerically a partial differential equation posed on an unbounded domain. We propose different strategies to construct so–called *discrete artificial boundary conditions* (ABCs) and present an efficient implementation by the sum–of–exponential ansatz. The derivation of the ABCs is based on the knowledge of the exact solution, the construction of asymptotic solutions or the usage of a continued fraction expansion to a second–order difference equation. Our approach is explained by means of three different types of partial differential equations arising in option pricing, in quantum mechanics and in (underwater) acoustics. Finally, we conclude with an illustrating numerical example from underwater acoustics showing the superiority of our new approach.

1 Introduction

It is a nonstandard task to solve numerically a partial differential equation posed on an unbounded domain. Usually finite differences are used to discretize the equation and *artificial boundary conditions* (ABCs) are introduced in order to confine the computational domain. If the solution on the computational domain coincides with the exact solution on the unbounded domain (restricted to the finite domain), one refers to these ABCs as *transparent boundary conditions* (TBCs).

However, ad-hoc discretizations of an *analytic TBC* may induce numerical reflections at this artificial boundary and also may destroy the stability properties of the underlying finite difference method. To overcome both problems so–called *discrete ABCs* (or *discrete TBCs*) are derived directly from the fully discretized problem on the unbounded domain. These discrete ABCs/TBCs are already adapted to the inner scheme and therefore the numerical stability is often better–behaved than for a discretized differential TBC. An additional motivation for this discrete approach arises from the fact that the numerical scheme often needs more boundary conditions than the analytical problem can provide (especially hyperbolic equations, systems of equations and high–order schemes).

In the literature the discrete approach did not gain much attention yet. The first *discrete derivation of artificial boundary conditions* was presented in [1, Section 5]. This discrete approach was also used by Schmidt and Deuflhard [2] for the Schrödinger equation, in [3], [4], [5] for linear hyperbolic systems and in [6] for the wave equation in one dimension, also with error estimates for the reflected part. In [4] a discrete (nonlocal) solution operator for general difference schemes (strictly hyperbolic systems, with constant coefficients in 1D) is constructed. Lill generalized in [7] the approach of Engquist and Majda [1] to boundary conditions for a convection–diffusion equation and drops the standard assumption that the initial data is compactly supported inside the computational domain.

In this work we will propose different strategies to construct these discrete ABCs by using the Z–transformation and exact or asymptotic solutions to the second–order linear difference equation:

$$\Delta^2 \, y_j - p(j) \, y_j = 0, \quad j \in \mathbb{Z}. \tag{1.1}$$

Here, $\Delta^2 y_j = y_{j+1} - 2\, y_j + y_{j-1}$ denotes the standard second–order difference operator.

We consider (1.1) with three different discrete potential terms:

A) constant coefficients: $p(j) = d, \quad d \in \mathbb{C}$,

B) Coulomb–type term: $p(j) = d + c/j, \quad c, d \in \mathbb{C}$,

C) affin–linear term: $p(j) = d + c\, j, \quad c, d \in \mathbb{C}$.

Equation A) can easily be solved explicitly. For the other two model equations it is not clear a-priori whether one can find *explicit solutions*.

However, it is a standard task [8, Chapter 7] to determine *asymptotic solutions* if the difference equation is of *Poincaré type*, i.e. the coefficient $p(j)$ in equation (1.1) must approach a constant value as $j \to \infty$. This is the case for the equation B) with the Coulomb–type term, but the difference equation of case C) (a general discrete Airy equation) does not satisfy this condition.

In §2 we will present the fields of applications of these three cases, namely the Black–Scholes equation for American options, a time–dependent Schrödinger equation with a Coulomb–like potential and with a linearly varying potential. Finite difference schemes are introduced in Section 3 to solve numerically these partial differential equations. For the derivation of the ABCs we apply the Z–transformation technique and need to solve in the sequel difference equations of the form (1.1). Afterwards, in §4, §5 and §6, we outline general procedures to construct ABCs and present different techniques to obtain exact and asymptotic solutions of these three model equations.

Since the discrete TBC includes a convolution with respect to time with a weakly decaying kernel, its numerical evaluation becomes very costly for large–time simulations. As a remedy we construct in §7 an *approximate discrete ABC* with a kernel having the form of a finite sum–of–exponentials, which can be evaluated by a very efficient recursion formula.

The Schrödinger equation with a linear varying potential term arises in (underwater) acoustics and we will present at the end of this chapter a concrete numerical example in Section 8 which will show the superiority of the new (approximated) discrete TBC.

2 Fields of Applications

2.1 The Black–Scholes Equation for American Options

The famous Black–Scholes equation is an effective model for option pricing. It was named after the pioneers Black, Scholes and Merton who suggested it 1973 [9], [10]. A derivation of the Black–Scholes equation can be found in [11] and for a more complete discussion in the context of discrete TBCs we refer the interested reader to [12].

An option is the right to buy ('call option') or to sell ('put option') an asset (typically a stock or a parcel of shares of a company) for a price E by the date T. European options can only be exercised at the expiration date T. For *American options* exercise is permitted at any time until the expiry date. While for European options the Black–Scholes equation results (after a standard transformation) in a boundary value problem, for American options it results in a free boundary problem (FBP) for the heat equation. In general, closed–form solutions do not exist (especially for American options) and the solution has to be computed numerically. The standard approach for solving the Black–Scholes equation for American options consists in transforming the original equation to a heat equation posed on a semi–unbounded domain with a free boundary [11].

The Black–Scholes Equation. Here we consider an *American call*. V denotes the value of an option and depends on the current value S of the underlying asset, and time t: $V = V(S,t)$.

$$\frac{\partial V}{\partial t} + \frac{\sigma^2}{2} S^2 \frac{\partial^2 V}{\partial S^2} + (r - D_0) S \frac{\partial V}{\partial S} - rV = 0, \quad 0 < S < S_f(t), \quad (2.1a)$$

$0 \le t < T$, where σ is the volatility of the asset price, r is the risk-free interest rate and T is the expiry date. We assume that dividends are paid with a continuous yields of constant level D_0. $S_f(t)$ denotes the free boundary ('early exercise boundary') separating the *holding region* ($S < S_f(t)$) and the *exercise region* ($S > S_f(t)$).

The final condition (*'payoff condition'*) at the expiry $t = T$ is

$$V(S,T) = (S - E)^+, \qquad 0 \le S < S_f(T), \qquad (2.1b)$$

with the notation $f^+ = \max(f, 0)$, $E > 0$ denotes the *exercise price* or 'strike', and $S_f(T) = \max(E, rE/D_0)$.

The asset–price boundary conditions at $S = 0$, and $S = S_f(t)$ are

$$V(0,t) = 0, \quad 0 \le t \le T, \qquad (2.1c)$$

$$V(S_f(t),t) = (S_f(t) - E)^+, \quad \frac{\partial V}{\partial S}(S_f(t),t) = 1, \quad 0 \le t \le T, \quad (2.1d)$$

i.e. at $S = 0$ the option is worthless. Note that we need two conditions at the free boundary $S = S_f(t)$. One condition is necessary for the solution of (2.1a) and the other is needed for determining the position of the *free boundary* $S = S_f(t)$ itself. At $S = S_f(t)$ one requires that $V(S,t)$ touches the payoff function tangentially.

The transformation to the heat equation. In the sequel we shall show how to transform (2.1a) into a diffusion equation (cf. [11,

§ 5.4]). First it is convenient to transform (2.1a)–(2.1d) to a forward in time equation by the change of variable $t = T - 2\tau/\sigma^2$. The new time variable τ stands for the *remaining life time* of the option (up to the scaling by $\sigma^2/2$). We denote the new variables by:

$$\widetilde{V}(S,\tau) = V(S,t) = V\big(S, T - \frac{2\tau}{\sigma^2}\big), \quad \widetilde{S}_f(\tau) = S_f\big(T - \frac{2\tau}{\sigma^2}\big),$$

$$\tilde{r} = \frac{2}{\sigma^2} r, \quad \widetilde{D}_0 = \frac{2}{\sigma^2} D_0, \quad \widetilde{T} = \frac{\sigma^2}{2} T.$$

The forward equation then reads:

$$\frac{\partial \widetilde{V}}{\partial \tau} = S^2 \frac{\partial^2 \widetilde{V}}{\partial S^2} + (\tilde{r} - \widetilde{D}_0) S \frac{\partial \widetilde{V}}{\partial S} - \tilde{r}\, \widetilde{V}, \quad 0 < S < \widetilde{S}_f(\tau), \tag{2.2a}$$

$0 \le \tau < \widetilde{T}$, with the initial condition

$$\widetilde{V}(S,0) = (S - E)^+, \qquad 0 \le S < \widetilde{S}_f(0) = S_0, \tag{2.2b}$$

and the boundary conditions

$$\lim_{S \to 0} \widetilde{V}(S,\tau) = 0, \; 0 \le \tau \le \widetilde{T}, \tag{2.2c}$$

$$\widetilde{V}(\widetilde{S}_f(\tau),\tau) = (\widetilde{S}_f(\tau) - E)^+, \; \frac{\partial \widetilde{V}}{\partial S}(\widetilde{S}_f(\tau),\tau) = 1, \; 0 \le \tau \le \widetilde{T}. \tag{2.2d}$$

The right hand side of (2.2a) is a well–known *Euler's differential equation* and therefore it is standard practice to transform (2.2a) to the heat equation. To do so, we let

$$\alpha = -\frac{1}{2}(\tilde{r} - \widetilde{D}_0 - 1), \quad \beta = -\frac{1}{4}(\tilde{r} - \widetilde{D}_0 + 1)^2 - \tilde{r},$$

and use the change of variables

$$S = Ee^x, \quad \widetilde{V}(S,\tau) = Ee^{\alpha x + \beta \tau} v(x,\tau).$$

Then problem (2.2a)–(2.2d) is equivalent to the free boundary problem for the heat equation:

$$\frac{\partial v}{\partial \tau} = \frac{\partial^2 v}{\partial x^2}, \quad -\infty < x < x_f(\tau), \quad 0 \le \tau < \widetilde{T}, \tag{2.3a}$$

with the initial condition

$$v(x,0) = \big(e^{\frac{1}{2}(\tilde{r} - \widetilde{D}_0 + 1)x} - e^{\frac{1}{2}(\tilde{r} - \widetilde{D}_0 - 1)x}\big)^+, \quad x < x_f(0), \tag{2.3b}$$

and the boundary conditions

$$\lim_{x\to-\infty} v(x,\tau) = 0, \quad 0 \le \tau \le \widetilde{T}, \tag{2.3c}$$

$$v(x_f(\tau),\tau) = g(x_f(\tau),\tau), \quad 0 \le \tau \le \widetilde{T}, \tag{2.3d}$$

$$e^{(\alpha-1)x-\beta\tau}\Big(\alpha v(x_f(\tau),\tau) + \frac{\partial v(x_f(\tau),\tau)}{\partial x}\Big) = 1,\ 0 \le \tau \le \widetilde{T}, \tag{2.3e}$$

where

$$g(x,\tau) = e^{-\alpha x-\beta\tau}(e^x - 1)^+.$$

It is known that the free boundary given by $x_f(\tau) = \ln(\widetilde{S}_f(\tau)/E)$ has the property $x_f(\tau) > 0$ for $0 \le \tau \le \widetilde{T}$.

2.2 The Schrödinger–Poisson System

The second example arises in quantum mechanics and details concerning the computation of solutions on unbounded domains can be found in [13]. In many applications one wants to calculate the evolution of an ensemble of particles over long time. These computations include the solution of the single particle Schrödinger equation obtained from a mean field approximation using Coulomb potentials [14]. The transient Schrödinger–Poisson problem describes the time evolution of the wave function ψ under the force of the self–consistent potential V caused by the charged electrons. It is an appropriate model for semiconductor heterostructures (cf. [14] and the references therein).

The Schrödinger–Poisson system. The transient *Schrödinger–Poisson system* (SPS) associated with a single particle system in vacuum reads for the complex–valued wave function $\psi(x,t)$ and the electrostatic potential $V(x,t)$:

$$i\hbar\partial_t\psi = -\frac{\hbar^2}{2m}\Delta_x\psi + V\psi, \qquad x \in \mathbb{R}^3, \quad t > 0, \tag{2.4a}$$

$$\Delta_x V = -\gamma\, n, \qquad x \in \mathbb{R}^3, \quad t > 0, \tag{2.4b}$$

where $n = |\psi(x,t)|^2$ denotes the particle density for a pure quantum state and $\gamma > 0$ (repulsive case) or $\gamma < 0$ (attractive case) depending on the considered type of Coulomb force. Here $\hbar$ denotes the Planck constant and m is the particle mass. Throughout this application we will be interested in the attractive case. Equations (2.4) are supplied with some initial data $\psi(x,0) = \psi^I(x)$ and the decay conditions

$$\lim_{|x|\to\infty} \psi(x,t) = 0, \qquad \lim_{|x|\to\infty} V(x,t) = 0.$$

The spherically symmetric Schrödinger–Poisson system. Since we want to keep the numerical effort to a minimum we only consider the case of a spherically symmetric *initial condition*: $\psi(x,0) = \psi^I(r)$. It can be shown that $\psi(x,t)$ is invariant under rotations and therefore a radial function at any time. For convenience we introduce the *reduced wave function* $u(r,t)$ by

$$\psi(x,t) = \frac{1}{\sqrt{4\pi}}\frac{u(r,t)}{r}, \tag{2.5}$$

and define the *effective charge* $\phi(r,t) = rV(x,t)$. The *SPS* reduces then to

$$i\hbar\partial_t u = -\frac{\hbar^2}{2m}\partial_r^2 u + \frac{\phi}{r}u, \qquad r>0, \quad t>0, \tag{2.6a}$$

$$\partial_r^2\phi = -\frac{\gamma}{4\pi}\frac{|u|^2}{r}, \qquad r>0, \quad t>0, \tag{2.6b}$$

together with the *homogeneous Dirichlet conditions at the origin*

$$u(0,t) = 0, \qquad \phi(0,t) = 0,$$

and the *decay conditions*

$$\lim_{r\to\infty} u(r,t) = 0, \qquad \lim_{r\to\infty}\phi(r,t) = \frac{\gamma}{4\pi}.$$

2.3 The Standard "Parabolic Equation"

The third example, a Schrödinger equation with a linear varying potential can be used for *standard "parabolic equation"* (SPE) [15] simulations in (underwater) acoustics and for radiowave propagation in the troposphere. Details about this example can be found in [16]. Here we focus on the application to underwater acoustics.

