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ON STABILITY OF THE CRANK-NICOLSON SCHEME WITH APPROXIMATE TRANSPARENT BOUNDARY CONDITIONS FOR THE SCHRÖDINGER EQUATION, PART I*

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Abstract. We consider initial-boundary value problems for a generalized time-dependent Schrödinger equation in 1D on the semi-axis and in 2D on a semi-bounded strip. For Crank-Nicolson finite-difference schemes, we suggest an alternative coupling to approximate transparent boundary conditions and present a condition ensuring unconditional stability. In the case of discrete transparent boundary conditions, we revisit the statement and the proof of stability together with the derivation of the conditions.

Key words. Stability, Crank-Nicolson, finite-difference scheme, transparent boundary conditions, time-dependent Schrödinger equation

AMS subject classifications. 65M06, 65M12, 35Q40

1. Introduction

The time-dependent Schrödinger equation is the fundamental equation in quantum mechanics and it has also a lot of applications in classical wave physics including optics, acoustics, etc. (where similar equations are called by other names: Fresnel's equation, parabolic wave equation, paraxial approximation, etc.). Our interest comes from long-term studies of microscopic description of low-energy nuclear fission dynamics (see in particular [8, 12]). Generally all these problems are described by initial-boundary value problems in unbounded domains (or the Cauchy problem in the whole space); in particular, for nuclear fission dynamics, a generalized 2D Schrödinger equation (with variable coefficients) in a semi-bounded strip is of interest.

To treat numerically such problems for the Schrödinger equation, finite-difference of finite element approximations are mainly applied but in bounded domains restricted by additional artificial boundaries, where *artificial boundary conditions* are imposed. For original initial-boundary value problems, *transparent boundary conditions* (TBCs) have been developed which are supposed to be satisfied by exact solutions; the TBCs are integro-differential relations, non-local in time and space (along the artificial boundaries). The natural and mathematically correct types of artificial boundary conditions are approximate TBCs (either non-local or local). It is well-known that their construction is not trivial since such approximate TBCs should ensure both stability of the resulting method in the bounded domain and small numerical reflections from the artificial boundary, see [1]-[4], [7, 9, 10, 13], [15]-[17], [19, 20].

Another approach, suggested in [5] and essentially developed in [11], consists in deriving directly *discrete TBCs* satisfied by solutions of the corresponding finite-difference schemes for the original initial-boundary value problem in an unbounded domain thus avoiding any explicit treatment of the integro-differential TBC (though, of course, the discrete TBCs are their mesh counterparts and non-standard approximations). This approach is proved to be very efficient in the sense that, whenever

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applicable, it guarantees both unconditional stability and complete absence of numerical reflections from the artificial boundary, what has been studied theoretically and confirmed by numerical experiments. For the related spatially discretized case, see also [21, 23].

For completeness, we should also mention some other approaches such as absorbing boundary conditions, absorbing and perfectly matching layers, complex absorbing potentials, etc.

The stability of the 1D Crank-Nicolson finite-difference scheme coupled to the discrete TBC is considered in the literature as established result, see [11]. Unfortunately, its statement is not completely satisfying (as containing a semi-norm rather than a norm of solutions) and the proof should be corrected (see details below). Moreover, the derivation of the discrete TBC in [11] gives rise to questions on the treatment of analytic branches of $\sqrt{w}$, and the resulting formulas have to be slightly corrected to hold for the whole range of parameters, which is especially significant for 2D extensions.

In this paper, we have tried to remove all these drawbacks, thus confirming more the value of the discrete TBCs. In Section 2, we first consider initial-boundary value problem for a generalized Schrödinger equation in 1D on the semi-axis. For the Crank-Nicolson finite-difference scheme on a non-uniform mesh, we suggest an alternative coupling to general (abstract) approximate TBC and present a condition on an operator in approximate TBC ensuring the unconditional stability of the resulting method with respect not only to initial data (as usual) but with respect to perturbations in the Crank-Nicolson equation and in the approximate TBC as well. This coupling is based on the symmetric (with respect to space and time) approximation of the space derivative appearing in the integro-differential TBC and involves the Crank-Nicolson equation at the same node in contrast to known one-sided approximations completely independent of the Crank-Nicolson equation.

The key Section 3 is devoted to revisiting the proof of stability in the case of discrete TBC together with its derivation. We begin with the Crank-Nicolson finite-difference scheme on an infinite mesh on the semi-axis, prove its unique solvability and stability with respect to initial data and and clarify the sense of the stability condition for the solution. We apply the method of reproducing functions to derive and to study the discrete TBC in the form suggested in Section 2. We present two distinct proofs of the stability condition in the case of the discrete TBC. The first proof is implicit, since this does not deal with any explicit expression for the operator in the discrete TBC and leads to the theoretically important conclusion that the discrete TBC (among all approximate TBCs) *automatically* yields the unconditionally stable scheme on the finite mesh. Note that this proof exploits the results for the Crank-Nicolson equation with the perturbation. The second proof is explicit since it exploits a suitable (though not genuinely explicit) expression for this operator; such a proof is also important since it can serve as a reference when considering various similar approximate TBC (including a simplified discrete TBC developed in [6]). We also derive the explicit expression for the operator in the discrete TBC (in the form suggested in Section 2) which only unessentially differs from one indirectly derived in [11] for the stable implementation of the discrete TBC and actually corrects the latter expression in order to make it valid in the whole range of parameters.

For applications in low-energy nuclear fission dynamics, 2D model is much more relevant than the oversimplified 1D one. That is the reason why finally in Section 4 we extend the listed results on the Crank-Nicolson scheme with approximate or discrete

TBCs to the case of generalized Schrödinger equation in 2D on a semi-bounded strip. In the case of the discrete TBC, we show that a mesh Fourier expansion with respect to the additional space variable is successfully applicable in order both to derive the discrete TBC and to prove the stability condition by reducing to the 1D situation that have been previously studied.

2. $1D$ Schrödinger equation and the Crank-Nicolson scheme with an approximate TBC

We first consider the simplified 1D version of the microscopic description of low-energy nuclear fission dynamics that can be written in term of the generalized time-dependent Schrödinger equation

$$i\hbar\frac{\partial\psi}{\partial t}=\mathcal{H}\psi \quad \text{for} \quad x>0 \quad \text{and } t>0, \tag{2.1}$$

involving the 1D Hamiltonian operator

$$\mathcal{H}\psi:=-\frac{\hbar^2}{2}\frac{\partial}{\partial x}\left(B\frac{\partial\psi}{\partial x}\right)+V\psi,$$

for the unknown complex-valued wave function $\psi=\psi(x,t)$. Hereafter, i is the imaginary unit, $\hbar>0$ is a physical constant (its value is not important in this study), B and V are given real-valued functions and $B(x)\geqslant B_0>0$.

We impose the following boundary condition and condition at infinity

$$\psi|_{x=0}=0 \quad \text{and} \quad \psi(x,t)\to 0 \quad \text{as } x\to\infty, \quad \text{for any } t>0, \tag{2.2}$$

together with the initial condition

$$\psi|_{t=0}=\psi^0(x) \quad \text{for } x>0. \tag{2.3}$$

We assume that, for some $X_0>0$

$$B(x)=B_{1\infty}>0, \quad V(x)=V_\infty \quad \text{and} \quad \psi^0(x)=0 \quad \text{for } x\geqslant X_0. \tag{2.4}$$

An integro-differential TBC for this problem can be written in the form, for any $X\geqslant X_0$ (for example see [11])

$$\frac{\partial\psi}{\partial x}(X,t)=-\frac{1-i}{\sqrt{\hbar B_{1\infty}}}e^{-i(V_\infty/\hbar)t}$$

$$\times\frac{1}{\sqrt{\pi}}\frac{d}{dt}\int_0^t\psi(X,\theta)e^{i(V_\infty/\hbar)\theta}\frac{d\theta}{\sqrt{t-\theta}}, \tag{2.5}$$

for $t>0$, which clearly is non-local in time; other equivalent forms are also available. Recall that the involved operator

$$\mathcal{D}_{0+}^{1/2}f(t):=\frac{1}{\sqrt{\pi}}\frac{d}{dt}\int_0^t f(\theta)\frac{d\theta}{\sqrt{t-\theta}} \quad \text{for} \quad t>0,$$

defines the classical left-hand Riemann-Liouville time derivative of order $1/2$ on the semi-axis $[0,\infty)$.

We fix some $X > X_0$ and introduce a non-uniform mesh $\overline{\omega}_{h,\infty}$ in x on $[0,\infty)$ with the nodes $0 = x_0 < \cdots < x_J = X < \dots$ and the steps $h_j := x_j - x_{j-1}$ such that $h_J \leqslant X - X_0$ and $h_j = h \equiv h_J$ for $j \geqslant J$. We also introduce a non-uniform mesh in t on $[0,\infty)$ with the nodes $0 = t_0 < \cdots < t_m < \dots$, $t_m \to \infty$ as $m \to \infty$, and the steps $\tau_m := t_m - t_{m-1}$. Let $\omega_{h,\infty} := \overline{\omega}_{h,\infty} \backslash \{0\}$, $h_{\min} := \min_{1 \leqslant j \leqslant J} h_j$ and $\omega^\tau := \overline{\omega}^\tau \backslash \{0\}$.