The standard parabolic equation in underwater acoustics. A standard task in oceanography is to calculate the acoustic pressure $p(z,r)$ emerging from a time–harmonic point source located in the water at $(z_s, 0)$. Here, $r>0$ denotes the radial range variable and $0<z<z_b$ the depth variable (assuming a cylindrical geometry). The water surface is at $z=0$, and the (horizontal) sea bottom at $z=z_b$. We denote the local sound speed by $c(z,r)$, the density by $\rho(z,r)$, and the attenuation by $\alpha(z,r)\geq 0$. The *complex refractive index* is given by $N(z,r) = c_0/c(z,r) + i\alpha(z,r)/k_0$ with a reference sound speed c_0

and the reference wave number $k_0 = 2\pi f/c_0$, where f denotes the frequency of the emitted sound.

The *SPE* in cylindrical coordinates (z, r) reads:

$$2ik_0\psi_r(z,r) + \rho\,\partial_z(\rho^{-1}\partial_z)\psi(z,r) + k_0^2(N^2(z,r)-1)\,\psi(z,r) = 0, \quad (2.7)$$

where ψ denotes the (complex valued) *outgoing acoustic field*

$$\psi(z,r) = \sqrt{k_0 r}\,p(z,r)\,e^{-ik_0 r}, \quad (2.8)$$

in the far field approximation ($k_0 r \gg 1$). This *Schrödinger equation* (2.7) is an evolution equation in r and a reasonable description of waves with a propagation direction within about 15° of the horizontal.

Here, the physical problem is posed on the unbounded z–interval $(0,\infty)$ and one wishes to restrict the computational domain in the z–direction by introducing an artificial boundary at the water–bottom interface ($z = z_b$), where the wave propagation in water has to be coupled to the wave propagation in the the bottom. At the water surface one usually employs a Dirichlet ("pressure release") BC: $\psi(0,r) = 0$.

Since the density is typically discontinuous at the water–bottom interface ($z = z_b$), one requires continuity of the pressure and the normal particle velocity:

$$\psi(z_b-, r) = \psi(z_b+, r), \quad (2.9a)$$

$$\frac{\psi_z(z_b-, r)}{\rho_w} = \frac{\psi_z(z_b+, r)}{\rho_b}, \quad (2.9b)$$

where $\rho_w = \rho(z_b-, r)$ is the water density just above the bottom and ρ_b denotes the constant density of the bottom. This situation is sketched in Fig. 1.

In this application we are especially interested in the case of a *linear squared refractive index* in the bottom region. For most underwater acoustics (and also radiowave propagation) problems the squared refractive index in the exterior domain increases with z. However, the usual TBC (see e.g. [17]) was derived for a homogeneous medium (i.e. all physical parameters are constant for $z > z_b$). This TBC is not matched to the behaviour of the refractive index and spurious reflections will occur. Instead we will derive a TBC that matches the squared refractive index gradient at $z = z_b$. We denote the physical parameters in the bottom with the subscript b and assume that the squared refractive index N_b below $z = z_b$ can be written as

$$N_b^2(z,r) = 1 + \beta + \mu(z - z_b), \quad z > z_b, \quad (2.10)$$

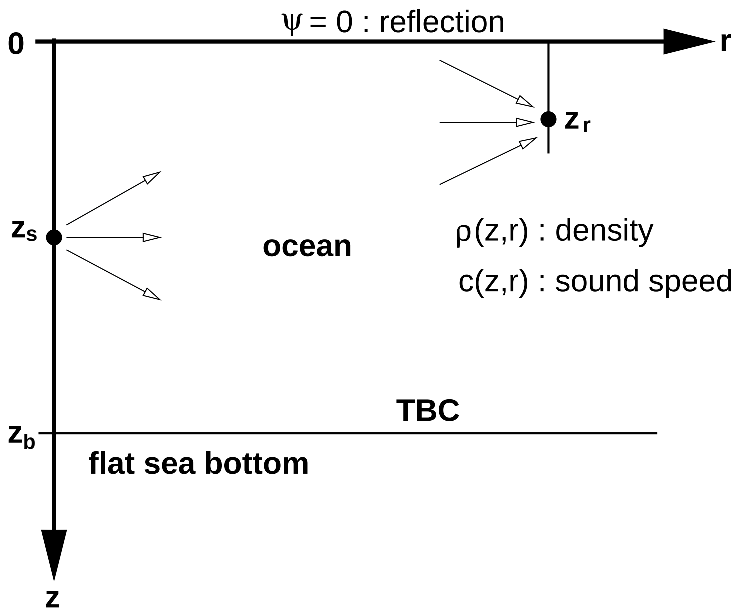

Figure 1: Underwater sound propagation in cylindrical coordinates.

with real parameters β and $\mu \neq 0$, i.e. no attenuation in the bottom: $\alpha_b = 0$. All other physical parameters are assumed to be constant in the bottom. Here, the slope $\mu > 0$ corresponds to a downward-refracting bottom (energy loss) and $\mu < 0$ represents the upward-refracting case, i.e. energy is returned from the bottom.

3 The Finite Difference Equations

In this section we derive the *discrete ABCs/TBCs* of the fully discretized problems based on a finite difference discretization. This strategy helps to minimize any numerical reflections at the boundary since the discrete ABC/TBC is matched to the finite difference scheme in the interior domain. Moreover, the stability of the resulting scheme is often better behaved (compared to the discretized analytic TBC).

While a uniform spatial grid is necessary in the exterior domain, the interior grid may be nonuniform in space. To derive the discrete ABCs/TBCs we make the *basic assumption* that the initial data is supported inside the computational domain. We note that a strategy to overcome this restriction could be found in [18].

The basic tool for the derivation of the discrete ABCs/TBCs is the *Z–transformation* of a series $\{f_j^{(n)}\}_{n\in\mathbb{N}_0}$ (with j fixed):

$$\mathcal{Z}\{f_j^{(n)}\} = \hat{f}_j(z) := \sum_{n=0}^{\infty} f_j^{(n)}\, z^{-n}, \quad z \in \mathbb{C}, \quad |z| > 1.$$

The Z–transformation is the discrete analogue of the Laplace–transformation and a collection of the most important properties is given in the Appendix.

3.1 The Black–Scholes Equation for American Options

With the uniform grid points $x_j = a + j\Delta x$, $\tau_n = n\Delta\tau$ and the approximation $v_j^{(n)} \approx v(x_j, \tau_n)$ the *Crank-Nicolson scheme* for solving the heat equation (2.3a) is

$$v_j^{(n+1)} - v_j^{(n)} = \rho \left(v_{j+1}^{(n+\frac{1}{2})} - 2v_j^{(n+\frac{1}{2})} + v_{j-1}^{(n+\frac{1}{2})} \right), \tag{3.1}$$

with the time averaging $v_j^{(n+\frac{1}{2})} = (v_j^{(n+1)} + v_j^{(n)})/2$ and the parabolic mesh ratio $\rho = \Delta\tau/(\Delta x)^2$.

We obtain the discrete TBC by solving the *discrete exterior problem*, i.e. (3.1) for $j \le 1$. To do so, we apply the Z–transformation to solve (3.1) for $j \le 1$ explicitly. We assume for the initial data, $v_j^{(0)} = 0,\ j \le 2$ and obtain the *transformed exterior scheme*

$$\Delta^2 \hat{v}_j(z) - \frac{2}{\rho}\frac{z-1}{z+1}\, \hat{v}_j(z) = 0, \quad j \le 1. \tag{3.2}$$

Obviously, (3.2) is a difference equation of the form (1.1) Case A).

3.2 The Schrödinger–Poisson System

For simplicity we use the uniform grid points

$$u_j^{(n)} \sim u(r_j, t_n), \quad \phi_j^{(n)} \sim \phi(r_j, t_n), \quad r_j = j\Delta r,\ t_n = n\Delta t,$$

with $0 \le j \le J$, $n \ge 0$. The *discretized SPS* (2.6) reads

$$i\hbar D_t^+ u_j^{(n)} = -\frac{\hbar^2}{2m} D_r^2 u_j^{(n+\frac{1}{2})} + \frac{\phi_j^{(n+\frac{1}{2})}}{r_j} u_j^{(n+\frac{1}{2})}, \quad j \ge 1, \tag{3.3a}$$

$$D_r^2 \phi_j^{(n+1)} = -\frac{\gamma}{4\pi} \frac{\left|u_j^{(n+1)}\right|^2}{r_j}, \quad j \ge 1, \tag{3.3b}$$

together with the discrete boundary conditions

$$u_0^{(n)} = 0, \qquad \lim_{j\to\infty} u_j^{(n)} = 0, \qquad \phi_0^{(n)} = 0, \qquad \phi_J^{(n)} = \frac{\gamma}{4\pi}. \tag{3.3c}$$

In (3.3) we have used the standard abbreviations for the forward, and second–order difference quotient:

$$D_t^+ u_j^{(n)} = \frac{u_j^{(n+1)} - u_j^{(n)}}{\Delta t}, \quad D_r^2 u_j^{(n)} = \frac{u_{j+1}^{(n)} - 2u_j^{(n)} + u_{j-1}^{(n)}}{(\Delta r)^2},$$

and the time averaging $u_j^{(n+\frac{1}{2})} = (u_j^{(n+1)} + u_j^{(n)})/2$.

On the unbounded domain $j \ge 0$ the nonlinear method (3.3) conserves the *discrete mass* and *discrete total energy* (cf. [13]). In order to obtain a mass and energy conserving *linear method* we now proceed to present a predictor–corrector scheme approximating the nonlinear Crank–Nicolson scheme (3.3). It only requires the solution of linear equations at each step and is of the same order as the nonlinear scheme (3.3). One step of this scheme will be of the form

$$(u_j^{(n)}, \phi_j^{(n)}) \to u_j^{(n,1)} \to \phi_j^{(n,1)} \to u_j^{(n,2)} \to \phi_j^{(n,2)} \to (u_j^{(n+1)}, \phi_j^{(n+1)}),$$

where $u_j^{(n,1)}$, $\phi_j^{(n,1)}$, $u_j^{(n,2)}$, $\phi_j^{(n,2)}$ denote intermediate values. For brevity we define the *difference operators* $D_{t,k}^+ u_j^{(n)} = (u_j^{(n,k)} - u_j^{(n)})/\Delta t$, and the *time averaging* $S_{t,k} u_j^{(n)} = (u_j^{(n,k)} + u_j^{(n)})/2$, $k = 1, 2$.

Given $u_j^{(n)}$, the *predictor step* to compute $u_j^{(n,1)}$, $\phi_j^{(n,1)}$ is then defined as

$$i\hbar D_{t,1}^+ u_j^{(n)} = -\frac{\hbar^2}{2m} D_r^2 S_{t,1} u_j^{(n)} + \frac{\phi_j^{(n)}}{r_j} S_{t,1} u_j^{(n)}, \quad j \ge 1, \tag{3.4a}$$

$$D_r^2 \phi_j^{(n,1)} = -\frac{\gamma}{4\pi} \frac{\left|u_j^{(n,1)}\right|^2}{r_j}, \quad j \ge 1. \tag{3.4b}$$

The standard *corrector step* for determining $u_j^{(n,2)}$, $\phi_j^{(n,2)}$ is

$$i\hbar D_{t,2}^{+} u_j^{(n)} = -\frac{\hbar^2}{2m} D_r^2 S_{t,2} u_j^{(n)} + \frac{S_{t,1}\phi_j^{(n)}}{r_j} S_{t,2} u_j^{(n)}, \quad j \geq 1, \tag{3.5a}$$

$$D_r^2 \phi_j^{(n,2)} = -\frac{\gamma}{4\pi} \frac{\left|u_j^{(n,2)}\right|^2}{r_j}, \quad j \geq 1. \tag{3.5b}$$

It is easily verified that the scheme (3.4)–(3.5) is second order consistent in time.

The Modulation Strategy. This predictor–corrector approximation to the Crank–Nicolson scheme preserves mass, but exhibits a spurious gain / loss of the total energy which is of order Δt^3 at each time step. Ringhofer and Soler [19] remedied this situation by *modulating the phase* of the second stage $u_j^{(n,2)}$ of the scheme by setting

$$u_j^{(n+1)} = u_j^{(n,2)} \exp(i\Delta t^3 \omega g_j), \qquad \phi_j^{(n+1)} = \phi_j^{(n,2)}, \quad j \geq 1, \tag{3.6}$$

where ω is a real parameter and $g_j = g(r_j)$ denotes an appropriate chosen real valued function bounded uniformly for $j \in \mathbb{N}$. Obviously, this correction does not change the discrete ℓ^2-norm of $u_j^{(k,2)}$, and therefore the mass conservation property is retained by this phase correction. Also, adding an order $\mathrm{O}(\Delta t^3)$ correction at each step does not destroy the overall second order accuracy of the method. For the detailed choice of the modulation parameters ω and g_j we refer to [13].