We define the backward, the modified forward and the central difference quotients with respect to x

$$\overline{\partial}_x W_j := \frac{W_j - W_{j-1}}{h_j}, \quad \widehat{\partial}_x W_j := \frac{W_{j+1} - W_j}{h_{j+1/2}}, \quad \overset{\circ}{\partial}_x W_j := \frac{W_{j+1} - W_{j-1}}{2h_{j+1/2}},$$

where $h_{j+1/2} := \frac{h_j + h_{j+1}}{2}$, together with the backward difference quotient, an averaging and the backward shift in time

$$\overline{\partial}_t \Phi^m := \frac{\Phi^m - \Phi^{m-1}}{\tau_m}, \quad \overline{s}_t \Phi^m := \frac{\Phi^{m-1} + \Phi^m}{2}, \quad \check{\Phi}^m := \Phi^{m-1}.$$

The standard 1D Crank-Nicolson finite-difference scheme for the generalized Schrödinger equation (2.1) is written as follows

$$i\hbar \overline{\partial}_t \Psi = \mathcal{H}_h \overline{s}_t \Psi, \tag{2.6}$$

with the 1D mesh Hamiltonian operator

$$\mathcal{H}_h W := -\frac{\hbar^2}{2} \widehat{\partial}_x \left(B_h \overline{\partial}_x W \right) + V_h W,$$

where $B_{hj} = B\left(x_{j-1/2}\right)$ with $x_{j-1/2} := x_j - h_j/2$ and $V_{hj} = V(x_j)$ (for definiteness).

In the literature, the standard way to deduce finite-difference schemes on a finite mesh $\overline{\omega}_h := \{x_j\}_{j=0}^J$ consists in exploiting discretization (2.6) on the mesh $\omega_h := \{x_j\}_{j=1}^{J-1}$ and coupling it to an approximation of the TBC (2.5) at the node x_J in order to obtain a closed problem for the values of Ψ on $\overline{\omega}_h \times \overline{\omega}^\tau$. The approximation can be deduced explicitly or implicitly but usually this is written independently from discretization (2.6) (see in particular [5, 6, 11, 13]).

We propose another approach which is first presented and studied for general (abstract) approximation of the TBC (2.5) in this section and is then analyzed in more detail for the discrete TBC in the next section. Let the relation

$$\left(\overset{\circ}{\partial}_x \overline{s}_t \Psi \right)_J^m = \mathcal{S}^m \left\{ \Psi_J^1, \dots, \Psi_J^m \right\} \quad \text{for any} \quad m \geqslant 1, \tag{2.7}$$

be an approximate TBC (2.5) at the node x_J. Notice that we suggest to exploit an approximation of $\frac{\partial \psi}{\partial x}$ in (2.5) that is symmetric both in x (instead of usual backward ones) and in t. Using initially the Crank-Nicolson discretization (2.6) on the mesh $\omega_h \cup \{x_J\}$, we apply it at the node x_J only in order to eliminate the values $\overline{s}_t \Psi_{J+1}$ involved in the left-hand side of (2.7). Namely since $\widehat{\partial}_x \overline{\partial}_x W_J = \frac{2}{h} \left(\overset{\circ}{\partial}_x W_J - \overline{\partial}_x W_J \right)$, from (2.6) at the node x_J we get

$$\frac{\hbar^2}{2} \left(\overset{\circ}{\partial}_x \overline{s}_t \Psi \right)_J = \frac{\hbar^2}{2} \left(\overline{\partial}_x \overline{s}_t \Psi \right)_J - \frac{h}{2B_{1\infty}} \left(i\hbar \overline{\partial}_t \Psi - V_\infty \overline{s}_t \Psi \right)_J. \tag{2.8}$$

This leads us to the following complete finite-difference scheme that couples the Crank-Nicolson discretization to the approximate TBC

$$i\hbar\overline{\partial}_t\Psi = \mathcal{H}_h\overline{s}_t\Psi \quad \text{on} \quad \omega_h\times\omega^\tau, \tag{2.9}$$

$$\Psi_0^m = 0 \quad \text{for} \quad m\geqslant 1, \tag{2.10}$$

$$\left[\overline{\partial}_x\overline{s}_t\Psi - \frac{h}{\hbar^2 B_{1\infty}}\left(i\hbar\overline{\partial}_t\Psi - V_\infty\overline{s}_t\Psi\right)\right]_J^m = \mathcal{S}^m\left\{\Psi_J^1,\dots,\Psi_J^m\right\} \quad \text{for} \quad m\geqslant 1, \tag{2.11}$$

$$\Psi^0 = \Psi_h^0 \quad \text{on} \quad \overline{\omega}_h, \tag{2.12}$$

where $\Psi_{hj}^0 = \psi^0(x_j)$ (for definiteness) and thus $\Psi_{hJ}^0 = 0$; we assume that $\Psi_{h0}^0 = 0$. Notice that the boundary condition (2.11) has the form of the well-known 4−point second order approximation to the non-homogeneous Neumann boundary condition (that would be the TBC (2.5) provided that its right-hand side were given), for example see [18].

We intend to study the important problem of stability of the finite-difference scheme (2.9)–(2.12) with respect to the initial data Ψ_h^0 and to perturbations in equation (2.9) and the boundary condition (2.11). To this end we replace (2.9) and (2.11) by their generalized versions

$$i\hbar\overline{\partial}_t\Psi = \mathcal{H}_h\overline{s}_t\Psi + F \quad \text{on} \quad \omega_h\times\omega^\tau, \tag{2.13}$$

$$\left[\overline{\partial}_x\overline{s}_t\Psi - \frac{h}{\hbar^2 B_{1\infty}}\left(i\hbar\overline{\partial}_t\Psi - V_\infty\overline{s}_t\Psi + G\right)\right]_J^m = \mathcal{S}^m\left\{\Psi_J^1,\dots,\Psi_J^m\right\} \quad \text{for } m\geqslant 1, \tag{2.14}$$

where the perturbations F and G are given functions defined on $\omega_h\times\omega^\tau$ and ω^τ. Note that it is also important to consider non-zero F for purely mathematical reasons (for example see the first proof of Proposition 3.6 below).

To state our result, we need to introduce two mesh counterparts of the inner product in the complex space $L^2(0,X)$:

$$(U,W)_{\omega_h} := \sum_{j=1}^{J-1} U_j W_j^* h_{j+1/2},$$

and

$$(U,W)_{\overline{\omega}_h} := (U,W)_{\omega_h} + U_J W_J^* \frac{h}{2},$$

together with the associated mesh norms $\|\cdot\|_{\omega_h}$ and $\|\cdot\|_{\overline{\omega}_h}$ (of course, for mesh functions respectively defined on ω_h or defined on $\overline{\omega}_h$ and equal zero at $x_0=0$). Hereafter z^*, $\operatorname{Re} z$ and $\operatorname{Im} z$ denote the complex conjugate, the real and the imaginary parts of $z\in\mathbb{C}$.

PROPOSITION 2.1. *Let Ψ_h^0 be a given function defined on $\overline{\omega}_h$ (such that $\Psi_{h0}^0 = \Psi_{hJ}^0 = 0$) and Ψ be a solution of the finite-difference scheme (2.13), (2.10), (2.14), (2.12). Assume that the operator $\mathcal{S}$ satisfies the inequality*

$$\operatorname{Im}\sum_{m=1}^{M}\mathcal{S}^m\left\{\Phi^1,\dots,\Phi^m\right\}\left(\overline{s}_t\Phi^m\right)^*\tau_m \geqslant 0 \quad \textit{for any } M\geqslant 1, \tag{2.15}$$

for any function Φ *defined on* $\overline{\omega}^\tau$ *such that* $\Phi^0=0$. *Then the following stability bound holds*

$$\max_{0\leqslant m\leqslant M}\|\Psi^m\|_{\overline{\omega}_h}$$

$$\leqslant\|\Psi_h^0\|_{\overline{\omega}_h}+\frac{2}{\hbar}\sum_{m=1}^M\|F^m\|_{\omega_h}\tau_m+\frac{\sqrt{2h}}{\hbar}\sum_{m=1}^M|G^m|\tau_m \quad \textit{for any } M\geqslant 1. \tag{2.16}$$

Proof. Proceeding in a standard manner, we take the $(\cdot,\cdot)_{\omega_h}$-inner-product of equation (2.13) and a function W defined on the mesh $\overline{\omega}_h$ such that $W_0=0$ and sum the result by parts (using the first assumption (2.4))

$$i\hbar\left(\overline{\partial}_t\Psi^m,W\right)_{\omega_h}=\frac{\hbar^2}{2}\sum_{j=1}^J B_{hj}(\overline{\partial}_x\overline{s}_t\Psi_j^m)\overline{\partial}_xW_j^*h_j+(V_h\overline{s}_t\Psi^m+F^m,W)_{\omega_h}$$

$$-\frac{\hbar^2}{2}B_{1\infty}\left(\overline{\partial}_x\overline{s}_t\Psi\right)_J^m W_J^{m*}. \tag{2.17}$$

Then applying the boundary condition (2.14), we obtain the identity

$$i\hbar\left(\overline{\partial}_t\Psi^m,W\right)_{\overline{\omega}_h}=\frac{\hbar^2}{2}\sum_{j=1}^J B_{hj}(\overline{\partial}_x\overline{s}_t\Psi_j^m)\overline{\partial}_xW_j^*h_j+(V_h\overline{s}_t\Psi^m,W)_{\overline{\omega}_h}$$

$$+(F^m,W)_{\omega_h}-\frac{h}{2}G^mW_J^*-\frac{\hbar^2B_{1\infty}}{2}\mathcal{S}^m\left\{\Psi_J^1,\dots,\Psi_J^m\right\}W_J^* \quad \text{for} \quad m\geqslant 1. \tag{2.18}$$

Now choosing $W=\overline{s}_t\Psi^m$ and separating the imaginary part of the result, we get the equality

$$\frac{\hbar}{2}\left(\overline{\partial}_t\|\Psi\|_{\overline{\omega}_h}^2\right)^m=\operatorname{Im}\left\{(F^m,\overline{s}_t\Psi^m)_{\omega_h}-\frac{h}{2}G^m(\overline{s}_t\Psi_J^m)^*\right\}$$

$$-\frac{\hbar^2B_{1\infty}}{2}\operatorname{Im}\left(\mathcal{S}^m\left\{\Psi_J^1,\dots,\Psi_J^m\right\}(\overline{s}_t\Psi_J^m)^*\right). \tag{2.19}$$

Multiplying this by $2\tau_m/\hbar$, summing up the result over $m=1,\dots,M$ and applying condition (2.15), we obtain the inequality

$$\|\Psi^M\|_{\overline{\omega}_h}^2\leqslant\|\Psi^0\|_{\overline{\omega}_h}^2+\frac{1}{\hbar}\sum_{m=1}^M\left(\|F^m\|_{\omega_h}+\sqrt{\frac{h}{2}}|G^m|\right)\left(\|\Psi^m\|_{\overline{\omega}_h}+\|\check{\Psi}^m\|_{\overline{\omega}_h}\right)\tau_m,$$

which implies the stability bound (2.16). ∎

COROLLARY 2.2. *Let condition (2.15) be valid. Then the finite-difference scheme (2.13), (2.10), (2.14), (2.12) is uniquely solvable at least provided that* $\mathcal{S}^m$ *is a linear operator for any* $m\geqslant 1$.

In particular, the scheme (2.9)-(2.12) is uniquely solvable, and its solution satisfies the equality

$$\max_{m\geqslant 0}\|\Psi^m\|_{\overline{\omega}_h}=\|\Psi_h^0\|_{\overline{\omega}_h}. \tag{2.20}$$

The equality ensures an important physical property that the total mass at each time level is not greater than the total initial one. Notice that, for $F=0$ and $G=0$, equality (2.19) implies that

$$\|\Psi^M\|_{\overline{\omega}_h}^2-\|\Psi_h^0\|_{\overline{\omega}_h}^2=-\hbar B_{1\infty}\,\mathrm{Im}\sum_{m=1}^{M}\mathcal{S}^m\left\{\Psi_J^1,\ldots,\Psi_J^m\right\}(\overline{s}_t\Psi_J^m)^*\tau_m \quad \text{for any } M\geqslant 1, \tag{2.21}$$

and thus, for validity of (2.20), it is *necessary* that condition (2.15) is valid at least for $\Phi=\Psi_J$. We clarify more the sense of the latter condition in the case of the discrete TBC in Corollary 3.3 below.

In [11], a bound similar to (2.20) is announced but containing only the level semi-norm $\|\cdot\|_{\omega_h}$ instead of the level norm $\|\cdot\|_{\overline{\omega}_h}$ (in the case of the discrete TBC, $B_h\equiv\mathrm{const}$ and the uniform mesh $\overline{\omega}_h$). In generally accepted sense, such a simplified bound *does not guarantee* the stability of the finite-difference scheme with respect to initial data, for example see [18]. Moreover, taking $\|\cdot\|_{\omega_h}$ instead of $\|\cdot\|_{\overline{\omega}_h}$ allows to establish neither the unique solvability (at least straightforwardly) nor a stability with respect to the boundary perturbation G.

For implementation, it is convenient to rewrite the boundary condition (2.11) in the equivalent form

$$\begin{aligned}\Psi_{J-1}^m+\Psi_{J-1}^{m-1}=(1+a_0-ia_1)\Psi_J^m+(1+a_0+ia_1)\Psi_J^{m-1}\\ -2h\mathcal{S}^m\left\{\Psi_J^1,\ldots,\Psi_J^m\right\} \quad \text{for} \quad m\geqslant 1,\end{aligned} \tag{2.22}$$

where the real parameters a_0 and a_1 are given by the formulas

$$a_0:=\frac{h^2V_\infty}{\hbar^2B_{1\infty}},\quad a_1:=\frac{2h^2}{\tau\hbar B_{1\infty}}>0. \tag{2.23}$$

3. The Crank-Nicolson scheme on the infinite mesh and the discrete TBC

In order to construct and to study discrete TBCs, we first turn to the Crank-Nicolson scheme on the infinite mesh for the original problem (2.1)–(2.3) on the semi-axis

$$i\hbar\overline{\partial}_t\Psi=\mathcal{H}_h\overline{s}_t\Psi+F \quad \text{on} \quad \omega_{h,\infty}\times\omega^\tau, \tag{3.1}$$

$$\Psi_0^m=0 \quad \text{for } m\geqslant 1, \tag{3.2}$$

$$\Psi^0=\Psi_h^0 \quad \text{on} \quad \overline{\omega}_{h,\infty}. \tag{3.3}$$

The given perturbation F is added to the right-hand side of (3.1) once again to analyze the stability of the scheme.

Let H_h be a Hilbert space consisting of complex-valued functions W defined on the mesh $\overline{\omega}_{h,\infty}$ such that $\sum_{j=1}^{\infty}|W_j|^2<\infty$ and $W_0=0$, equipped with the inner product $(U,W)_{H_h} := \sum_{j=1}^{\infty} U_j W_j^* h_{j+1/2}$. Since $h_j = h$ for $j \geqslant J$, clearly the conditions $\sum_{j=1}^{\infty} |W_j|^2 < \infty$ and $\|W\|_{H_h}^2 = \sum_{j=1}^{\infty} |W_j|^2 h_{j+1/2} < \infty$ are equivalent.

Proposition 3.1. *Let $F^m \in H_h$ for any $m \geqslant 1$ and $\Psi_h^0 \in H_h$. Then there exists a unique solution to the scheme (3.1)-(3.3) such that $\Psi^m \in H_h$ for any $m \geqslant 0$, and the following stability bound holds*

$$\max_{0\leqslant m\leqslant M} \|\Psi^m\|_{H_h} \leqslant \|\Psi_h^0\|_{H_h} + \frac{2}{\hbar} \sum_{m=1}^{M} \|F^m\|_{H_h} \tau_m \quad \text{for any } M \geqslant 1. \tag{3.4}$$

Moreover, in the particular case $F = 0$, the mass conservation law holds

$$\|\Psi^m\|_{H_h}^2 = \|\Psi_h^0\|_{H_h}^2 \quad \text{for any } m \geqslant 1. \tag{3.5}$$

Proof. We extend $\mathcal{H}_h$ to an operator in H_h by setting

$$\overset{\circ}{\mathcal{H}}_h W_j := \mathcal{H}_h W_j, \quad \text{for } j \geqslant 1, \quad \text{and} \quad \overset{\circ}{\mathcal{H}}_h W_0 := 0.$$

Since $h_j = h$ for $j \geqslant J$ and

$$\sup_{j\geqslant 1} \left(|B_{hj}| + |V_{hj}| \right) < \infty, \tag{3.6}$$

see (2.4), the operator $\overset{\circ}{\mathcal{H}}_h$ is bounded in H_h. Moreover, $\overset{\circ}{\mathcal{H}}_h$ is self-adjoint since

$$\left(\overset{\circ}{\mathcal{H}}_h W, U \right)_{H_h} = \frac{\hbar^2}{2} \sum_{j=1}^{\infty} B_{hj} \left(\overline{\partial}_x W_j \right) \overline{\partial}_x U_j^* h_j + (V_h W, U)_{H_h} \quad \text{for any } W, U \in H_h. \tag{3.7}$$

To establish this equality, one can first transform the finite sum $\sum_{j=1}^{j_1} (\mathcal{H}_h W)_j U_j^* h_{j+1/2}$ by summing by parts (compare with (2.17)) and second pass to the limit as $j_1 \to \infty$, using properties (3.6) and $W_j \to 0$ as $j \to \infty$, for $W \in H_h$.

Now we rewrite equation (3.1) together with the boundary condition (3.2) as an operator equation in H_h

$$i\hbar \overline{\partial}_t \Psi = \overset{\circ}{\mathcal{H}}_h \overline{s}_t \Psi + F \quad \text{on} \quad \omega^\tau. \tag{3.8}$$

Another form of this equation is as follows

$$\left(I + i \frac{\tau}{2\hbar} \overset{\circ}{\mathcal{H}}_h \right) \Psi^m = \left(I - i \frac{\tau}{2\hbar} \overset{\circ}{\mathcal{H}}_h \right) \check{\Psi}^m - i \frac{\tau}{\hbar} F^m \quad \text{for} \quad m \geqslant 1. \tag{3.9}$$

Hereafter I denotes the identity operator. Since

$$\left\| \left(I + i \frac{\tau}{2\hbar} \overset{\circ}{\mathcal{H}}_h \right) W \right\|_{H_h}^2 = \|W\|_{H_h}^2 - \frac{\tau}{\hbar} \operatorname{Im} \left(\overset{\circ}{\mathcal{H}}_h W, W \right)_{H_h} + \left\| \frac{\tau}{2\hbar} \overset{\circ}{\mathcal{H}}_h W \right\|_{H_h}^2 \geqslant \|W\|_{H_h}^2,$$

by virtue of the self-adjointness of $\overset{\circ}{\mathcal{H}}_h$, the inverse operator

$$\left(I + i \frac{\tau}{2\hbar} \overset{\circ}{\mathcal{H}}_h \right)^{-1},$$

exists, and its norm is not greater than 1. Thus, taking into account that, for $\check{\Psi}^m \in H_h$, the right-hand side of (3.9) is in H_h, we obtain that (3.9) has a unique solution $\Psi^m \in H_h$. The unique solvability of the scheme (3.1)-(3.3) with $\Psi^m \in H_h$, for any $m \geqslant 0$, is established.