Since the problem (2.6a) is posed on an unbounded domain we have to introduce an artificial boundary at $j = J$ for the numerical solution. Here we use the approach of a discrete TBC first assuming a constant potential term: $V_j^{(n)} = \phi_j^{(n)}/r_j = \text{const}$ for $j \geq J$ (exterior domain). Afterwards we extend these calculations to the case of a Coulomb–type potential, i.e. $\phi_j^{(n)}/r_j \sim \text{const}\,/r_j$, $j \to \infty$. It will turn out that the discrete TBC for zero potential is the lowest order approximation to the discrete TBC for the Coulomb–type potential. To derive the discrete TBC we assume $u_j^{(0)} = 0$, $j \geq J-1$, and rewrite the scheme (3.3a) in the form:

$$-i\rho(u_j^{(n+1)} - u_j^{(n)}) = \Delta^2(u_j^{(n+1)} + u_j^{(n)}) + w\frac{\phi_j^{(n+\frac{1}{2})}}{r_j}(u_j^{(n+1)} + u_j^{(n)}), \tag{3.7}$$

with the mesh ratio ρ and the abbreviation w given by

$$\rho = \frac{4m}{\hbar}\frac{\Delta r^2}{\Delta t}, \qquad w = -\frac{2m}{\hbar^2}\Delta r^2.$$

i) Constant potential term outside the computational domain. We start with assuming that $V_j^{(n)} = \phi_j^{(n)}/r_j = \text{const}$ for $j \geq J$ (exterior domain). The Z–transformed finite difference scheme (3.7) for $j \geq J$ reads

$$\Delta^2 \hat{u}_j(z) + i\rho\Big[\frac{z-1}{z+1} + i\kappa\Big]\hat{u}_j(z) = 0, \quad \kappa = \frac{\Delta t}{2}\frac{V_R}{\hbar}, \tag{3.8}$$

i.e. (3.8) represents a difference equation of the form (1.1) case A).

ii) Coulomb–type potential term outside the computational domain. We now assume that $\phi_j^{(n)} = \phi_j^{(n,1)} = \phi_j^{(n,2)} = \phi_\infty$, $j \geq J$ and write the discrete Z–transformed exterior problem (3.7) as

$$\Delta^2 \hat{u}_j(z) + \Big[i\rho\,\frac{z-1}{z+1} + w\frac{\phi_\infty}{j\Delta r}\Big]\hat{u}_j(z) = 0, \quad j \geq J. \tag{3.9a}$$

Clearly, (3.9a) has the form (1.1) case B) with

$$d = -i\rho\,\frac{z-1}{z+1}, \quad c = -w\frac{\phi_\infty}{\Delta r}. \tag{3.9b}$$

3.3 The Standard "Parabolic Equation"

In order to solve the Schrödinger equation (2.7) numerically we use a *Crank-Nicolson* finite difference scheme which is of second order (in Δz and Δr) and unconditionally stable. We choose the uniform grid $z_j = jh$, $r_n = nk$ with $h = \Delta z$, $k = \Delta r$ and the approximations $\psi_j^{(n)} \approx \psi(z_j, r_n)$, $\rho_j \approx \rho(z_j)$. The discretized SPE (2.7) then reads:

$$\begin{aligned} &-iR(\psi_j^{(n+1)} - \psi_j^{(n)}) = \\ &\rho_j \Delta_z^0(\rho_j^{-1}\Delta_z^0)(\psi_j^{(n+1)} + \psi_j^{(n)}) + w\big((N^2)_j^{(n)} - 1\big)(\psi_j^{(n+1)} + \psi_j^{(n)}), \end{aligned} \tag{3.10}$$

with $\Delta_z^0 \psi_j^{(n)} = \psi_{j+1/2}^{(n)} - \psi_{j-1/2}^{(n)}$, the ratio $R = 4k_0h^2/k$ and $w = k_0^2h^2$.

To derive the discrete TBC at $z_b = Jh$ we assume vanishing initial data $\psi_j^{(0)} = 0$, $j \geq J-1$ and use the linear potential term $(N^2)_j^{(n)} - 1 = \beta + \mu h(j-J)$, and solve the *discrete exterior problem*

$$\begin{aligned} &-iR(\psi_j^{(n+1)} - \psi_j^{(n)}) = \\ &\qquad \Delta^2\psi_j^{(n+1)} + \Delta^2\psi_j^{(n)} + w\big[\beta + \mu h(j-J)\big](\psi_j^{(n+1)} + \psi_j^{(n)}), \end{aligned} \tag{3.11}$$

$j \geq J$. Hence, the Z–transformed finite difference scheme (3.11), is a *general discrete Airy equation* of the form (cf. case C)):

$$\Delta^2 y_j - (d + c\, j)\, y_j = 0, \quad c, d \in \mathbb{C}. \tag{3.12a}$$

with

$$d = -2i\zeta(z) + \mu k_0^2 h^3 J, \quad c = -\mu k_0^2 h^3, \tag{3.12b}$$

$$\zeta(z) = \frac{R}{2} \frac{z-1}{z+1} - i\frac{\beta}{2} k_0^2 h^2. \tag{3.12c}$$

Transparent Boundary Conditions. Here, we review from [20] the derivation of the analytic TBC at $z = z_b$. We assume that the initial data $\psi^I = \psi(z, 0)$ is supported in the *computational domain* $0 < z < z_b$ and use the Laplace transform (2.7) for $z > z_b$:

$$\hat{\psi}_{zz}(z, s) + [\mu k_0^2 (z - \tilde{z}_b) + 2ik_0 s]\hat{\psi}(z, s) = 0, \quad z > z_b, \tag{3.13}$$

with $\tilde{z}_b = z_b - \beta/\mu$. To solve (3.13) in the *exterior domain* $z > z_b$ we set $\sigma^3 = -\mu k_0^2$ and $\tau = 2ik_0/\sigma^2$. Then (3.13) can be written as

$$\hat{\psi}_{zz}(z, s) + \sigma^2 \big[\sigma(z - \tilde{z}_b) + \tau s\big]\hat{\psi}(z, s) = 0, \quad z > z_b. \tag{3.14}$$

Introducing the change of variables $\zeta_s(z) = \sigma(z - \tilde{z}_b) + \tau s$, $U(\zeta_s(z)) = \hat{\psi}(z, s)$, we can write (3.14) in the form of an *Airy equation*:

$$U''(\zeta_s(z)) + \zeta_s(z)\, U(\zeta_s(z)) = 0, \quad z > z_b. \tag{3.15}$$

The decaying solution of (3.15) for $z \to \infty$, for fixed s, Re $s > 0$ is

$$\hat{\psi}(z, s) = C_1(s)\ \mathrm{Ai}(\zeta_s(z)), \quad z > z_b, \tag{3.16}$$

if we define the physically relevant branch of σ to be

$$\sigma = \begin{cases} (\mu k_0^2)^{1/3} e^{-i\pi/3}, & \mu > 0, \\ (-\mu k_0^2)^{1/3}, & \mu < 0. \end{cases} \tag{3.17}$$

Elimination of $C_1(s)$ gives

$$\hat{\psi}(z, s) = \hat{\psi}(z_b+, s)\, \frac{\mathrm{Ai}(\zeta_s(z))}{\mathrm{Ai}(\zeta_s(z_b))}, \quad z > z_b. \tag{3.18}$$

Finally, differentiation w.r.t. z yields with the matching conditions (2.9) the *transformed analytic TBC* at $z = z_b$:

$$\hat{\psi}_z(z_b-, s) = \frac{\rho_w}{\rho_b} s\, \hat{\psi}(z_b-, s)\, W(s), \qquad W(s) = \sigma\, \frac{\mathrm{Ai}'(\zeta_s(z_b))}{s\,\mathrm{Ai}(\zeta_s(z_b))}, \tag{3.19}$$

i.e. the *analytic TBC* at $z = z_b$ reads:

$$\psi_z(z_b, r) = \frac{\rho_w}{\rho_b} \int_0^r \psi_r(z_b, r')\, g_\mu(r - r')\, dr'. \tag{3.20}$$

The kernel g_μ is obtained by an inverse Laplace transformation of $W(s)$ (cf. [21]):

$$g_\mu(r) = \sigma \left\{ \frac{\mathrm{Ai}'(\zeta_0(z_b))}{\mathrm{Ai}(\zeta_0(z_b))} + \sum_{j=1}^{\infty} \frac{e^{-(a_j - \zeta_0(z_b))r/\tau}}{a_j - \zeta_0(z_b)} \right\}, \tag{3.21}$$

where $\zeta_0(z_b) = \sigma\beta/\mu$ and the (a_j) are the zeros of the Airy function Ai which are all located on the negative real axis. This TBC is *nonlocal* in the range variable r and can be discretized, e.g. in conjunction with a finite difference scheme for (2.7). The constant term in g_μ acts like a Dirac function and the infinite series represents the continuous part. As Levy noted in [20] the kernel g_μ decays extremely fast for $\mu > 0$ and for negative μ it decays slowly at short ranges and then oscillates.

Discretization of the continuous TBC. To incorporate the analytic TBC (3.20) in a finite difference scheme we make the approximation that $\psi_r(z_b, r')$ is constant on each subinterval $r_n < r' < r_{n+1}$ and integrate the kernel g_μ exactly. In the following we review the discretization from [20] and start with the discretization in range:

$$\psi_z(z_b, r_n) = \frac{\rho_w}{\rho_b} \sum_{m=0}^{n-1} \frac{\psi_b^{(n-m)} - \psi_b^{(n-m-1)}}{k} G_m, \tag{3.22}$$

where we set $\psi_b^{(n)} = \psi(z_b, r_n)$ and G_m is given by

$$\begin{aligned} G_m &= \int_{r_m}^{r_{m+1}} g_\mu(\eta)\, d\eta \\ &= k\sigma \frac{\mathrm{Ai}'(\zeta_0(z_b))}{\mathrm{Ai}(\zeta_0(z_b))} + \frac{2ik_0}{\sigma} \sum_{j=1}^{\infty} \frac{e^{-(a_j - \zeta_0(z_b))r/\tau}}{(a_j - \zeta_0(z_b))^2} \Big|_{r=r_m}^{r=r_{m+1}}. \end{aligned} \tag{3.23}$$

This leads after rearranging to

$$k\frac{\rho_b}{\rho_w}\psi_z(z_b, r_n) = -\psi_b^{(0)} G_n + \psi_b^{(n)} G_0 + \sum_{m=1}^{n-1} \psi_b^{(n-m)} (G_m - G_{m-1}). \tag{3.24}$$

In [20] Levy used an *offset grid* in depth, i.e. $\tilde{z}_j = (j+\frac{1}{2})h$, $\tilde{\psi}_j^{(n)} \approx \psi(\tilde{z}_j, r_n)$, $j=-1,\dots,J$, where the water–bottom interface lies between the grid points $j=J-1$ and J:

$$\psi_b^{(m)} = \psi(z_b, r_m) \approx \frac{\tilde{\psi}_J^{(m)} + \tilde{\psi}_{J-1}^{(m)}}{2}, \quad \psi_z(z_b, r_n) \approx \frac{\tilde{\psi}_J^{(n)} - \tilde{\psi}_{J-1}^{(n)}}{h}. \tag{3.25}$$

This finally yields (recall that $\tilde{\psi}_J^{(0)} = \tilde{\psi}_{J-1}^{(0)} = 0$) the following *discretized TBC* for the SPE:

$$(1-b_0)\tilde{\psi}_J^{(n)} - (1+b_0)\tilde{\psi}_{J-1}^{(n)} = \sum_{m=1}^{n-1} b_m (\tilde{\psi}_J^{(n-m)} + \tilde{\psi}_{J-1}^{(n-m)}), \tag{3.26}$$

with

$$b_0 = \frac{1}{2}\frac{h}{k}\frac{\rho_w}{\rho_b} G_0, \quad b_m = \frac{1}{2}\frac{h}{k}\frac{\rho_w}{\rho_b}(G_m - G_{m-1}). \tag{3.27}$$

Note that the constant term in (3.23) enters only b_0. Since $a_j \sim -\bigl(\frac{3\pi}{8}(4j-1)\bigr)^{2/3}$ for $j \to \infty$ the series (3.23) defining G_m has good convergence properties for positive range r but for $r=0$ the convergence is very slow. To overcome this problem we use the identity

$$\sum_{j=1}^{\infty} \frac{1}{(a_j - \zeta_0(z_b))^2} = \left(\frac{\mathrm{Ai}'(\zeta_0(z_b))}{\mathrm{Ai}(\zeta_0(z_b))}\right)^2 - \zeta_0(z_b), \tag{3.28}$$

which can be derived analogously to the one in [20].

In a numerical implementation one has to limit the summation in (3.21) and therefore the TBC is no more fully transparent. Moreover, the stability of the resulting scheme is not clear since the discretized TBC (3.26) is not matched to the finite difference scheme (3.10) in the interior domain.

4 Discrete TBCs via Exact Solutions

We will now show how to find exact solutions for the presented difference equations in order to formulate the TBCs.

It is well–known how to solve second–order linear difference equations with *constant coefficients* (this is the case for the transformed Crank–Nicolson scheme (3.2) for solving the Black–Scholes equation for American options). In contrast, second–order linear difference equations with *variable coefficients* cannot be solved in closed form in most cases. However, if one wants to solve a difference equation with *polynomial coefficients*, one approach is to find the solution by the *"method of generating functions"*; i.e., a generating function for a solution of the difference equation can be shown to satisfy a differential equation, which may be solvable in terms of known functions.