Finally, exploiting the self-adjointness property (3.7) it is a simple matter to derive from (3.8) the equality

$$\frac{\hbar}{2}\overline{\partial}_t \left(\|\Psi\|^2_{H_h}\right) = \mathrm{Im}\,(F, \overline{s}_t\Psi)_{H_h} \quad \text{on} \quad \omega^\tau, \tag{3.10}$$

compare with (2.19). This clearly implies the stability bound (3.4) and, for $F=0$, the conservation law (3.5). ∎

REMARK 3.1. Proposition 3.1 remains valid for any real-valued coefficients B_h and V_h satisfying (3.6).

REMARK 3.2. Relations (3.4) and (3.5) also follow from (3.9) by virtue of the well-known unitarity of the operator $(I+iA)^{-1}(I-iA)$ for any bounded self-adjoint operator A.

COROLLARY 3.2. *Bound (3.4) implies the uniform-norm bound*

$$\sup_{m\geqslant 0}\max_{j\geqslant 0}\left|\Psi_j^m\right| \leqslant \frac{1}{\sqrt{h_{\min}}}\left(\|\Psi_h^0\|_{H_h} + \frac{2}{\hbar}\sum_{m=1}^{\infty}\|F^m\|_{H_h}\tau_m\right),$$

which is non-trivial provided that the series in the right-hand side is convergent, in particular, for $F=0$.

COROLLARY 3.3. *Let $F_J^m = 0$ and $\Psi_j^0 = 0$ for $j \geqslant J$ and $m \geqslant 1$. If the solution to the scheme (3.1)-(3.3) such that $\Psi^m \in H_h$, for any $m \geqslant 0$, satisfies relation (2.7) with some operator $\mathcal{S}$, then we have, for any $M \geqslant 1$*

$$\hbar B_{1\infty}\,\mathrm{Im}\sum_{m=1}^{M}\mathcal{S}^m\left\{\Psi_J^1,\ldots,\Psi_J^m\right\}(\overline{s}_t\Psi_J^m)^*\tau_m = \|\Psi^M\|^2_{\omega_{h,\infty}\setminus\omega_h}$$

$$:= \frac{h}{2}|\Psi_J^M|^2 + \sum_{j=J+1}^{\infty}|\Psi_j^M|^2 h \geqslant 0. \tag{3.11}$$

Actually, by virtue of equation (3.1) at the node x_J with $F_J^m = 0$, relation (2.7) is equivalent to the boundary condition (2.11); thus the solution to the scheme (3.1)-(3.3) solves the scheme (2.13), (2.10)-(2.12) too. Subtracting equalities (3.10) and (2.19) (with $G=0$) we obtain, for any $m \geqslant 1$

$$\frac{\hbar}{2}\overline{\partial}_t\left(\|\Psi\|^2_{\omega_{h,\infty}\setminus\omega_h}\right)^m = \frac{\hbar^2 B_{1\infty}}{2}\,\mathrm{Im}\left(\mathcal{S}^m\left\{\Psi_J^1,\ldots,\Psi_J^m\right\}(\overline{s}_t\Psi_J^m)^*\right),$$

which yields (3.11).

Clearly, the identity holds

$$\|W\|^2_{H_h} = \|W\|^2_{\overline{\omega}_h} + \|W\|^2_{\omega_{h,\infty}\setminus\omega_h} \quad \text{for any} \quad W \in H_h,$$

and therefore the latter corollary clarifies the sense of condition (2.15) in the case of the discrete TBC for $\Phi = \Psi_J$.

Now we turn to the explicit construction of the discrete TBC of the form (2.7) and proofs of property (2.15) for this.

To construct the discrete TBC, following [11] we consider the auxiliary finite-difference problem on the uniform part of the infinite mesh

$$i\hbar\overline{\partial}_t\Psi = \mathcal{H}_{h,\infty}\overline{s}_t\Psi \quad \text{on} \quad (\omega_{h,\infty}\backslash\omega_h)\times\omega^\tau, \tag{3.12}$$

$$\Psi_{J-1} \quad \text{is given}, \quad |\Psi_{J-1}|_\infty := \sup_{m\geqslant 0}|\Psi^m_{J-1}| < \infty, \tag{3.13}$$

$$\sup_{j\geqslant J-1,\, m\geqslant 0}|\Psi^m_j| < \infty, \tag{3.14}$$

$$\Psi^0_j = 0 \quad \text{for} \quad j\geqslant J-1, \tag{3.15}$$

which involves the limiting mesh Hamiltonian operator

$$\mathcal{H}_{h,\infty}W := -\frac{\hbar^2}{2}B_{1\infty}\widehat{\partial}_x\overline{\partial}_x W + V_\infty W \quad \text{on} \quad \omega_{h,\infty}\backslash\omega_h.$$

Hereafter in this section we assume that the time mesh $\overline{\omega}^\tau$ is uniform as well, that is, $\tau_m = \tau$ for any $m\geqslant 1$. Clearly, condition (3.14) on the uniform boundedness of the solution is implied by Corollary 3.2.

Since the coefficients are constants and the meshes are uniform, it becomes possible to solve explicitly this auxiliary problem.

To this end, we apply the method of reproducing functions (for example see [14, 22]); this is close to but simpler than the $\mathcal{Z}-$transform based on the Laurent series and used in [5, 11]. Namely, for a sequence $\{\Phi^m\}_{m=0}^\infty$ (that is, a complex-valued function on the mesh $\overline{\omega}^\tau$), we consider the power series

$$\widetilde{\Phi}(z) \equiv \mathcal{T}[\Phi](z) := \sum_{m=0}^{\infty}\Phi^m z^m,$$

in a neighborhood of the point $z=0$ on $\mathbb{C}$. In particular, if $|\Phi|_\infty < \infty$, this series converges for $|z|<1$, the bound holds

$$|\widetilde{\Phi}(z)| \leqslant \frac{|\Phi|_\infty}{1-|z|} \quad \text{for} \quad |z|<1, \tag{3.16}$$

and $\widetilde{\Phi}(z)$ is analytic for $|z|<1$.

Conversely, for a function p analytic in a disk $\{|z|<r_0\}$, the inverse transform $\Phi = \mathcal{T}^{-1}[p]$ that maps p into the sequence $\{\Phi^m\}_{m=0}^\infty$ of its Taylor coefficients

$$\Phi^m = \frac{1}{2\pi}\int_0^{2\pi}\frac{p(z)}{z^m}\bigg|_{z=re^{i\varphi}}d\varphi, \tag{3.17}$$

for any $0<r<r_0$, is well-defined.

Taking into account conditions (3.14) and (3.15), for $|z|<1$, we calculate

$$\mathcal{T}\left[i\hbar\overline{\partial}_t\Psi_j - \mathcal{H}_{h,\infty}\overline{s}_t\Psi_j\right](z) = i\hbar\frac{1-z}{\tau}\widetilde{\Psi}_j(z) - \frac{1+z}{2}\mathcal{H}_{h,\infty}\widetilde{\Psi}_j(z)$$
$$= \frac{1+z}{2}\frac{\hbar B_{1\infty}}{2h^2}\Big(\widetilde{\Psi}_{j+1}(z) - 2\gamma(z)\widetilde{\Psi}_j(z) + \widetilde{\Psi}_{j-1}(z)\Big) \quad \text{for} \quad j\geqslant J, \tag{3.18}$$

where the coefficient $\gamma(z)$ is expressed by the formula

$$\gamma(z):=1+a_0-ia_1\frac{1-z}{1+z},$$

and a_0 and a_1 have been introduced in (2.23). Hereafter, for $j\geqslant J-1$, we extend $\Psi_j^m\big|_{m=-1}:=0$ so that $\overline{\partial}_t\Psi_j^0=\overline{s}_t\Psi_j^0=0$. Equation (3.12) implies the difference equation

$$\widetilde{\Psi}_{j+1}(z)-2\gamma(z)\widetilde{\Psi}_j(z)+\widetilde{\Psi}_{j-1}(z)=0 \quad\text{for}\quad j\geqslant J. \tag{3.19}$$

The corresponding characteristic equation has the form

$$\nu^2(z)-2\gamma(z)\nu(z)+1=0,\quad z\neq -1; \tag{3.20}$$

its roots are

$$\nu_{1,2}(z)=\gamma(z)+\sqrt{\gamma^2(z)-1},$$

where $\sqrt{\cdot}$ is a two-valued function. We choose $\nu_1(z)$ such that $0<|\nu_1(z)|\leqslant 1$ and then $|\nu_2(z)|\geqslant 1$ since $\nu_1(z)\nu_2(z)=1$.

Since $\nu_1+\nu_2=2\gamma$, it is easy to see that $|\nu_1(z)|=1$ (and thus $|\nu_2(z)|=1$ too) if and only if $\gamma(z)$ is real and $|\gamma(z)|\leqslant 1$. The formula

$$\gamma(z)=1+a_0-2a_1\frac{\operatorname{Im} z}{|z+1|^2}+ia_1\frac{|z|^2-1}{|z+1|^2},$$

yields that

$$0<|\nu_1(z)|<1,\quad |\nu_2(z)|>1 \quad\text{for}\quad |z|\neq 1.$$

Consequently the general solution to the difference equation (3.19) has the form

$$\widetilde{\Psi}_j(z)=c_1(z)\nu_1^{j-J+1}(z)+c_2(z)\nu_2^{j-J+1}(z) \quad\text{for}\quad j\geqslant J-1,$$

with arbitrary $c_1(z)$ and $c_2(z)$. By virtue of (3.14) and (3.16) we find that $c_2(z)\equiv 0$ and thus recalling (3.13) we obtain

$$\widetilde{\Psi}_j(z)=\widetilde{\Psi}_{J-1}(z)\nu_1^{j-J+1}(z) \quad\text{for}\quad j\geqslant J-1. \tag{3.21}$$

We need to study properties of ν_1 and ν_2 in more detail. Let $\overset{-}{\sqrt{w}}$ be the analytic branch of $\sqrt{w}$ in $\mathbb{C}$ with the cross-cut along the semi-axis $\operatorname{Re} w>0$, $\operatorname{Im} w=0$ such that $\overset{-}{\sqrt{-1}}=i$.

LEMMA 3.4. *The functions ν_1 and ν_2 are analytic in the open unit disk $\{|z|<1\}$ and are expressed there by the formulas*

$$\nu_1(z)=\gamma(z)+\overset{-}{\sqrt{\gamma^2(z)-1}},\quad \nu_2(z)=\gamma(z)-\overset{-}{\sqrt{\gamma^2(z)-1}}.$$

Proof. The above defined linear-fractional function $\zeta=\gamma(z)$ establishes a one-to-one correspondence between the unit circumference $\{|z|=1\}$ with the punctured point $z=-1$ and the axis $\{\operatorname{Im}\zeta=0\}$ as well as between the open unit disk and the lower semi-plane $\{\operatorname{Im}\zeta<0\}$.

The function $\mathrm{Z}^{-1}(\zeta) := \zeta + \sqrt{\zeta^2 - 1}$ is the two-valued inverse of the elementary Zhukovskii function $\mathrm{Z}(z) := \frac{1}{2}\left(z + \frac{1}{z}\right)$, for example see [14]. Its branches

$$\mathrm{Z}_1^{-1}(\zeta) := \zeta + \sqrt[*]{\zeta^2 - 1} \quad \text{such that} \quad |\mathrm{Z}_1^{-1}(\zeta)| < 1,$$

and

$$\mathrm{Z}_2^{-1}(\zeta) := \zeta - \sqrt[*]{\zeta^2 - 1} = \frac{1}{\mathrm{Z}_1^{-1}(\zeta)} \quad \text{such that} \quad |\mathrm{Z}_2^{-1}(\zeta)| > 1,$$

are well-defined for any ζ excepting real ζ with $|\zeta| \leqslant 1$. [For the exceptional values of ζ, obviously $\mathrm{Z}^{-1}(\zeta) = \zeta$ for $\zeta = \pm 1$ and $\mathrm{Z}^{-1}(\zeta) = \zeta \pm i|\zeta^2 - 1|^{1/2}$ for $|\zeta| < 1$, $\operatorname{Im}\zeta = 0$, with $|\mathrm{Z}^{-1}(\zeta)| = 1$.]

Moreover, assume that $\arg(\zeta^2 - 1) \in [0, 2\pi)$. Then clearly $\arg \sqrt[*]{\zeta^2 - 1}$ is selected from two values $\frac{1}{2}\arg(\zeta^2 - 1) + \pi k$, $k = 0, 1$, by the condition

$$\cos\left(\arg \sqrt[*]{\zeta^2 - 1} - \arg\zeta\right) < 0.$$

Straightforwardly we check that

$$\arg \sqrt[*]{\zeta^2 - 1} = \frac{1}{2}\arg(\zeta^2 - 1) \in \begin{cases} \left(0, \frac{\pi}{2}\right] & \text{for } \arg\zeta \in \left(\pi, \frac{3\pi}{2}\right], \\ \left(\frac{\pi}{2}, \pi\right) & \text{for } \arg\zeta \in \left(\frac{3\pi}{2}, 2\pi\right). \end{cases} \tag{3.22}$$

Clearly, the function $w = \zeta^2 - 1$ establishes a one-to-one correspondence between the lower semi-plane $\{\operatorname{Im}\zeta < 0\}$ and the whole complex plane with the cross-cut along the ray $\operatorname{Re} w \geqslant -1$, $\operatorname{Im} w = 0$. In the image, $\sqrt[*]{\zeta^2 - 1} = \sqrt[-]{\zeta^2 - 1}$. Therefore the functions $\sqrt[*]{\zeta^2 - 1}$ and $\mathrm{Z}_l^{-1}(\zeta)$ are analytic in the lower semi-plane $\{\operatorname{Im}\zeta < 0\}$, and the functions $\nu_l(z) = \mathrm{Z}_l^{-1}(\gamma(z))$ are analytic in the open unit disk $\{|z| < 1\}$, for $l = 1, 2$.

We now turn to consequences of formula (3.21). ∎

Proposition 3.5.

1. *The solution to the problem (3.12)-(3.15) is given by the formula*

$$\Psi_j = \mathcal{T}^{-1}\left[\nu_1^{j-J+1}(z)\widetilde{\Psi}_{J-1}(z)\right] \quad \textit{for} \quad j \geqslant J - 1. \tag{3.23}$$

In the case where condition (3.13) is replaced by the more general one

$$\Psi_{j_0} \textit{ is given}, \quad |\Psi_{j_0}|_\infty < \infty,$$

with some $j_0 \geqslant J - 1$, the following generalized formula for the solution holds

$$\Psi_j = \mathcal{T}^{-1}\left[\nu_1^{j-j_0}(z)\widetilde{\Psi}_{j_0}(z)\right] \quad \textit{for} \quad j \geqslant J - 1. \tag{3.24}$$

2. *Conversely, for any function Φ defined on $\overline{\omega}^\tau$ such that $\Phi^0 = 0$ and $|\Phi|_\infty < \infty$, the function*

$$\Psi_j := \mathcal{T}^{-1}\left[\nu_1^{j-j_0}(z)\widetilde{\Phi}(z)\right] \quad \textit{for} \quad j \geqslant J - 1, \tag{3.25}$$

with $j_0 \geqslant J - 1$, satisfies equation (3.12), the boundary condition $\Psi|_{j=j_0} = \Phi$ and the initial condition (3.15) as well as satisfies

$$\sum_{j=J-1}^{\infty} |\Psi_j^m|^2 < \infty \quad \textit{for} \quad m \geqslant 1.$$

Proof. 1. Formula (3.21) together with Lemma 3.4 immediately lead to formula (3.23). Formula (3.24) is proved quite similarly (recall that $\nu_1(z)\neq 0$).

2. Function (3.25) is well-defined and satisfies (3.15) (since $\widetilde{\Phi}(0)=0$). By relations (3.18) and (3.20), this also satisfies the equality

$$\mathcal{T}\left[i\hbar\overline{\partial}_t\Psi_j-\mathcal{H}_{h,\infty}\overline{s}_t\Psi_j\right](z)=0 \quad\text{for}\quad j\geqslant J \quad\text{and}\quad |z|<1,$$

and thus equation (3.12) too.

By the Cauchy bound (following from formula (3.17)) and bound (3.16), we obtain, for any $j\geqslant j_0$ and $m\geqslant 1$

$$|\Psi_j^m|\leqslant\frac{\max_{|z|=r}|\nu_1^{j-j_0}(z)\widetilde{\Phi}(z)|}{r^m}\leqslant\frac{q(r)^{j-j_0}|\Phi|_\infty}{r^m(1-r)}\quad\text{for any}\quad 0<r<1,$$

where $q(r):=\max_{|z|=r}|\nu_1(z)|<1$. [For $J-1\leqslant j<j_0$, the same estimate with $q(r):=\min_{|z|=r}|\nu_1(z)|$ holds.] Consequently

$$\sum_{j=j_0}^{\infty}|\Psi_j^m|^2\leqslant\left(\frac{|\Phi|_\infty}{r^m(1-r)}\right)^2\frac{1}{1-q^2(r),}$$

which completes the proof. ∎

Let us return back to the derivation of the discrete TBC. From formula (3.21) we obtain

$$\widetilde{\Psi}_{j+1}(z)-\widetilde{\Psi}_{j-1}(z)=\left(\nu_1(z)-\frac{1}{\nu_1(z)}\right)\widetilde{\Psi}_j(z),$$

and thus

$$\mathcal{T}\left[\left(\overset{\circ}{\partial}_x\overline{s}_t\Psi\right)_J\right]=\frac{1}{2h}(\nu_1-\nu_2)(z)\widetilde{\overline{s}_t\Psi}_J(z)=\frac{1+z}{4h}(\nu_1-\nu_2)(z)\widetilde{\Psi}_J(z). \tag{3.26}$$

By the well-known formula for the product of two power series, this leads us to the discrete TBC of type (2.7) in the first form

$$\left(\overset{\circ}{\partial}_x\overline{s}_t\Psi\right)_J=\frac{1}{2h}Q*\overline{s}_t\Psi_J, \tag{3.27}$$

where $Q:=\mathcal{T}^{-1}[\nu_1-\nu_2]$ and

$$(Q*T)^m:=\sum_{q=0}^{m}Q^qT^{m-q}\quad\text{for}\quad m\geqslant 0,$$

is the convolution of sequences $\{Q^m\}_{m=0}^\infty$ and $\{T^m\}_{m=0}^\infty$. The sequence Q is well-defined according to Lemma 3.4 and could be calculated explicitly following [11]. But we omit such an explicit expression since it will be not required neither theoretically nor computationally; in particular, for implementation we rewrite (3.27) in the more suitable form (3.31) below.

We are in a position to prove inequality (2.15) in the case of the discrete TBC (3.27). We present two distinct proofs for this crucial result. The first proof is implicit since this exploits only the fact that the solution $\Psi^m\in H_h$, for any $m\geqslant 0$, to the scheme

(3.1)-(3.3) on the infinite mesh, with any F such that $F_j^m = 0$ for $j \geqslant J$ and $m \geqslant 1$ and with $\Psi^0 \equiv 0$, satisfies a relation of form (2.7) without using any explicit expression for $\mathcal{S}^m\left\{\Psi_J^1, \ldots, \Psi_J^m\right\}$. Thus we see that the discrete TBC (among all approximate TBCs of form (2.7)) *automatically* yields the unconditionally stable scheme on the finite mesh.