4.1 The Black–Scholes Equation for American Options

The two linearly independent solutions of the resulting *second–order difference equation* (3.2) take the form $\hat{v}_j(z) = \nu_{1,2}^j(z)$, $j \leq 1$, where $\nu_{1,2}(z)$ are the solutions of the quadratic equation

$$\nu^2 - 2\Big[1 + \frac{1}{\rho}\frac{z-1}{z+1}\Big]\nu + 1 = 0. \tag{4.1}$$

Since we are seeking decreasing modes as $j \to -\infty$ we have to require $|\nu_1| > 1$ and obtain the Z–transformed *discrete TBC* as

$$\hat{v}_1(z) = \nu_1(z)\,\hat{v}_0(z). \tag{4.2}$$

It only remains to inverse Z–transform $\nu_1(z)$ in order to obtain the discrete TBC from (4.2). This can be performed explicitly (cf. [22]) and the discrete TBC becomes:

$$v_1^{(n)} = \ell^{(n)} * v_0^{(n)} = \sum_{k=1}^{n} \ell^{(n-k)} v_0^{(k)}, \quad n \geq 1, \tag{4.3}$$

with convolution coefficients $\ell^{(n)}$ given in [22]. Since the asymptotical behaviour $\ell^{(n)} \sim 4(-1)^n/\rho$ of the convolution coefficients may lead to subtractive cancellation in (4.3) we prefer to use the following *summed coefficients* in the implementation

$$s^{(n)} := \ell^{(n)} + \ell^{(n-1)}, \quad n \geq 1, \quad s^{(0)} := \ell^{(0)}. \tag{4.4}$$

The *discrete TBC* then reads

$$v_1^{(n)} - s^{(0)} v_0^{(n)} = \sum_{k=1}^{n-1} s^{(n-k)} v_0^{(k)} - v_1^{(n-1)}, \quad n \geq 1. \tag{4.5}$$

with the convolution coefficients

$$\begin{aligned} s^{(0)} &= 1 + \frac{1+\sqrt{1+2\rho}}{\rho}, \quad s^{(1)} = 1 - \frac{1}{\rho} - \frac{1}{\rho\sqrt{1+2\rho}}, \\ s^{(n)} &= -\frac{\sqrt{1+2\rho}}{\rho}\,\frac{\widetilde{P}_n(\mu) - \lambda^{-2}\widetilde{P}_{n-2}(\mu)}{2n-1}, \quad n \geq 2, \end{aligned} \tag{4.6}$$

where $\widetilde{P}_n(\mu) := \lambda^{-n} P_n(\mu)$ denotes the *"damped" Legendre polynomials* ($\widetilde{P}_0 \equiv \lambda^{-1}$, $\widetilde{P}_{-1} \equiv 0$). The parameters λ, μ are given by

$$\lambda = \frac{\sqrt{1+2\rho}}{\sqrt[+]{1-2\rho}}, \qquad \mu = \frac{1}{\sqrt{1+2\rho}\,\sqrt[+]{1-2\rho}}. \tag{4.7}$$

Alternatively, the convolution coefficients can be computed by the recursion formula

$$s^{(n+1)} = \frac{2n-1}{n+1}\mu\lambda^{-1}s^{(n)} - \frac{n-2}{n+1}\lambda^{-2}s^{(n-1)}, \quad n \geq 2, \tag{4.8}$$

after calculating $s^{(n)}$, $n = 0, 1, 2$ by formula (4.6).

For a derivation of the discrete TBC for a class of difference schemes for a general convection diffusion equation we refer to [22, Chapter 2].

4.2 The Schrödinger–Poisson System

Unfortunately, the exact solution to the discrete Schrödinger equation with a Coulomb–type potential (case ii)) is not known explicitly. However, in the case of a constant potential (case i)) we can easily write down an explicit solution:

The two linearly independent solutions of the second–order difference equation (3.8) are $\hat{u}_j(z) = \nu_{1,2}^j(z)$, $j \geq J$, where $\nu_{1,2}(z)$ solve

$$\nu^2 - 2\left[1 - \frac{i\rho}{2}\Big(\frac{z-1}{z+1} + i\kappa\Big)\right]\nu + 1 = 0. \tag{4.9}$$

For the decreasing mode (as $j \to \infty$) we have to require $|\nu_1(z)| < 1$ and obtain the *Z–transformed discrete TBC* as

$$\hat{u}_{J-1}(z) = \nu_1^{-1}(z)\,\hat{u}_J(z). \tag{4.10}$$

It only remains to inverse transform (4.10) and in a tedious calculation this can be achieved explicitly [23]. However, since the magnitude of $\ell^{(n)} := \mathcal{Z}^{-1}\left\{\nu_1^{-1}(z)\right\}$ does not decay as $n \to \infty$ (Im $\ell^{(n)}$ behaves like const $\cdot(-1)^n$ for large n), it is more convenient to use a modified formulation of the discrete TBC (cf. [18]). Therefore we introduce the *summed coefficients*

$$s^{(n)} = \mathcal{Z}^{-1}\left\{\hat{s}(z)\right\}, \text{ with } \hat{s}(z) := \frac{z+1}{z}\hat{\ell}(z), \tag{4.11}$$

which satisfy

$$s^{(0)} = \ell^{(0)}, \quad s^{(n)} = \ell^{(n)} + \ell^{(n-1)}, \quad n \geq 1.$$

The *discrete TBC* for the discretization (3.7) now reads (cf. [23]):

$$u_{J-1}^{(n)} - s^{(0)} u_J^{(n)} = \sum_{k=1}^{n-1} s^{(n-k)} u_J^{(k)} - u_{J-1}^{n-1}, \quad n \geq 1, \tag{4.12}$$

with

$$\begin{gathered} s^{(n)} = \big[1 - i\frac{\rho}{2} + \frac{\sigma}{2}\big]\delta_n^0 + \big[1 + i\frac{\rho}{2} + \frac{\sigma}{2}\big]\delta_n^1 + \alpha\, e^{-in\varphi}\, \frac{P_n(\mu) - P_{n-2}(\mu)}{2n-1}\,, \\ \varphi = \arctan \frac{2\rho(\sigma+2)}{\rho^2 - 4\sigma - \sigma^2}, \quad \mu = \frac{\rho^2 + 4\sigma + \sigma^2}{\sqrt{(\rho^2+\sigma^2)(\rho^2+[\sigma+4]^2)}}, \\ \sigma = -wV_R, \quad \alpha = \frac{i}{2}\sqrt[4]{(\rho^2+\sigma^2)(\rho^2+[\sigma+4]^2)}\, e^{i\varphi/2}. \end{gathered} \tag{4.13}$$

P_n denotes the Legendre polynomials ($P_{-1} \equiv P_{-2} \equiv 0$) and δ_n^j the Kronecker symbol. The P_n only have to be evaluated at one value $\mu \in \mathbb{R}$, and hence the numerically stable recursion formula for the Legendre polynomials can be used. Using asymptotic properties of the Legendre polynomials one finds the decay rate $s^{(n)} = \mathrm{O}(n^{-3/2})$.

4.3 The Standard "Parabolic Equation"

We show that in the case of the discrete Airy equation (3.12a) the exact solution can be found explicitly by the method of generating functions. We define the *generating function* to be

$$g(\xi) = \sum_{j=-\infty}^{\infty} y_j \xi^j. \tag{4.14}$$

We multiply (3.12a) with ξ^{j-1} and sum it up for $j \in \mathbb{Z}$:

$$\sum_{j=-\infty}^{\infty} y_j \xi^{j-2} - (2+d) \sum_{j=-\infty}^{\infty} y_j \xi^{j-1} + \sum_{j=-\infty}^{\infty} y_j \xi^j - c \sum_{j=-\infty}^{\infty} j y_j \xi^{j-1} = 0.$$

This results in the following ordinary differential equation for g:

$$g'(\xi) - \frac{1 - (2+d)\xi + \xi^2}{c\xi^2}\, g(\xi) = 0,$$

for which the solution is

$$g(\xi) = \xi^{-\frac{2+d}{c}}\, e^{(\xi - \frac{1}{\xi})/c} = \xi^{-\frac{2+d}{c}} \sum_{\nu=-\infty}^{\infty} J_\nu(\tfrac{2}{c}) \xi^\nu.$$

Hence, the exact decaying solution of (3.12a) is the *Bessel function* $J_\nu(\frac{2}{c})$ (regarded as function of its order ν), i.e. the discrete Airy equation is nothing else but the recurrence relation for $J_\nu(\frac{2}{c})$. It is well–known [24] that the recurrence equation for the Bessel functions

$$J_{\nu+1}(z) - 2\,\frac{\nu}{z}\,J_\nu(z) + J_{\nu-1}(z) = 0, \tag{4.15}$$

still holds for complex orders ν and complex arguments z.

Thus the decaying solution to (3.12a) can be represented as (cf. [24, Chapter 3.1]):

$$y_j = J_{j+\frac{2+d}{c}}(\tfrac{2}{c}) = \frac{1}{c^{j+\frac{2+d}{c}}} \sum_{n=0}^{\infty} \frac{(-1)^n}{c^{2n}\,n!\,\Gamma(j+\frac{2+d}{c}+n+1)}, \quad c,d \in \mathbb{C}. \tag{4.16}$$

We also observe that (4.14) is not a generating function in the strict sense but a *Laurent series*, which is uniformly convergent, i.e. differentiating each term is permissible (cf. [24]). Note that this generating function approach is not suitable for determining the growing solution of (3.12a) for $j \to \infty$. This solution is the so–called *"Neumann–Function"* (or Bessel function of the second kind) which is also known to satisfy the recursion equation of the Bessel functions.

Remark. A difference equation more general than (3.12a) was examined by Barnes [25] in 1904. He also considered (3.12a) and found (through a different construction) the solution (4.16).

Comparing (3.12a) with the recurrence relation of the Bessel function $J_\nu(\sigma)$ yields the condition

$$\frac{\nu}{\sigma} = 1 - i\zeta(z) - \mu\frac{k_0^2}{2}h^3(j-J) \overset{!}{=} \frac{j+\text{offset}}{\sigma}, \tag{4.17}$$

and we conclude that the exact solution of (3.12a) is

$$\hat{\psi}_j(z) = J_{\nu_j(z)}(\sigma), \tag{4.18}$$

with

$$\nu = \nu_j(z) = \sigma(1-i\zeta(z)) + j - J, \quad \sigma = -\big(\mu\frac{k_0^2}{2}h^3\big)^{-1} \in \mathbb{R}. \tag{4.19}$$

From (4.18) we obtain the *transformed discrete TBC* at $z_b = Jh$:

$$\hat{\psi}_{J-1}(z) = \hat{g}_{\mu,J}(z)\hat{\psi}_J(z) \tag{4.20a}$$

with

$$\hat{g}_{\mu,J}(z) = \frac{J_{\nu_{J-1}(z)}(\sigma)}{J_{\nu_J(z)}(\sigma)} = \frac{J_{\sigma(1-i\zeta(z))-1}(\sigma)}{J_{\sigma(1-i\zeta(z))}(\sigma)}. \tag{4.20b}$$

Finally, an inverse Z–transformation yields the *discrete TBC*

$$\psi_{J-1}^{(n)} - \ell_J^{(0)} \psi_J^{(n)} = \sum_{m=1}^{n-1} \psi_J^{(n-m)}\, \ell_J^{(m)}, \tag{4.21}$$

with $\ell_J^{(n)} = \mathcal{Z}^{-1}\left\{\hat{g}_{\mu,J}(z)\right\}$ given by

$$\ell_J^{(n)} = \frac{\tau^n}{2\pi} \int_0^{2\pi} \hat{g}_{\mu,J}(\tau e^{i\varphi}) e^{in\varphi}\, d\varphi, \quad n \in \mathbb{Z}_0, \quad \tau > 0. \tag{4.22}$$

Since this inverse Z–transformation cannot be done explicitly, we use a numerical inversion technique based on FFT (cf. [18]); for details of this routine we refer the reader to [22]. Note that the Bessel functions in (4.20) with complex order and (possibly large) real argument can be evaluated numerically by special software packages (see e.g. [26]).

Analogously, to §4.2 we introduce the *summed coefficients*

$$s_J^{(n)} = \mathcal{Z}^{-1}\left\{\hat{s}_J(z)\right\}, \text{ with } \hat{s}_J(z) := \frac{z+1}{z}\hat{\ell}_J(z), \tag{4.23}$$

i.e. in physical space, the discrete TBC is:

$$\psi_{J-1}^{(n)} - s_J^{(0)} \psi_J^{(n)} = \sum_{m=1}^{n-1} s_J^{(n-m)} \psi_J^{(m)} - \psi_{J-1}^{(n-1)}, \quad n \geq 1. \tag{4.24}$$

Remark. For brevity of the presentation, we omit the discussion of an adequate discrete treatment of the typical density shock at $z = z_b$ and refer the reader to [17] for a detailed discussion of various strategies.

5 Discrete ABCs through Asymptotic Solutions

If the exact solution is not known or too complicated (i.e. too expensive for an efficient numerical calculation) then one can use asymptotic solutions of the second–order difference equation (1.1) (cf. [8, Chapter 7] and the references therein).

If the coefficient $p(j)$ in (1.1) has the finite limit $p = \lim_{j\to\infty} p(j)$ one calls (1.1) a *Poincaré difference equation* and

$$\Phi(t) = t^2 - (2+p)t + 1 \tag{5.1}$$

the *characteristic polynomial* of (1.1). The idea of Poincaré [27]is now that the solutions of a Poincaré difference equation behave asymptotically for large j similar to the solutions of the corresponding constant coefficent difference equation

$$\Delta^2 y_j - p\, y_j = 0, \quad j \in \mathbb{Z}.$$

We formulate the classical *Theorem of Poincaré* (for the special case of this second–order difference equation):

Theorem 5.1 (Poincaré Theorem,[8]) *Suppose that the zeros t_1, t_2 of the characteristic polynomial* (5.1) *have distinct moduli. Then for any nontrivial solution y_j of* (1.1)

$$\lim_{j\to\infty} \frac{y_{j+1}}{y_j} = t_k$$

for $k = 1$ or $k = 2$.

This theorem was improved 1921 by Perron [28]:

Theorem 5.2 (Perron Theorem,[8]) *Assume that $p(j) \neq 0$ for all $j \in \mathbb{N}_0$. Then under the assumptions of Theorem 5.1, Equation* (1.1) *has a fundamental set of solutions $\{y_j^{(1)}, y_j^{(2)}\}$ with the property*

$$\lim_{j\to\infty} \frac{y_{j+1}^{(k)}}{y_j^{(k)}} = t_k, \quad k = 1, 2$$

Remark. If equation (1.1) has characteristic roots with equal moduli then Poincaré's Theorem may fail (cf. Example of Perron [8, Example 7.12]).

In the case of the Schrödinger–Poisson problem we have a difference equation of Poincaré–type. However, the applicability of the above two theorems is limited; they only yield the first term approximation of the asymptotic solution. Therefore we apply standard perturbation techniques of asymptotic analysis to the equation

$$\Delta^2 y_j = 0, \quad j \in \mathbb{Z}.$$

Remark. We remark that the same approach is given in [8, Chapter 7.3], but the Theorem [8, Theorem 7.17.] does not apply to our case of the Coulomb–type potential.

If the classic theorems of Poincaré and Perron cannot be applied to (3.12a) it is not straight forward to obtain information about the asymptotic behaviour of the solutions to this equation. This is the case for the discrete Airy equation. One ansatz is the one of Mickens [29] and another approach is due to Wong and Li [30]. They obtain asymptotic solutions to the second–order difference equation

$$y_{j+2} + j^p \, a(j) \, y_{j+1} + j^q \, b(j) \, y_j = 0, \tag{5.2}$$

where p, q are integers and $a(j)$, $b(j)$ have expansions of the form

$$a(j) = \sum_{s=0}^{\infty} \frac{a_s}{j^s}, \qquad b(j) = \sum_{s=0}^{\infty} \frac{a_s}{j^s}, \tag{5.3}$$

with nonzero leading coefficients: $a_0 \neq 0$, $b_0 \neq 0$.

5.1 The Schrödinger–Poisson System

We consider the difference equation (3.9a) which is the discrete Z–transformed exterior problem. Motivated by (4.10), we want to obtain the *transformed discrete TBC* in the form:

$$\hat{u}_{J-1}(z) = \hat{\ell}(z) \, \hat{u}_J(z). \tag{5.4}$$

In the sequel we will construct some expressions for $\hat{\ell}(z)$ by determining asymptotic solutions to (3.9a) through different approaches.

Approach of Mickens. Following the approach [31], the asymptotic solution of (3.9a) written as

$$\hat{u}_{j+1}(z) - 2\Big[A_0 + \frac{A_1}{j}\Big]\hat{u}_j(z) + \hat{u}_{j-1}(z) = 0, \quad j \geq J, \tag{5.5}$$

takes the form

$$\hat{u}_j(z) \sim j^\theta e^{B_0 j} \Big[1 + \sum_{k=1}^{\infty} \frac{B_k}{j^k}\Big], \tag{5.6}$$

where the parameters θ and B_k are expressible in terms of $A_0 = A_0(z)$,

A_1. The parameters θ, B_0, B_1 can be obtained by

$$\cosh(B_0) = A_0, \text{ i.e. } B_0 = \ln\bigl(A_0 \pm \sqrt{A_0^2 - 1}\bigr), \tag{5.7a}$$

$$\theta = \frac{A_1}{\sinh(B_0)}, \tag{5.7b}$$

$$B_1 = \frac{\theta(\theta - 1)}{2} \coth(B_0). \tag{5.7c}$$

In our case we obtain

$$e^{B_0} = \nu_1(z), \tag{5.8a}$$

$$\theta = \frac{2m\Delta r}{\hbar^2} \frac{\phi_\infty}{\nu_1(z) - \nu_1^{-1}(z)}, \tag{5.8b}$$

$$B_1 = \frac{\theta(\theta - 1)}{2} \frac{\nu_1(z) + \nu_1^{-1}(z)}{\nu_1(z) - \nu_1^{-1}(z)}, \tag{5.8c}$$

where $\nu_1(z)$ is the solution to (4.9) for the Schrödinger equation with zero potential (i.e. $\kappa = 0$) with $|\nu_1(z)| < 1$.

Approach of Wong & Li. Alternatively, one can use the *approach of Wong and Li* [32] to obtain a formula for the asymptotic behaviour of the solutions to this second–order difference equation of Poincaré type. To do so, we rewrite (3.9a) in the form

$$\hat{u}_{j+2} + a(j)\, \hat{u}_{j+1} + \hat{u}_j = 0, \quad j \geq J, \tag{5.9}$$

with $a(j) = -2[A_0 + A_1/(j+1)]$. Now $a(j)$ has a power expansion

$$a(j) = \sum_{k=0}^{\infty} \frac{a_k}{j^k},$$

with coefficients:

$$a_0 = -2A_0, \quad a_k = 2A_1(-1)^k, \quad k \geq 1.$$

Then the decaying asymptotic solution (cf. [32]) is of the form

$$\hat{u}_j \sim \nu_1(z)^j j^\alpha \sum_{k=0}^{\infty} \frac{c_k}{j^k}, \qquad j \to \infty, \tag{5.10}$$

where α can be calculated as

$$\alpha = \frac{a_1 \nu_1(z)}{a_0 \nu_1(z) + 2} = \frac{A_1 \nu_1(z)}{A_0 \nu_1(z) - 1} = \frac{2A_1}{\nu_1(z) - \nu_1^{-1}(z)}. \tag{5.11}$$

Without loss of generality, we assume that $c_0 = 1$ and determine the values of the coefficients $c_1,\ c_2, \dots$ by formula (2.3) in [32] or more illustrative by substituting the solution (5.10) in (5.9):

$$\nu_1^2\Big(1+\frac{2}{j}\Big)^{\alpha}\sum_{k=0}^{\infty}\frac{c_k}{(j+2)^k}+a(j)\nu_1\Big(1+\frac{1}{j}\Big)^{\alpha}\sum_{k=0}^{\infty}\frac{c_k}{(j+1)^k}+\sum_{k=0}^{\infty}\frac{c_k}{j^k}=0.$$

We now obtain after a Taylor expansion in $1/j$ and setting all the linearly independent terms equal to zero, by a lengthy calculation

$$c_1 = \frac{\alpha^2 + A_0A_1\alpha - \alpha - A_1\nu_1 + A_1^2}{2(A_0\nu_1 - 1)}, \tag{5.12a}$$

$$\begin{aligned} c_2 = {} & \frac{c_1^2}{2} + \frac{A_0\nu_1 - \alpha}{2(A_0\nu_1 - 1)}\, c_1 + \frac{1 - A_1\nu_1 - A_0A_1 - A_0^2}{3(A_0\nu_1 - 1)}\, c_1 \\ & + \frac{(A_0^3c_1 + \nu_1 - A_0)A_1}{6(A_0\nu_1 - 1)} + \frac{(A_0^2 - A_1\nu_1 + A_1A_0 - 3)A_1^2}{12(A_0\nu_1 - 1)}, \end{aligned} \tag{5.12b}$$

etc..

This result can be checked easily with a symbolic package like MAPLE. After some basic manipulations one observes that these two approaches lead to the same asymptotic solution of the equation (3.9a).

5.2 The Standard "Parabolic Equation"

It is a nontrivial task to determine asymptotic solutions of the discrete Airy equation (3.12a) since equation (3.12a) is not of Poincaré type.

Approach of Wong & Li. We increase the index of (3.12a) by one to put it in the form of (5.2) and make the following identifications:

$$\begin{aligned} &a_0 = -c, \quad a_1 = -(2+c+d), \quad a_s = 0,\ s \ge 2, \\ &b_0 = 1, \quad b_s = 0,\ s \ge 1, \quad p = 1, \quad q = 0. \end{aligned}$$

Then the two formal series solutions (cf. [30]) are given by

$$y_j^{(1)} = \frac{c^{-j}}{(j-2)!}\, j^{-2-(2+d)/c}\sum_{s=0}^{\infty}\frac{c_s^{(1)}}{j^s}, \tag{5.13a}$$

$$y_j^{(2)} = (j-2)!\, c^j\, j^{1+(2+d)/c}\sum_{s=0}^{\infty}\frac{c_s^{(2)}}{j^s}. \tag{5.13b}$$

To determine the values of the coefficients $c_1^{(1)}$, $c_2^{(1)}$, $c_3^{(1)}, \ldots$ we substitute the decaying solution $y_j^{(1)}$ in (5.2):

$$\frac{1}{cj}\Big(\frac{j+1}{j+2}\Big)^{\theta}\sum_{s=0}^{\infty}\frac{c_s^{(1)}}{(j+2)^s}+c(j-1)\Big(\frac{j+1}{j}\Big)^{\theta}\sum_{s=0}^{\infty}\frac{c_s^{(1)}}{j^s} = \big(c(\theta-1)+cj\big)\sum_{s=0}^{\infty}\frac{c_s^{(1)}}{(j+1)^s}, \quad (5.14)$$

with $\theta = 2+(2+d)/c$. We now obtain after a Taylor expansion in $1/j$ and setting all the linearly independent terms equal to zero, by a lengthy but elementary calculation, the results:

$$c_1^{(1)} = -c_0^{(1)}\big[c^{-2}-\theta+\frac{\theta}{2}(\theta-1)\big], \quad (5.15a)$$

$$\begin{aligned} c_2^{(1)} &= \frac{c_0^{(1)}}{2}\big[\theta c^{-2}+\frac{\theta}{2}(\theta-1)-\frac{\theta}{6}(\theta-1)(\theta-2)\big] \\ &\quad -\frac{c_1^{(1)}}{2}\big[c^{-2}-2+\frac{\theta}{2}(\theta-1)\big], \end{aligned} \quad (5.15b)$$

$$\begin{aligned} c_3^{(1)} &= -\frac{c_0^{(1)}}{3}\Big[\big(2\theta+\frac{\theta}{2}(\theta-1)\big)c^{-2}-\frac{\theta}{6}(\theta-1)(\theta-2) \\ &\qquad -\frac{\theta}{24}(\theta-1)(\theta-2)(\theta-3)\Big] \\ &\quad +\frac{c_1^{(1)}}{3}\big[(2+\theta)c^{-2}-2+\theta+\frac{\theta}{2}(\theta-1)-\frac{\theta}{6}(\theta-1)(\theta-2)\big] \\ &\quad -\frac{c_2^{(1)}}{3}\big[c^{-2}-5+\theta+\frac{\theta}{2}(\theta-1)\big], \end{aligned} \quad (5.15c)$$

etc..

Similarly we obtain for the increasing solution $y_j^{(2)}$ the first three coefficients

$$c_1^{(2)} = c_0^{(2)}\big[c^{-2}-\eta+\frac{\eta}{2}(\eta-1)\big], \quad (5.16a)$$

$$\begin{aligned} c_2^{(2)} &= -\frac{c_0^{(2)}}{2}\big[(\eta-1)c^{-2}-\eta+\eta(\eta-1)-\frac{\eta}{6}(\eta-1)(\eta-2)\big] \quad (5.16b) \\ &\quad +\frac{c_1^{(2)}}{2}\big[c^{-2}+3-2\eta-\frac{\eta}{2}(\eta-1)\big], \end{aligned}$$

$$
\begin{aligned}
c_3^{(2)} = \frac{c_0^{(2)}}{3}\Big[&\big(1+\frac{\eta}{2}(\eta-1)\big)c^{-2}-\eta+\frac{3}{2}\eta(\eta-1)\\
&-\frac{\eta}{2}(\eta-1)(\eta-2)+\frac{\eta}{24}(\eta-1)(\eta-2)(\eta-3)\Big]\\
-&\frac{c_1^{(2)}}{3}\big[(\eta-1)c^{-2}-7-6\eta+2\eta(\eta-1)-\frac{\eta}{6}(\eta-1)(\eta-2)\big]\\
+&\frac{c_2^{(2)}}{3}\big[c^{-2}+9-3\eta+\frac{\eta}{2}(\eta-1)\big],
\end{aligned}
\tag{5.16c}
$$

with $\eta = 1 + (2+d)/c$. Here $c_0^{(1)}$, $c_0^{(2)}$ denote arbitrary constants.

We recall that the Z–transformed scheme in the exterior $j \geq J-1$, given by (3.12b), is a discrete Airy equation of the form (3.12a) with

$$
c = 2\sigma^{-1}, \quad d = -2i\zeta(z) - cJ, \text{ i.e. } \theta = 2 + \frac{2+d}{c} = 2 + \nu_0.
$$

Using the asymptotic solution $y_j^{(1)}$ from (5.13a) we thus obtain the *transformed discrete ABC*

$$
\hat{\psi}_{J-1}(z) = \hat{k}_{\mu,J}(z)\hat{\psi}_J(z), \tag{5.17a}
$$

with

$$
\hat{k}_{\mu,J}(z) = \frac{y_{J-1}^{(1)}}{y_J^{(1)}} = c(J-2)\Big(\frac{J}{J-1}\Big)^{\theta} \frac{\sum_{s=1}^{\infty} \frac{c_s^{(1)}}{(J-1)^s}}{\sum_{s=1}^{\infty} \frac{c_s^{(1)}}{J^s}}. \tag{5.17b}
$$

Asymptotic Expansion of Explicit Solution. Another approach is to use an asymptotic expansion for the exact solution. We will explain this using the discrete Airy equation (3.12). We use the following asymptotic representation of Bessel functions for large values of the order ν (cf. [24]):

$$
J_\nu(z) \approx \frac{e^{\nu+\nu\log(z/2)-(\nu+1/2)\log\nu}}{\sqrt{2\pi}}, \quad |\nu| \to \infty,\ |\arg\nu| \leq \pi - \delta. \tag{5.18}
$$

Using the formula (5.18) leads to the *transformed discrete ABC*

$$
\hat{\psi}_{J-1}(z) = \hat{h}_{\mu,J}(z)\hat{\psi}_J(z), \tag{5.19a}
$$

with

$$
\hat{h}_{\mu,J}(z) = \frac{2}{e}\sigma^{-1}\sqrt{\nu_J(\nu_J-1)}\Big(\frac{\nu_J}{\nu_J-1}\Big)^{\nu_J}, \tag{5.19b}
$$

and ν_J, σ given by (4.19).

6 The Continued Fraction Approach

Finally, for a third approach to construct a discrete ABC, we use a formulation as a *continued fraction*. This approach is suitable for general second–order difference equations, since the exact solvability of the difference equation is not necessary. One can deduce such an expression for the quotient of two spatially neighboured Z–transformed solutions as a continued fraction directly from the difference scheme (i.e. without knowing the solution). This approach is often better than evaluating the quotient of two asymptotic solutions (obtained by any of the previous approaches) at two neighboured grid points. For the numerical implementation one can use the *modified Lentz's method* [33] which is an efficient general method for evaluating continued fractions. The calculations in [13] and [16] showed that the numerical evaluation of the continued fraction formula is stable for all considered parameter values.