The second proof is explicit in the sense that this exploits the expression $\mathcal{S}^m\left\{\Psi_J^1, \ldots, \Psi_J^m\right\} = (Q * \overline{s}_t \Psi)^m$ with Q given above. Such a proof is also important since can serve as the reference one while considering other similar approximate TBC (for example, a simplified discrete TBC developed in [6]).

Proposition 3.6. *For the discrete TBC (3.27), inequality (2.15) holds.*

Proof. 1. The first (implicit) proof. Let us fix any $M \geqslant 1$ and values $\Phi^0 = 0, \Phi^1, \ldots, \Phi^M$. We extend Φ to the whole of $\overline{\omega}^\tau$ by any way such that $|\Phi|_\infty < \infty$. For $j \geqslant J-1$, we define the function Ψ by formula (3.25) for $j_0 = J$. For $0 \leqslant j < J-1$ and $m \geqslant 0$, we set $\Psi_j^m := 0$ (actually the values of Ψ on $(\omega^h \backslash \{x_{J-1}\}) \times \omega^\tau$ could be defined arbitrarily) and then $F := i\hbar \overline{\partial}_t \Psi - \mathcal{H}_h \overline{s}_t \Psi$.

By virtue of Claim 2 in Proposition 3.5, the constructed function Ψ satisfies the problem (3.12)-(3.15) and therefore the scheme (3.1)-(3.3) with $F = 0$ on $(\omega_{h,\infty} \backslash \omega_h) \times \omega^\tau$ and $\Psi_h^0 = 0$. Finally Corollary 3.3 implies inequality (2.15) since $\Psi_J^m = \Phi^m$ for $0 \leqslant m \leqslant M$.

2. The second (explicit) proof. Let us fix any $M \geqslant 1$ and values $\Phi^m|_{m=-1,0} = 0$, $\Phi^1, \ldots, \Phi^M$. We extend Φ by the formula

$$\Phi^m := (-1)^{m-M} \Phi^M \quad \text{for} \quad m \geqslant M+1. \tag{3.28}$$

Then $\overline{s}_t \Phi^m = 0$ for $m = 0$ and $m \geqslant M+1$ and

$$S := \sum_{m=1}^{M} (Q * \overline{s}_t \Phi)^m (\overline{s}_t \Phi^m)^* = \sum_{m=0}^{\infty} (Q * \overline{s}_t \Phi)^m (\overline{s}_t \Phi^m)^*. \tag{3.29}$$

Clearly, also

$$p(z) := \mathcal{T}[\overline{s}_t \Phi](z) = \frac{1+z}{2} \sum_{m=1}^{M-1} \Phi^m z^m + \frac{1}{2} \Phi^M z^M,$$

is simply a polynomial with degree not greater than M.

According to the formula expressing the product of two sequences in terms of their $\mathcal{T}-$transforms (for example see Chapter II, Section 2 in [22]), we have, for any $0 < r < 1$

$$S = \frac{1}{2\pi} \int_0^{2\pi} \mathcal{T}[Q * \overline{s}_t \Phi]\left(re^{i\varphi}\right) (\mathcal{T}[\overline{s}_t \Phi])^* \left(r^{-1} e^{i\varphi}\right) d\varphi,$$

that is,

$$S = \frac{1}{2\pi} \int_0^{2\pi} (\nu_1 - \nu_2)\left(re^{i\varphi}\right) p\left(re^{i\varphi}\right) p^*\left(r^{-1} e^{i\varphi}\right) d\varphi.$$

For $|z| < 1$, by Lemma 3.4 we obviously have

$$(\nu_1 - \nu_2)(z) = 2\, \bar{\sqrt{\gamma^2(z) - 1}}; \tag{3.30}$$

therefore

$$|(\nu_1-\nu_2)(z)|\leqslant 2(|\gamma(z)|+1) \quad \text{and} \quad \operatorname{Im}(\nu_1-\nu_2)(z)>0,$$

see also (3.22). Consequently we get, for $\frac{1}{2}\leqslant r<1$

$$S=\frac{1}{2\pi}\int_0^{2\pi}(\nu_1-\nu_2)\left(re^{i\varphi}\right)\left|p\left(e^{i\varphi}\right)\right|^2 d\varphi+O(\rho(r)),$$

with

$$\rho(r):=\int_0^{2\pi}\left(|\gamma(re^{i\varphi})|+1\right)d\varphi\,(1-r)\geqslant 0,$$

and then $\operatorname{Im} S\geqslant O(\rho(r))$.

Let $0<\varepsilon<1$. By definition of $\gamma(z)$, the estimates hold

$$|\gamma(z)|\leqslant C_\varepsilon \quad \text{for} \quad \frac{1}{2}\leqslant|z|<1,\quad 0\leqslant\arg z\leqslant\pi-\varepsilon \quad \text{and} \quad \pi+\varepsilon\leqslant\arg z\leqslant 2\pi,$$

and

$$\sup_{|z|<1}|\gamma(z)(1+z)|\leqslant C_0.$$

Applying them (preliminarily dividing the integral over $[0,2\pi]$ in the definition of $\rho(r)$ over $[0,2\pi]$ into two corresponding summands) and the inequality $1-|z|\leqslant|z+1|$, we find

$$\rho(r)\leqslant 2(\pi-\varepsilon)(C_\varepsilon+1)(1-r)+2\varepsilon(C_0+1).$$

Passing to the (upper) limit first as $r\to 1_-$ and second as $\varepsilon\to 0_+$, we obtain that $\rho(r)\to 0$ as $r\to 1_-$. This implies the desired property $\operatorname{Im} S\geqslant 0$. ∎

Note that in [11] in a similar situation the zero extension of Φ instead of (3.28) was applied; but clearly the zero extension does not ensure the validity of formula (3.29).

For implementation, we rewrite the discrete TBC (3.27) in the second form, see the right-hand equality (3.26)

$$\left(\overset{\circ}{\partial}_x\bar{s}_t\Psi\right)_J=\frac{1}{2h}R*\Psi_J, \tag{3.31}$$

where $R:=\mathcal{T}^{-1}\left[\frac{1+z}{2}(\nu_1-\nu_2)(z)\right]$, that is, in form (2.7) with

$$\mathcal{S}^m\left\{\Psi_J^1,\dots,\Psi_J^m\right\}:=\frac{1}{2h}(R*\Psi_J)^m=\frac{1}{2h}\sum_{q=0}^{m-1}R^q\Psi_J^{m-q} \quad \text{for any} \quad m\geqslant 1.$$

Now we calculate the sequence R (notice that we accomplish that directly rather than base on an explicit expression for Q in (3.27) as in [11]). Preliminarily rewriting $\gamma(z)$ in the form

$$\gamma(z)=1+\frac{az+a^*}{z+1} \quad \text{with} \quad a:=a_0+ia_1,$$

we get

$$\gamma^2(z)-1=\frac{\alpha z^2+2\beta z+\alpha^*}{(z+1)^2},$$

where the parameters α and β are given by the formulas

$$\alpha:=a(2+a)=\left[a_0(2+a_0)-a_1^2\right]+i2(1+a_0)a_1,\quad \beta:=2a_0+|a|^2=a_0^2+2a_0+a_1^2. \tag{3.32}$$

Furthermore, we rewrite

$$\alpha z^2+2\beta z+\alpha^*=\alpha^*\left[(\varkappa z)^2-2\mu\varkappa z+1\right],$$

where

$$\mu:=\frac{\beta}{|\alpha|}\in(-1,1),\quad \varkappa:=-e^{i\arg\alpha}\ \text{ with }\ \arg\alpha\in(0,2\pi); \tag{3.33}$$

here the property $\mu\in(-1,1)$ follows from the elementary inequality $\beta^2<|\alpha|^2$. Thus

$$\gamma^2(z)-1=\alpha^*\,\frac{(\varkappa z)^2-2\mu\varkappa z+1}{(z+1)^2},$$

and since $\gamma^2(z)-1\to\alpha^*=\gamma^2(0)-1$ as $z\to 0$, we obtain, for sufficiently small z

$$\sqrt[-]{\gamma^2(z)-1}=\sqrt[-]{\alpha^*}\,\frac{\sqrt[+]{(\varkappa z)^2-2\mu\varkappa z+1}}{z+1}, \tag{3.34}$$

where now $\sqrt[+]{w}$ is another analytic branch of $\sqrt{w}$, say, in the disk $\{|w-1|<1\}$ such that $\sqrt[+]{1}=1$. The formula

$$\sqrt[-]{\alpha^*}=\sqrt[-]{\gamma^2(0)-1}=-|\alpha|^{1/2}e^{-i(\arg\alpha)/2},$$

is valid, see (3.22) (here the choice $\arg\alpha\in(0,2\pi)$ is applied).

Formulas (3.30) and (3.34) imply that

$$\frac{z+1}{2}(\nu_1-\nu_2)(z)=\sqrt[-]{\alpha^*}\,\frac{(\varkappa z)^2-2\mu\varkappa z+1}{\sqrt[+]{(\varkappa z)^2-2\mu\varkappa z+1}}.$$

The well-known formula for the reproducing function of the Legendre polynomials $\{p_m\}_{m=0}^{\infty}$ holds, for any $|\mu|\leqslant 1$ and sufficiently small ζ

$$\sum_{m=0}^{\infty}p_m(\mu)\zeta^m=\frac{1}{\sqrt[+]{\zeta^2-2\mu\zeta+1}},$$

for example see Chapter VII, Section 2 in [14]. Consequently, for any integer l, $\varkappa\in\mathbb{C}$ and sufficiently small z (with $\varkappa z\neq 0$ for $l<0$)

$$\sum_{m=l}^{\infty}\varkappa^m p_{m-l}(\mu)z^m=\frac{(\varkappa z)^l}{\sqrt[+]{(\varkappa z)^2-2\mu\varkappa z+1}}.$$

Thus

$$\frac{1+z}{2}(\nu_1-\nu_2)(z)=\sqrt[-]{\alpha^*}\sum_{m=0}^{\infty}\varkappa^m\left[p_m(\mu)-2\mu p_{m-1}(\mu)+p_{m-2}(\mu)\right]z^m,$$

where $p_m(\mu)\equiv 0$ for $m<0$. Applying the recurrence relation for the Legendre polynomials

$$\mu p_{m-1}(\mu)=\frac{m-1}{2m-1}p_{m-2}(\mu)+\frac{m}{2m-1}p_m(\mu) \quad \text{for} \quad m\geqslant 0, \tag{3.35}$$

we find

$$\frac{1+z}{2}(\nu_1-\nu_2)(z)=-\bar{\sqrt{\alpha^*}}\sum_{m=0}^{\infty}\frac{\varkappa^m}{2m-1}(p_m-p_{m-2})(\mu)z^m.$$

Therefore the following result has been proved.