6.1 The Schrödinger–Poisson System

If we rewrite the transformed discrete exterior problem (3.9a) as

$$\frac{\hat{u}_{J-1}(z)}{\hat{u}_J(z)} = 2\Big[A_0 + \frac{A_1}{j}\Big] - \frac{1}{\frac{\hat{u}_J(z)}{\hat{u}_{J+1}(z)}},$$

it is obvious that we have the following continued fraction

$$\frac{\hat{u}_{J-1}(z)}{\hat{u}_J(z)} = 2\Big[A_0+\frac{A_1}{J}\Big] - \frac{1}{2[A_0+\frac{A_1}{J+1}]-}\cdots\frac{1}{2[A_0+\frac{A_1}{J+M}]-}\;\frac{\hat{u}_{J+M+1}(z)}{\hat{u}_{J+M}(z)}.$$

For decreasing solutions the last quotient may be neglected if $M \to \infty$, i.e. we obtain the expansion

$$\hat{\ell}(z) = 2\Big[A_0 + \frac{A_1}{J}\Big] - \frac{1}{2[A_0+\frac{A_1}{J+1}]-}\;\frac{1}{2[A_0+\frac{A_1}{J+2}]-\cdots}. \tag{6.1}$$

This continued fractions formula (6.1) offers another way to evaluate the quotient $\hat{\ell}(z)$ needed in the transformed discrete TBC (4.10).

Finally we want to end with a short note about the implementation of the discrete TBC using the asymptotic expansions or the continued fraction approach. As in the case for the constant potential in the exterior domain (cf. (4.11)) it is favourable to use

$$\hat{s}(z) := \frac{z+1}{z}\,\hat{\ell}(z). \tag{6.2}$$

An inverse Z–transformation yields finally the *discrete TBC*

$$u_{J-1}^{(n)} - s^{(0)} u_J^{(n)} = \sum_{k=1}^{n-1} s^{(n-k)} u_J^{(k)} - u_{J-1}^{(n-1)}, \quad n \geq 1. \tag{6.3}$$

with

$$s^{(n)} = \mathcal{Z}^{-1}\left\{\hat{s}(z)\right\} = \frac{\tau^n}{2\pi} \int_0^{2\pi} \hat{s}(\tau e^{i\varphi}) e^{in\varphi}\, d\varphi, \quad n \in \mathbb{Z}_0, \quad \tau > 0. \tag{6.4}$$

This inverse Z–transformation (6.4) must be performed numerically (cf. §4.3).

Remark. We remark that this discrete TBC (6.3) can also used for both the predictor (3.4a) and the corrector step (3.5a) for the Schrödinger equation. In the exterior domain they are

$$i\hbar D_{t,k}^{+} u_j^{(n)} = -\frac{\hbar^2}{2m} D_r^2 S_{t,k} u_j^{(n)} + \frac{\phi_\infty}{r_j} S_{t,k} u_j^{(n)}, \quad j \geq J, \tag{6.5}$$

$k = 1, 2$, i.e. after a (slightly modified) Z–transformation they are of the form (3.9a) and a discrete TBC analogue to (6.3) can be applied.

6.2 The Standard "Parabolic Equation"

Following [24, Section 5.6] we can easily deduce an expression for the quotient of Bessel functions as a continued fraction from the recurrence formula (4.15). If we rewrite (4.15) as

$$\frac{J_{\nu-1}(z)}{J_\nu(z)} = 2\nu z^{-1} - \frac{1}{\frac{J_\nu(z)}{J_{\nu+1}(z)}},$$

it is obvious that

$$\frac{J_{\nu-1}(z)}{J_\nu(z)} = 2\nu z^{-1} - \frac{1}{2(\nu+1)z^{-1}} {}_{-}\dots{}_{-} \frac{1}{2(\nu+M)z^{-1}} {}_{-} \frac{J_{\nu+M-1}(z)}{J_{\nu+M}(z)}.$$

This holds for general values of ν and it can be shown, with the help of the theory of Lommel polynomials [24, Section 9.65], that for $M \to \infty$, the last quotient may be neglected, so that

$$\frac{J_{\nu-1}(z)}{J_\nu(z)} = 2\nu z^{-1} - \frac{1}{2(\nu+1)z^{-1}} {}_{-} \frac{1}{2(\nu+2)z^{-1}} {}_{-} \dots. \tag{6.6}$$

This continued fractions formula offers another way to evaluate the quotient of two Bessel functions needed in the transformed discrete TBC.

In the sequel we will focus exclusively on this example of the Standard "parabolic equation". However, the approximation technique described in the following Section 7 applies generally to boundary conditions of convolution type.

7 The Approximation by the Sum of Exponentials

An ad-hoc implementation of the discrete convolution (4.24) with convolution coefficients $s_J^{(n)}$ from (4.23) (or obtained by any of the above approaches) has still one disadvantage. The boundary condition is non–local and therefore computationally expensive. In fact, the evaluation of (4.24) is as expensive as for an discretization of the TBC (3.20). As a remedy, we proposed in [34] the sum–of–exponentials ansatz (for a comparison of the computational efforts see Fig. 7). In the sequel we will briefly review this approach which can also be used for more general "parabolic equations" [35].

In order to derive a fast numerical method to calculate the discrete convolutions in (4.24), we approximate the coefficients $s_J^{(n)}$ by the following (*sum of exponentials*):

$$s_J^{(n)} \approx \tilde{s}_J^{(n)} := \begin{cases} s_J^{(n)}, & n = 0, 1 \\ \displaystyle\sum_{l=1}^{L} b_l \, q_l^{-n}, & n = 2, 3, \dots, \end{cases} \tag{7.1}$$

where $L \in \mathbb{N}$ is a fixed number. Evidently, the approximation properties of $\tilde{s}_J^{(n)}$ depend on L, and the corresponding set $\{b_l, q_l\}$. Below we propose a deterministic method of finding $\{b_l, q_l\}$ for fixed L.

Remark. The "split" definition of $\{\tilde{s}_J^{(n)}\}$ in (7.1) is motivated by the fact that the implementation of the discrete TBCs (4.24) involves a convolution sum with k ranging only from 1 to $m = n-1$. Since the first coefficient $s_J^{(0)}$ does not appear in this convolution, it makes no sense to include it in our sum–of–exponential approximation, which aims at simplifying the evaluation of the convolution. The "special form" of $s_J^{(0)}$ and $s_J^{(1)}$ (in the case of a constant potential, cf. (4.13)) suggests to even exclude $s_J^{(1)}$ from this approximation.

Let us fix L and consider the formal power series:

$$g(x) := s_J^{(2)} + s_J^{(3)} x + s_J^{(4)} x^2 + \dots, \quad |x| \le 1. \tag{7.2}$$

If there exists the $[L-1|L]$ *Padé approximation*

$$\tilde{g}(x) := \frac{P_{L-1}(x)}{Q_L(x)} \tag{7.3}$$

of (7.2), then its Taylor series

$$\tilde{g}(x) = \tilde{s}_J^{(2)} + \tilde{s}_J^{(3)} x + \tilde{s}_J^{(4)} x^2 + \dots \tag{7.4}$$

satisfies the conditions

$$\tilde{s}_J^{(n)} = s_J^{(n)}, \qquad n = 2, 3, \dots, 2L+1, \tag{7.5}$$

due to the definition of the Padé approximation rule.

Theorem 7.1 ([34]) *Let $Q_L(x)$ have L simple roots q_l with $|q_l| > 1, \quad l = 1, \dots, L$. Then*

$$\tilde{s}_J^{(n)} = \sum_{l=1}^{L} b_l \, q_l^{-n}, \qquad n = 2, 3, \dots, \tag{7.6}$$

where

$$b_l := -\frac{P_{L-1}(q_l)}{Q'_L(q_l)} \, q_l \neq 0, \qquad l = 1, \dots, L. \tag{7.7}$$

It follows from (7.5) and (7.6) that the set $\{b_l, q_l\}$ defined in Theorem 7.1 can be used in (7.1) at least for $n = 2, 3, .., 2L+1$. The main question now is: Is it possible to use these $\{b_l, q_l\}$ also for $n > 2L+1$? In other words, what quality of approximation

$$\tilde{s}_J^{(n)} \approx s_J^{(n)}, \qquad n > 2L+1 \tag{7.8}$$

can we expect?

The above analysis permits us to give the following description of the approximation to the convolution coefficients $s_J^{(n)}$ by the representation (7.1) if we use a $[L-1|L]$ Padé approximant to (7.2): the first $2L$ coefficients are reproduced exactly, see (7.5); however, the asymptotic behaviour of $s_J^{(n)}$ and $\tilde{s}_J^{(n)}$ (as $n \to \infty$) differs strongly (algebraic versus exponential decay). A typical graph of $|s_J^{(n)} - \tilde{s}_J^{(n)}|$ versus n for $L = 27$ is shown in Fig. 3 in Section 8.

Fast Evaluation of the Discrete Convolution. Let us consider the approximation (7.1) of the discrete convolution kernel appearing in the DTBC (4.24). With these "exponential" coefficients the convolution

$$C^{(n)} := \sum_{m=1}^{n-1} \tilde{s}_J^{(n-m)} \psi_J^{(m)}, \quad \tilde{s}_J^{(n)} = \sum_{l=1}^{L} b_l \, q_l^{-n}, \tag{7.9}$$

$|q_l| > 1$, of a discrete function $\psi_J^{(m)}$, $m = 1, 2, \ldots$, with the kernel coefficients $\tilde{s}_J^{(n)}$, can be calculated by recurrence formulas, and this will reduce the numerical effort significantly (cf. Fig. 7 in Section 8).

A straightforward calculation (cf. [34]) yields:

Theorem 7.2 ([34]) *The value $C^{(n)}$ from* (7.9) *for $n \geq 2$ is represented by*

$$C^{(n)} = \sum_{l=1}^{L} C_l^{(n)}, \tag{7.10}$$

where

$$C_l^{(1)} \equiv 0,$$
$$C_l^{(n)} = q_l^{-1} C_l^{(n-1)} + b_l \, q_l^{-1} \psi_J^{(n-1)}, \tag{7.11}$$

$n = 2, 3, \ldots \; l = 1, \ldots, L.$

Finally we summarize the approach by the following *algorithm*:

1. calculate $s_J^{(n)}$, $n = 0, \ldots, N-1$, via an explicit formula or a numerical inverse Z–transformation;
2. calculate $\tilde{s}_J^{(n)}$ via Padé–algorithm;
3. the corresponding coefficients b_l, q_l are used for the efficient calculation of the discrete convolutions.

Remark. We note that the Padé approximation must be performed with high precision ($2L - 1$ digits mantissa length) to avoid a 'nearly breakdown' by ill conditioned steps in the Lanczos algorithm. If such problems still occur or if one root of the denominator is smaller than 1 in absolute value, the orders of the numerator and denominator polynomials are successively reduced.

8 Numerical Example

In the example of this section we will consider the SPE for comparing the numerical result from using our new (approximated) discrete TBC to the solution using the discretized TBC of Levy [20]. We used the environmental test data from [21] and the Gaussian beam from [17] as starting field ψ^I. Below we present the so–called *transmission loss* $-10\log_{10}|p|^2$, where the acoustic pressure p is calculated from (2.8). We computed a *reference solution* on a three times larger computational domain confined with the discrete TBC from [17].

Example. As an illustrating example we chose the typical *downward refracting case* (i.e. energy loss to the bottom): $\mu = 2\cdot 10^{-4}\,\mathrm{m}^{-1}$. The source at $z_s = 91.44\,\mathrm{m}$ is emitting sound with a frequency $f = 300\,\mathrm{Hz}$ and the receiver is located at the depth $z_r = 27.5\,\mathrm{m}$. The TBC is applied at $z_b = 152.5\,\mathrm{m}$ and the discretization parameters are given by $\Delta r = 10\,\mathrm{m}$, $\Delta z = 0.5\,\mathrm{m}$. It contains no attenuation: $\alpha = 0$. We consider a range-independent situation for $0 < r < 50\,\mathrm{km}$, i.e. 5000 range steps. The sound speed varies linearly from $c(0\,\mathrm{m}) = 1536.5\,\mathrm{m\,s}^{-1}$ to $c(152.5\,\mathrm{m}) = 1539.24\,\mathrm{m\,s}^{-1}$. The reference sound speed c_0 is chosen to be equal to $c(z_b)$ such that $\beta = 0$ in (2.10).

For this choice of parameters the mesh ratio becomes $R \approx 0.12246$ and the parameter $\sigma \approx -53345.32$; that is, the value of ν_J defined in (4.19) is much too large for the routines like COULCC [26] for evaluating Bessel functions. On the other hand, using the asymptotic formula (5.19) is not advisable since for large ν_J we have $\hat{h}_{\mu,J}(z) \sim 2(1 - i\zeta(z))$ which is only the first term in the continued fraction expansion (6.6). Therefore, we decided to evaluate the ratio of the two Bessel functions in (4.20) by the continued fraction formula (6.6) together with the sum–of–exponentials ansatz (7.1). We note that all approaches fulfilled for moderate choices of ν_J the growth condition (8.2) needed for stability.

We computed the first 1000 terms in the expansion (6.6) and used a radius $\tau = 1.04$ with 2^{10} sampling points for the numerical inverse Z–transformation (4.22). The choice of an appropriate radius τ is a delicate problem: it may not be too close to the convergence radius of (6.6) due to the approximation error and τ too large raises problems with rounding errors during the rescaling process. For a discussion of that topic we refer the reader to [34, Section 2] and [36]. In order to calculate the convolution coefficients b_n (discretized TBC of Levy) we used the MATLAB routine from [37] to compute the first 100 zeros of the Airy function. Alternatively, using precomputed values from the call `evalf(AiryAiZeros(1..100));` in MAPLE with high precision yielded indistinguishable results.

First we examine the convolution coefficients of the two presented approaches. Fig. 2 shows a comparison of the coefficients b_n from the discretized TBC (3.26) with the coefficients $s_J^{(n)}$ from the approximated discrete TBC. The coefficients b_n decay even faster than the

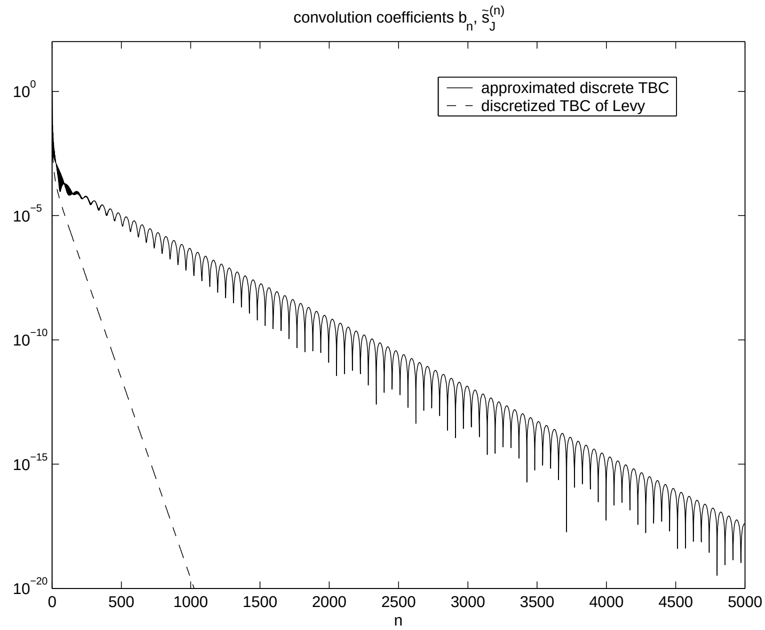

Figure 2: Comparison of the convolution coefficients b_n of the discretized TBC (3.26) and $\tilde{s}_J^{(n)}$ from the approximated discrete TBC (with $L = 27$).

coefficients $s_J^{(n)}$. In Fig. 3 we plot both the exact convolution coefficients $s_J^{(n)}$ and the error $|s_J^{(n)} - \tilde{s}_J^{(n)}|$ versus n for $L = 27$ (observe the different scales).

Now we investigate the *stability* of our numerical scheme for the

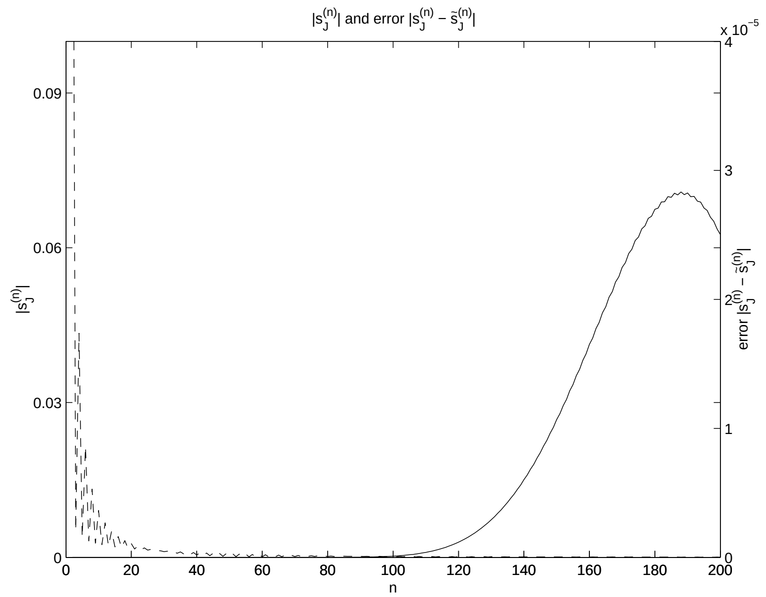

Figure 3: Convolution coefficients $s_J^{(n)}$ (left axis, dashed line) and error $|s_J^{(n)} - \tilde{s}_J^{(n)}|$ of the convolution coefficients (right axis); ($L = 27$).

SPE (3.10) along with a surface condition and the discrete TBC (4.21):

$$\left\{ \begin{array}{rcl} -iR(\psi_j^{(n+1)} - \psi_j^{(n)}) & = & \rho_j \Delta_z^0 (\rho_j^{-1} \Delta_z^0)(\psi_j^{(n+1)} + \psi_j^{(n)}) \\ & & +w\big[(N^2)_j^{(n)} - 1\big](\psi_j^{(n+1)} + \psi_j^{(n)}), \\ & & \qquad j = 1, \ldots, J-1, \\ \psi_j^{(0)} & = & \psi^I(z_j), \; j = 0, 1, 2, \ldots, J-1, J; \\ \text{with } \psi_{J-1}^{(0)} & = & \psi_J^{(0)} = 0, \\ \psi_0^{(n)} & = & 0, \\ \hat{\psi}_{J-1}(z) & = & \hat{g}_{\mu,J}(z) \hat{\psi}_J(z), \end{array} \right. \tag{8.1}$$

where $\hat{g}_{\mu,J}(z)$ is given by (4.20). The following theorem bounds the exponential growth of solutions to the numerical scheme for a fixed discretization:

Theorem 8.1 ([16]) *Let the boundary kernel $\hat{g}_{\mu,J}$ satisfy*

$$\operatorname{Im} \hat{g}_{\mu,J}(\gamma e^{i\varphi}) \leq 0, \quad \forall\, 0 \leq \varphi \leq 2\pi, \tag{8.2}$$

for some (sufficiently large) $\gamma \geq 1$ (i.e. the system is dissipative). Assume also that $\hat{g}_{\mu,J}(z)$ is analytic for $|z| \geq \gamma$. Then, the solution of

(8.1) *satisfies the a-priori estimate*

$$\|\psi^{(n)}\|_2 \le \|\psi^0\|_2\, \gamma^n, \quad n \in \mathbb{N}, \tag{8.3}$$

where

$$\|\psi^{(n)}\|_2^2 := h \sum_{j=1}^{J-1} |\psi_j^{(n)}|^2 \rho_j^{-1}, \tag{8.4}$$

denotes the discrete weighted ℓ^2–norm.

Remark. Above we have assumed that the Z–transformed boundary kernel $\hat{g}_{\mu,J}(z)$ is analytic for $|z| \ge \beta$. Hence its imaginary parts is a harmonic functions there. Since the average of $\hat{g}_{\mu,J}(z)$ on the circles $z = \beta e^{i\varphi}$ equals $g_{\mu,J}^{(0)} = \hat{g}_{\mu,J}(z=\infty)$, condition (8.2) implies Im $\hat{g}_{\mu,J}(z=\infty) \le 0$. Then we have the following simple consequence of the maximum principle for the Laplace equation:

If condition (8.2) holds for some γ_0, it also holds for all $\gamma > \gamma_0$.

We want to check the *growth condition* (8.2) for this example. For $\gamma = 1$ we have $\max\{\mathrm{Im}\,(\hat{g}_{\mu,J}(\gamma\, e^{i\varphi})\} = 0.153$ and, with $\gamma = 1.01$, we obtain $\max\{\mathrm{Im}\,(\hat{g}_{\mu,J}(\gamma\, e^{i\varphi})\} = -0.002$ (see Fig. 4). Hence, the Z–transformed kernel $\hat{g}_{\mu,J}(\gamma\, e^{i\varphi})$ of the approximated discrete TBC satisfies the condition (8.2) for $\gamma \ge 1.01$ (for this discretization).

In Fig. 5 and Fig. 6 we compare the transmission loss results for the discretized TBC and the approximated discrete TBC in the range from 0 to 50 km. The transmission loss curve of the solution using the approximated discrete TBC is indistinguishable from the one of the reference solution while the solution with the discretized TBC still deviates significantly from it (and is more oscillatory) for the chosen discretization. The result in Fig. 6 does not change if we compute more zeros of the Airy function.

Evaluating the convolution appearing in the discretized TBC (3.26) is quite expensive for long-range calculations. Therefore we extended the range interval up to 250 km and shall now illustrate the difference in the computational effort for both approaches in Fig. 7: The computational effort for the discretized TBC is quadratic in range, since the evaluation of the boundary convolutions dominates for large ranges. On the other hand, the effort for the approximated discrete TBC only increases linearly. The line (- - -) does not change considerably for different values of L since the evaluation of the sum–of–exponential convolutions has a negligible effort compared to solving the PDE in the interior domain.

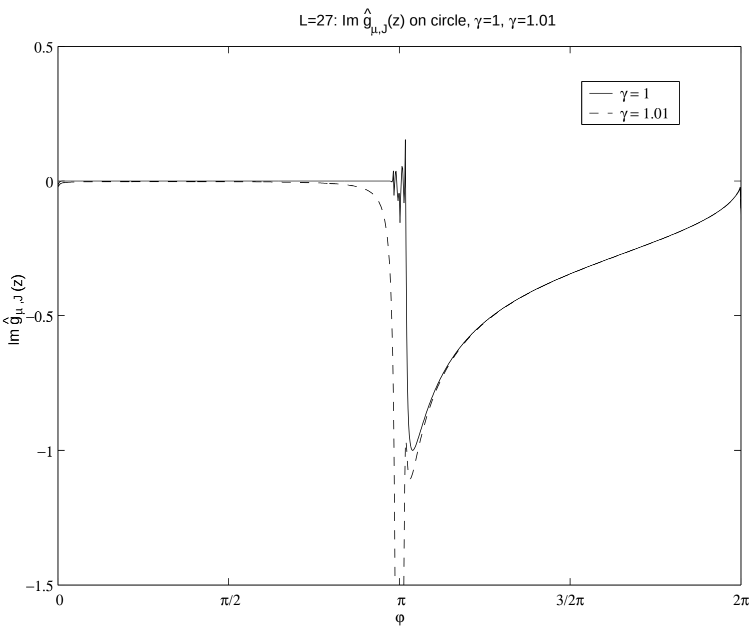

Figure 4: Growth condition $\hat{g}_{\mu,J}(z)$, $z = \gamma\, e^{i\varphi}$ $(L = 27)$.

Conclusion

We have proposed a variety of general strategies to derive discrete ABCs/TBCs for the Black-Scholes equation for American options and the Schrödinger equation with a linear or Coulomb–type potential term in the exterior domain. The derivation was based on the knowledge of the exact solution, the construction of asymptotic solutions or the usage of a continued fraction expansion. Our approach has two advantages over the standard approach of discretizing the continuous TBC: higher accuracy and efficiency; while discretized TBCs have usually quadratic effort, the sum–of–exponential approximation to discrete ABCs/TBCs has only linear effort. Moreover, we have provided in the case of the standard "parabolic equation" a simple criteria to check the stability of our method and gave an illustrating numerical example from underwater acoustics showing the superiority of our new approach.

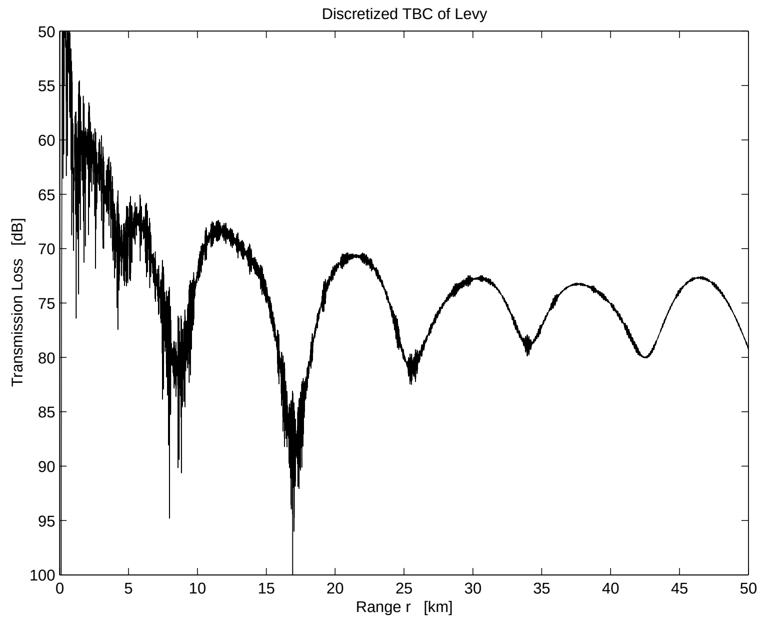

Figure 5: Transmission loss at $z_r = 27.5\,\mathrm{m}$.

9 Future Directions

It can easily be seen that the solutions to this discretization (3.12) do not have the same asymptotic properties as the solutions of the continuous Airy equation (3.15) which motivated the construction of a *nonstandard discretization scheme* (cf. [29], [38]). The logical consequence would be to study discrete TBC to the nonstandard discretization. This will be a topic of future work.

Acknowledgments

The author acknowledges support by the DFG Research Center "Mathematics for key technologies" MATHEON in Berlin.