PROPOSITION 3.7. *The sequence R in the discrete TBC (3.31) is given by the formula*

$$R^m:=|\alpha|^{1/2}e^{-i(\arg\alpha)/2}\frac{\varkappa^m}{2m-1}(p_m-p_{m-2})(\mu) \quad \textit{for} \quad m\geqslant 0,$$

where the parameters α, μ and $\varkappa$ are given by formulas (2.23), (3.32) with $a=a_0+ia_1$ and (3.33). Recall that $\{p_m\}_{m=0}^{\infty}$ are the Legendre polynomials and $p_m\equiv 0$ for $m<0$.

Note that, in particular, the initial elements of R are expressed by the formulas

$$R^0=-|\alpha|^{1/2}e^{-i(\arg\alpha)/2}, \quad R^1=|\alpha|^{1/2}e^{i(\arg\alpha)/2}\mu.$$

Recall that the recurrence relation for the elements of R is known [11] (based on relation (3.35)).

One can verify that formula (2.22) together with those from the last proposition are equivalent to and only slightly differ from the corresponding formulas derived in [11] for the stable implementation of the discrete TBC but only in the case $\mathrm{Re}\,\alpha<0$ (since in [11] the choice $\arg(-\mathrm{Re}\,\frac{\alpha}{4}+i\,\mathrm{Im}\,\frac{\alpha}{4})=\arctan\frac{\mathrm{Im}\,\alpha}{-\mathrm{Re}\,\alpha}$ is adopted). In the case $\mathrm{Re}\,\alpha\geqslant 0$ the formulas from [11] have to be corrected. Note that even in the simplest case $V_\infty=0$ (that is, $a_0=0$), we have $\mathrm{Re}\,\alpha<0$ in 1D case but in general we need to cover the case of $\mathrm{Re}\,\alpha$ of arbitrary sign in 2D case below. We should also mention that the treatment of the analytic branches of $\sqrt{w}$ in [11] (for example, concerning the counterpart of formula (3.34)) gives rise to questions.

4. 2D Schrödinger equation and the Crank-Nicolson scheme with approximate or discrete TBC

For applications in low-energy nuclear fission dynamics, 1D model is oversimplified and 2D model is much more relevant, see [8, 12]. In this section, we show that the above 1D results and ideas can be rather easily extended to a 2D situation of physical interest.

So we turn to the generalized time-dependent 2D Schrödinger equation

$$i\hbar\frac{\partial\psi}{\partial t}=\mathcal{H}\psi \quad \text{for} \quad (x,y)\in\Omega \quad \text{and} \quad t>0, \tag{4.1}$$

involving the 2D Hamiltonian operator

$$\mathcal{H}\psi:=-\frac{\hbar^2}{2}\left[\frac{\partial}{\partial x}\left(B_{11}\frac{\partial\psi}{\partial x}\right)+\frac{\partial}{\partial x}\left(B_{12}\frac{\partial\psi}{\partial y}\right)+\frac{\partial}{\partial y}\left(B_{21}\frac{\partial\psi}{\partial x}\right)+\frac{\partial}{\partial y}\left(B_{22}\frac{\partial\psi}{\partial y}\right)\right]+V\psi,$$

where $\Omega:=(0,\infty)\times(0,Y)$ is a semi-bounded strip, the real matrix $\{B_{jk}(x,y)\}_{j,k=1}^2$ is symmetric and positive definite uniformly in Ω and $V(x,y)$ is real in Ω.

We impose the following boundary condition and condition at infinity

$$\psi|_{\partial\Omega}=0 \quad \text{and} \quad \|\psi(x,\cdot,t)\|_{L^2(0,Y)}\to 0 \quad \text{as} \quad x\to\infty, \quad \text{for any} \quad t>0, \tag{4.2}$$

together with the initial condition

$$\psi|_{t=0}=\psi^0(x,y) \quad \text{in } \Omega. \tag{4.3}$$

We assume that for some $X_0>0$

$$B_{11}(x,y)=B_{1\infty}>0, \quad B_{12}(x,y)=B_{21}(x,y)=0, \quad B_{22}(x,y)=B_{2\infty}>0,$$
$$V(x,y)=V_\infty \quad \text{and} \quad \psi^0(x,y)=0 \quad \text{for} \quad x\geqslant X_0, \quad y\in[0,Y]. \tag{4.4}$$

Expanding the solution for $x\geqslant X_0$ with respect to the orthonormalized system $\left\{\sqrt{\frac{2}{Y}}\sin\frac{\pi l y}{Y}\right\}_{l=1}^{\infty}$ on $(0,Y)$, for the corresponding Fourier coefficients, we get disjoint 1D Schrödinger equations of the form (2.1) with the auxiliary potentials $V_{\infty l}:=V_\infty+\frac{\hbar^2}{2}\left(\frac{\pi l}{Y}\right)^2 B_{2\infty}$ replacing V_∞. Therefore the 2D integro-differential TBC can be represented in the form of the expansion, for any $X\geqslant X_0$

$$\frac{\partial\psi}{\partial x}(X,y,t)=-\frac{1-i}{\sqrt{\hbar B_{1\infty}}}\sqrt{\frac{2}{Y}}\sum_{l=1}^{\infty}e^{-i(V_{\infty l}/\hbar)t}$$

$$\times\frac{1}{\sqrt{\pi}}\frac{d}{dt}\int_0^t \psi^{(l)}(X,\theta)e^{i(V_{\infty l}/\hbar)\theta}\frac{d\theta}{\sqrt{t-\theta}}\sin\frac{\pi l y}{Y}, \tag{4.5}$$

for $0<y<Y$ and $t>0$, with the Fourier coefficients

$$\psi^{(l)}(X,\theta):=\sqrt{\frac{2}{Y}}\int_0^Y \psi(X,y,\theta)\sin\frac{\pi l y}{Y}\,dy.$$

This TBC is non-local with respect to both y and t. In what follows, the similar approach will be applied to derive a discrete 2D TBC.

We continue to exploit the meshes, the mesh operators and the mesh norms in x and t introduced in Section 2 and in addition define two mesh averaging operators with respect to x

$$\bar{s}_x W_j=\frac{W_{j-1}+W_j}{2}, \quad \widehat{s}_x W_j:=\frac{h_j W_j+h_{j+1}W_{j+1}}{2h_{j+1/2}};$$

they are related by the identity

$$(\widehat{s}_x W,U)_{\omega_h}=\sum_{j=1}^{J}W_j\bar{s}_x U_j h_j-\frac{1}{2}(W_1U_0h_1+W_JU_Jh_J). \tag{4.6}$$

We also introduce the mesh $\overline{\omega}_\delta$ in y on $[0,Y]$ with the nodes $0=y_0<\cdots<y_K=Y$ and the steps $\delta_k:=y_k-y_{k-1}$. Let $\omega_\delta:=\overline{\omega}_\delta\setminus\{0,Y\}$ and $\delta_{\min}:=\min_{1\leqslant k\leqslant K}\delta_k$. We define the backward and the modified forward difference quotients together with two mesh averaging operators with respect to y

$$\bar{\partial}_y U_k:=\frac{U_k-U_{k-1}}{\delta_k}, \quad \widehat{\partial}_y U_k:=\frac{U_{k+1}-U_k}{\delta_{k+1/2}}, \quad \bar{s}_y U_k=\frac{U_{k-1}+U_k}{2},$$

and

$$\widehat{s}_y U_k := \frac{\delta_k U_k + \delta_{k+1} U_{k+1}}{2\delta_{k+1/2}},$$

where $\delta_{k+1/2} := (\delta_k + \delta_{k+1})/2$.

Let $\overset{\circ}{H}(\overline{\omega}_\delta)$ be the space of the complex-valued functions defined on the mesh $\overline{\omega}_\delta$ and equal zero at the nodes $y = 0, Y$, equipped with the inner product

$$(U, W)_{\omega_\delta} := \sum_{k=1}^{K-1} U_k W_k^* \delta_{k+1/2},$$

and the associated norm $\|\cdot\|_{\omega_\delta}$.

We define the product meshes $\overline{\omega}_{\mathbf{h},\infty} := \overline{\omega}_{h,\infty} \times \overline{\omega}_\delta$ on $\overline{\Omega} = [0,\infty) \times [0, Y]$, $\overline{\omega}_{\mathbf{h}} := \overline{\omega}_h \times \overline{\omega}_\delta$ on $[0, X] \times [0, Y]$ and also $\omega_{\mathbf{h},\infty} := \omega_{h,\infty} \times \omega_\delta$ and $\omega_{\mathbf{h}} := \omega_h \times \omega_\delta$.