A The Z–Transformation

The main tool of this work is the Z–transformation which is the discrete analogue of the Laplace–transformation. The Z–transformation

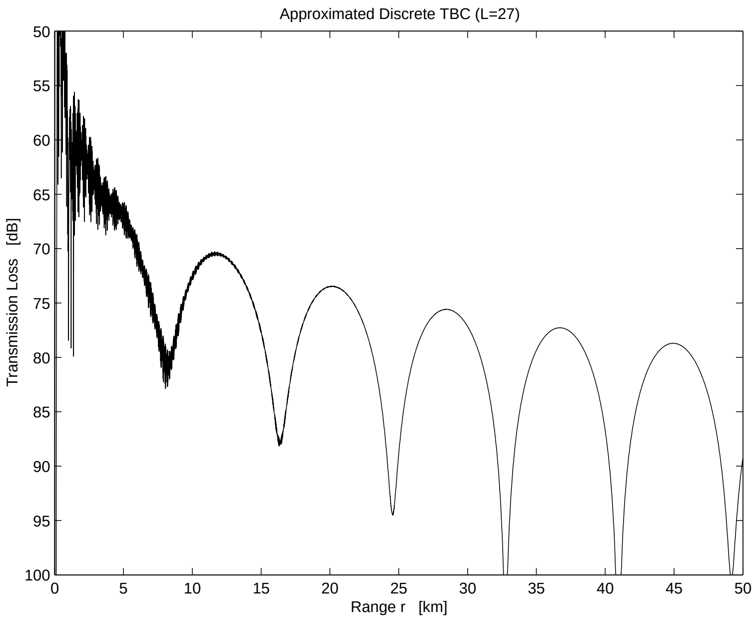

Figure 6: Transmission loss at $z_r = 27.5\,\mathrm{m}$.

can be applied to the solution of linear difference equations in order to reduce the solutions of such equations into those of algebraic equations in the complex z–plane. In this work we used it to solve the finite difference schemes in the exterior domain in order to construct the discrete ABCs/TBCs. The Z–transformation is described in more detail in [39]. It is defined in the following way:

Definition 1 (Z–transformation [39]) *The formal connection between a sequence and a complex function given by the correspondence*

$$\mathcal{Z}\{f_n\} = \hat{f}(z) := \sum_{n=0}^{\infty} f_n \, z^{-n}, \quad z \in \mathbb{Z}, \quad |z| > R_{\hat{f}}, \tag{1.1}$$

is called Z–transformation. The function $\hat{f}(z)$ is called Z–transformation of the sequence $\{f_n\}$, $n = 0, 1, \ldots$ and $R_{\hat{f}} \geq 0$ denotes the radius of convergence.

The discrete analogue of the Differentiation Theorem for the Laplace transformation is the *shifting theorem*:

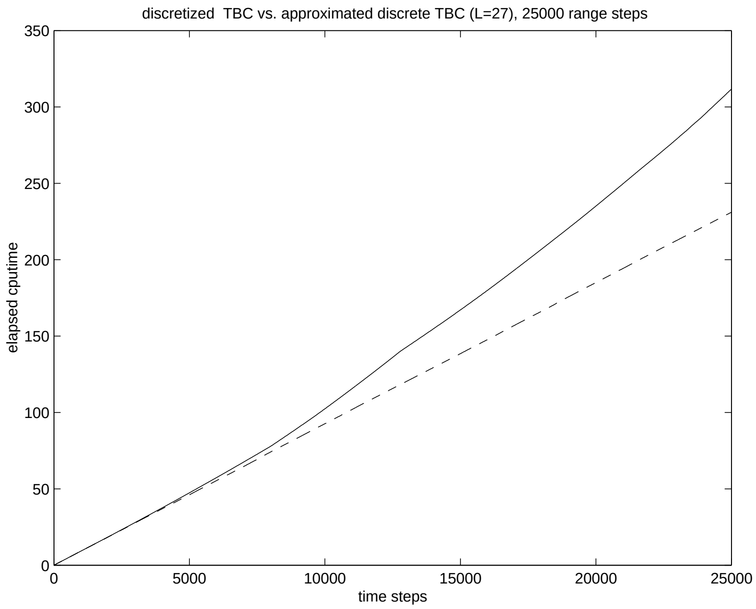

Figure 7: Comparison of CPU times: the discretized TBC of Levy (3.26) has quadratic effort (—), while the sum–of–exponential approximation to the discrete TBC has only linear effort (- - -).

Theorem A.1 (Shifting Theorem[39]) *If the sequence* $\{f_n\}$ *is exponentially bounded, i.e. there exist* $C > 0$ *and* c_0 *such that*

$$|f_n| \le C\, e^{c_0 n}, \qquad n = 0, 1, \ldots,$$

then the Z*–transformation* $\hat{f}(z)$ *is given by the Laurent series* (1.1) *and for the shifted sequence* $\{g_n\}$ *with* $g_n = f_{n+1}$ *holds*

$$\mathcal{Z}\{f_{n+1}\} = z\hat{f}(z) - zf_0. \tag{1.2}$$

The initial values enter into the transformation of the shifted sequence. As a useful consequence of the shifting theorem we have:

$$\mathcal{Z}\{f_{n+1} \pm f_n\} = (z \pm 1)\hat{f}(z) - zf_0. \tag{1.3}$$

The convolution $f_n * g_n$ of two sequences $\{f_n\}$, $\{g_n\}$, $n = 0, 1, \ldots$ is defined by $\sum_{k=0}^{n} f_k\, g_{n-k}$. For the Z–transformation of a convolution of two sequences we formulate the following theorem:

Theorem A.2 (Convolution Theorem [39]) *If $\hat{f}(z) = \mathcal{Z}\{f_n\}$ exists for $|z| > R_{\hat{f}} \geq 0$ and $\hat{g}(z) = \mathcal{Z}\{g_n\}$ for $|z| > R_{\hat{g}} \geq 0$, then there also exists $\mathcal{Z}\{f_n * g_n\}$ for $|z| > \max(R_{\hat{f}}, R_{\hat{g}})$ with*

$$\mathcal{Z}\{f_n * g_n\} = \hat{f}(z)\,\hat{g}(z). \tag{1.4}$$

Note that (1.4) is nothing else but an expresssion for the Cauchy product of two power series.

Now we present two basic rules for calculating the *inverse Z–transformation* which are essential for formulating the discrete TBCs.

Theorem A.3 (Inverse Z–transformation [39]) *If $\{f_n\}$ is an exponentially bounded sequence and $\hat{f}(z)$ the corresponding Z–transformation then the inverse Z–transformation is given by*

$$f_n = \mathcal{Z}^{-1}\left\{\hat{f}(z)\right\} = \frac{1}{2\pi i}\oint_{\mathcal{C}} \hat{f}(z)\,z^{n-1}dz, \qquad n = 0, 1, \ldots, \tag{1.5}$$

where $\mathcal{C}$ is a circle around the origin with sufficiently large radius.

Other inversion formulas can be obtained by using the fact that $\hat{f}(z^{-1})$ is a Taylor series or if $\hat{f}(z)$ is a rational function of z, analytic at ∞. The most important formula is the *inverse Z–transformation of a product*:

$$\mathcal{Z}^{-1}\left\{\hat{f}(z)\,\hat{g}(z)\right\} = f_n * g_n = \sum_{k=0}^{n} f_k\,g_{n-k}. \tag{1.6}$$

Theorem A.4 (Initial Value Theorem [39]) *If $\hat{f}(z) = \mathcal{Z}\{f_n\}$ exists then*

$$f_0 = \lim_{z\to\infty} \hat{f}(z). \tag{1.7}$$

z can tend to ∞ on the real axis or on an arbitrary path, since $\hat{f}(z)$ is analytic at $z = \infty$.

This theorem, when repeatedly applied to $\hat{f}(z)$, $\hat{f}(z) - f_0$, $\hat{f}(z) - f_0 - f_1 z^{-1}$, etc., yields a method for the inversion of the Z–transformation:

$$f_n = \lim_{z\to\infty} z^n \Big[\hat{f}(z) - \sum_{k=0}^{n-1} f_k z^{-k}\Big], \quad n = 0, 1, 2, \ldots. \tag{1.8}$$

References

[1] B. Engquist and A. Majda, "Radiation Boundary Conditions for Acoustic and Elastic Wave Calculations," *Comm. Pure Appl. Math.* **32** (1979), 313–357.

[2] F. Schmidt and P. Deuflhard, "Discrete transparent boundary conditions for the numerical solution of Fresnel's equation," *Comput. Math. Appl.* **29** (1995), 53–76.

[3] C.W. Rowley and T. Colonius, "Discretely Nonreflecting Boundary Conditions for Linear Hyperbolic Systems," *J. Comp. Phys.* **157** (2000), 500–538.

[4] L. Wagatha, "On Boundary Conditions for the Numerical Simulation of Wave Propagation," *Appl. Num. Math.* **1** (1985), 309–314.

[5] J.C. Wilson, "Derivation of boundary conditions for the artificial boundaries associated with the solution of certain time dependent problems by Lax–Wendroff type difference schemes," *Proc. Edinb. Math. Soc.* **II. Ser. 25** (1982), 1–18.

[6] L. Halpern, "Absorbing Boundary Conditions for the Discretization Schemes for the One–Dimensional Wave Equation," *Math. Comp.* **38** (1982), 415–429.

[7] G. Lill, *Diskrete Randbedingungen an künstlichen Rändern* (Ph.D. Thesis, Technische Hochschule Darmstadt, 1992).

[8] S.N. Elaydi, *An introduction to difference equations* (Springer, New York, 1996).

[9] F. Black and M. Scholes, "The pricing of options and corporate liabilities," *J. Polit. Econ.* **81** (1973), 637–659.

[10] R.C. Merton, "Theory of rational option pricing," *Bell J. Econ. Manag. Sci.*, **4** (1973), 141–183.

[11] P. Wilmott, S. Howison, and J. Dewynne, *The Mathematics of Financial Derivatives, A Student Introduction* (Cambridge University Press, 2002).

[12] M. Ehrhardt and R.E. Mickens, "Discrete Artificial Boundary Conditions for the Black–Scholes Equation of American Options," (in preparation).

[13] M. Ehrhardt and A. Zisowsky, "Fast Calculation of Energy and Mass preserving solutions of Schrödinger–Poisson systems on

unbounded domains," *Preprint No. 162 of the DFG Research Center* MATHEON *Berlin, 2004*, (submitted to J. Comp. Appl. Math.).

[14] P. Markowich, C. Ringhofer and C. Schmeiser, *Semiconductor equations* (Springer, New York, 1990).

[15] F.D. Tappert, "The parabolic approximation method," in: *Wave Propagation and Underwater Acoustics*, Lecture Notes in Physics 70, eds. J.B. Keller and J.S. Papadakis, (Springer, New York, 1977), 224–287.

[16] M. Ehrhardt and R.E. Mickens, "Solutions to the Discrete Airy Equation: Application to Parabolic Equation Calculations," *J. Comp. Appl. Math.* **172** (2004), 183–206.

[17] A. Arnold and M. Ehrhardt, "Discrete transparent boundary conditions for wide angle parabolic equations in underwater acoustics," *J. Comp. Phys.* **145** (1998), 611–638.

[18] M. Ehrhardt and A. Arnold, "Discrete Transparent Boundary Conditions for the Schrödinger Equation," *Riv. Mat. Univ. Parma* **6** (2001), 57–108.

[19] C. Ringhofer and J. Soler, "Discrete Schrödinger–Poisson Systems preserving Energy and Mass," *Appl. Math. Lett.* **13** (2000), 27–32.

[20] M.F. Levy, *Parabolic equation models for electromagnetic wave propagation* (IEE Electromagnetic Waves Series 45, 2000).

[21] T.W. Dawson, D.J. Thomson and G.H. Brooke, "Non–local boundary conditions for acoustic PE predictions involving inhomogeneous layers," *Proceedings of the Third European Conference on Underwater Acoustics*, FORTH–IACM, Heraklion, Greece, 1996, 183–188.

[22] M. Ehrhardt, *Discrete Artificial Boundary Conditions* (Ph.D. Thesis, Technische Universität Berlin, 2001).

[23] A. Arnold, "Numerically Absorbing Boundary Conditions for Quantum Evolution Equations," *VLSI Design* **6** (1998), 313–319.

[24] G.N. Watson, *A treatise on the theory of Bessel functions* (Cambridge University Press, Cambridge, 1966).

[25] E.W. Barnes, "On the homogeneous linear difference equation of the second order with linear coefficients," *Messenger* **34** (1904), 52–71.

[26] I.J. Thompson and A.R. Barnett, "Coulomb and Bessel Functions of Complex Arguments and Order," *J. Comp. Phys.* **46** (1986), 490–509.

[27] H. Poincaré, "Sur Les Equation Linéaires aux Differentielles Ordinaires et aux Différence Finies," *Amer. J. Math.* **7** (1885), 203–258.

[28] O. Perron, "Über Summengleichungen und Poincarésche Differenzengleichungen," *Math. Annalen* **84** (1921), 1–15.

[29] R.E. Mickens, "Asymptotic properties of solutions to two discrete Airy equations," *J. Difference Equ. Appl.* **3** (1998), 231–239.

[30] R. Wong and H. Li, "Asymptotic expansions for second–order linear difference equations. II," *Stud. Appl. Math.* **87** (1992), 289–324.

[31] R.E. Mickens, "Asymptotic properties of solutions to discrete Coulomb equations," *Comput. Math. Appl.* **36** (1998), 285–289.

[32] R. Wong and H. Li, "Asymptotic expansions for second–order linear difference equations," *J. Comput. Appl. Math.* **41** (1992), 65–94.

[33] W.J. Lentz, "Generating Bessel Functions in Mie Scattering Calculations Using Continued Fractions," *Appl. Opt.* **15** (1976), 668–671.

[34] A. Arnold, M. Ehrhardt and I. Sofronov, "Discrete transparent boundary conditions for the Schrödinger equation: Fast calculation, approximation, and stability," *Comm. Math. Sci.* **1** (2003), 501–556.

[35] M. Ehrhardt and A. Arnold, "Discrete Transparent Boundary Conditions for Wide Angle Parabolic Equations: Fast Calculation and Approximation," *Proceedings of the Seventh European Conference on Underwater Acoustics*, July 3–8, 2004, TU Delft, The Netherlands, 9–14.

[36] A. Zisowsky, *Discrete Transparent Boundary Conditions for Systems of Evolution Equations* (Ph.D. Thesis, Technische Universität Berlin, 2003).

[37] S. Zhang and J. Jin, *Computation of special functions: with over 100 computer programs in FORTRAN* (John Wiley & Sons, New York, 1996). (MATLAB routines: `http://ceta.mit.edu/comp_spec_func/`)

[38] R.E. Mickens, "Asymptotic solutions to a discrete Airy equation," *J. Difference Equ. Appl.* **7** (2001), 851–858.

[39] G. Doetsch, *Anleitung zum praktischen Gebrauch der Laplace–Transformation und der Z–Transformation* (R. Oldenburg Verlag München, Wien, 1967).