We exploit the 2D mesh Hamiltonian operator

$$\mathcal{H}_{\mathbf{h}} W :=$$
$$-\frac{\hbar^2}{2}\left\{\widehat{\partial}_x\left(B_{11h}\overline{\partial}_x W + \widehat{\partial}_x \widehat{s}_y (B_{12h}\overline{s}_x \overline{\partial}_y W)\right) + \widehat{s}_x \widehat{\partial}_y (B_{21h}\overline{\partial}_x \overline{s}_y W) + \widehat{\partial}_y\left(B_{22h}\overline{\partial}_y W\right)\right\}$$
$$+ V_h W,$$

where the coefficients are given by the formulas

$$B_{11hjk} = \widehat{s}_y B_{11}(x_{j-1/2}, y_{k-1/2}), \quad B_{22hjk} = \widehat{s}_x B_{22}(x_{j-1/2}, y_{k-1/2}),$$
$$B_{12hjk} = B_{21hjk} = B_{12}(x_{j-1/2}, y_{k-1/2}),$$

with $y_{k-1/2} := y_k - \delta_k/2$, and $V_{hjk} = \widehat{s}_x \widehat{s}_y V(x_{j-1/2}, y_{k-1/2})$. Actually this finite-difference discretization is a simplification of the finite element one based on the bilinear elements for the rectangular mesh $\overline{\omega}_{\mathbf{h}}$ (conserving, in particular, its $L^2(\Omega)$ and $H^1(\Omega)$ optimal error estimates), see [24]. Other operators $\mathcal{H}_{\mathbf{h}}$ can be also exploited.

Let the relation

$$\left.\left(\overset{\circ}{\partial}_x \overline{s}_t \Psi\right)^m\right|_{j=J} = \mathcal{S}^m\left\{\Psi_J^1, \ldots, \Psi_J^m\right\} \text{ on } \omega_\delta, \tag{4.7}$$

be an approximate 2D TBC (4.5) at the node x_J for $m \geqslant 1$. Here Ψ_J^p is the collection $\Psi_J^p = \{\Psi_{Jk}^p\}_{k=0}^K$, $1 \leqslant p \leqslant m$, so that in general the relation is non-local not only in time (as in 1D case) but in y as well.

The approach described in Section 2 leads us to the following complete finite-difference scheme on the finite mesh $\overline{\omega}_{\mathbf{h}} \times \overline{\omega}^\tau$ which couples the Crank-Nicolson discretization to the approximate TBC

$$i\hbar \overline{\partial}_t \Psi = \mathcal{H}_{\mathbf{h}} \overline{s}_t \Psi \text{ on } \omega_{\mathbf{h}} \times \omega^\tau, \tag{4.8}$$

$$\Psi^m|_{j=0} = 0, \quad \Psi^m|_{k=0,K} = 0 \text{ for } m \geqslant 1, \tag{4.9}$$

$$\left.\left[\overline{\partial}_x \overline{s}_t \Psi - \frac{h}{\hbar^2 B_{1\infty}}\left(i\hbar \overline{\partial}_t \Psi + \frac{\hbar^2}{2} B_{2\infty} \widehat{\partial}_y \overline{\partial}_y \overline{s}_t \Psi - V_\infty \overline{s}_t \Psi\right)\right]^m\right|_{j=J}$$
$$= \mathcal{S}^m\left\{\Psi_J^1, \ldots, \Psi_J^m\right\} \text{ on } \omega_\delta \text{ for } m \geqslant 1, \tag{4.10}$$

$$\Psi^0 = \Psi_{\mathbf{h}}^0 \text{ on } \overline{\omega}_{\mathbf{h}}, \tag{4.11}$$

where $\Psi^0_{\mathbf{h}jk}=\psi^0(x_j,y_k)$ (for definiteness) and thus $\Psi^0_{\mathbf{h}}\big|_{j=J}=0$; we assume that the two conjunction conditions $\Psi^0_{\mathbf{h}}\big|_{j=0}=0$ and $\Psi^0_{\mathbf{h}}\big|_{k=0,K}=0$ are valid. Notice once more that the boundary condition (4.10) has the form of the well-known 2D second order approximation (exploiting an 8-point stencil in all the directions x, y and t) to the non-homogeneous Neumann boundary condition, for example see [18].

To study the stability problem for this finite-difference scheme, we replace (4.8) and (4.10) by their generalized versions

$$i\hbar\overline{\partial}_t\Psi=\mathcal{H}_{\mathbf{h}}\overline{s}_t\Psi+F \quad \text{on} \quad \omega_{\mathbf{h}}\times\omega^{\tau}, \tag{4.12}$$

$$\left[\overline{\partial}_x\overline{s}_t\Psi-\frac{h}{\hbar^2B_{1\infty}}\left(i\hbar\overline{\partial}_t\Psi+\frac{\hbar^2}{2}B_{2\infty}\widehat{\partial}_y\overline{\partial}_y\overline{s}_t\Psi-V_\infty\overline{s}_t\Psi+G\right)\right]^m\Bigg|_{j=J}$$
$$=\mathcal{S}^m\left\{\Psi^1_J,\dots,\Psi^m_J\right\} \quad \text{on} \quad \omega_\delta \quad \text{for} \quad m\geqslant 1, \tag{4.13}$$

where the perturbations F and G are given functions defined on $\omega_{\mathbf{h}}\times\omega^{\tau}$ and $\omega_\delta\times\omega^{\tau}$.

To state the result, we need to introduce two mesh counterparts of the inner product in the complex space $L^2((0,X)\times(0,Y))$:

$$(U,W)_{\omega_{\mathbf{h}}}:=\sum_{j=1}^{J-1}\sum_{k=1}^{K-1}U_{jk}W^*_{jk}h_{j+1/2}\delta_{k+1/2},$$

$$(U,W)_{\overline{\omega}_{\mathbf{h}}}:=(U,W)_{\omega_{\mathbf{h}}}+\sum_{k=1}^{K-1}U_{Jk}W^*_{Jk}\frac{h}{2}\delta_{k+1/2},$$

together with the associated mesh norms $\|\cdot\|_{\omega_{\mathbf{h}}}$ and $\|\cdot\|_{\overline{\omega}_{\mathbf{h}}}$.

PROPOSITION 4.1. *Let $\Psi^0_{\mathbf{h}}$ be any function defined on $\overline{\omega}_{\mathbf{h}}$ (satisfying $\Psi^0_{\mathbf{h}}\big|_{j=J}=0$ and the above conjunction conditions) and Ψ be a solution of the finite-difference scheme (4.12), (4.9), (4.13), (4.11). Assume that the operator $\mathcal{S}$ satisfies the inequality*

$$\operatorname{Im}\sum_{m=1}^{M}\left(\mathcal{S}^m\left\{\Phi^1,\dots,\Phi^m\right\},\overline{s}_t\Phi^m\right)_{\omega_\delta}\tau_m\geqslant 0 \quad \textit{for any } M\geqslant 1, \tag{4.14}$$

for any function Φ defined on $\overline{\omega}_\delta\times\overline{\omega}^{\tau}$ such that $\Phi^0=0$ and $\Phi|_{k=0,K}=0$. Then the following stability bound holds

$$\max_{0\leqslant m\leqslant M}\|\Psi^m\|_{\overline{\omega}_{\mathbf{h}}}\leqslant\|\Psi^0_{\mathbf{h}}\|_{\overline{\omega}_{\mathbf{h}}}+\frac{2}{\hbar}\sum_{m=1}^{M}\|F^m\|_{\omega_{\mathbf{h}}}\tau_m+\frac{\sqrt{2h}}{\hbar}\sum_{m=1}^{M}\|G^m\|_{\omega_\delta}\tau_m \quad \textit{for any } M\geqslant 1. \tag{4.15}$$

Proof. We take the $(\cdot,\cdot)_{\omega_{\mathbf{h}}}$-inner-product of equation (4.12) with any function W defined on the mesh $\overline{\omega}_{\mathbf{h}}$ such that $W|_{j=0}=0$ and $W|_{k=0,K}=0$. Then we sum the result by parts (using assumption (4.4)), apply identity (4.6) (and a similar identity with respect to y), exploit the boundary condition (4.13) and obtain the identity

$$i\hbar\left(\overline{\partial}_t\Psi^m,W\right)_{\overline{\omega}_{\mathbf{h}}}=\frac{\hbar^2}{2}\sum_{j=1}^{J}\sum_{k=1}^{K}\Big\{\widetilde{B}_{11}\overline{s}_y\left[(\overline{\partial}_x\overline{s}_t\Psi^m)\overline{\partial}_xW^*\right]+\widetilde{B}_{12}(\overline{s}_x\overline{\partial}_y\overline{s}_t\Psi^m)\overline{\partial}_x\overline{s}_yW^*$$
$$+\widetilde{B}_{21}(\overline{\partial}_x\overline{s}_y\overline{s}_t\Psi^m)\overline{s}_x\overline{\partial}_yW^*+\widetilde{B}_{22}\overline{s}_x\left[(\overline{\partial}_y\overline{s}_t\Psi^m)\overline{\partial}_yW^*\right]\Big\}_{jk}h_j\delta_k+(V_h\overline{s}_t\Psi^m,W)_{\overline{\omega}_{\mathbf{h}}}$$
$$+(F^m,W)_{\omega_{\mathbf{h}}}-\frac{h}{2}(G^m,W_J)_{\omega_\delta}-\frac{\hbar^2B_{1\infty}}{2}\left(\mathcal{S}^m\left\{\Psi_J^1,\ldots,\Psi_J^m\right\},W_J\right)_{\omega_\delta}\quad\text{for } m\geqslant 1, \tag{4.16}$$

where $\widetilde{B}_{jk}:=B(x_{j-1/2},y_{k-1/2})$. The rest of the proof is similar to one for Proposition 2.1 and thus is omitted. ∎

Corollary 4.2. *Let condition (4.14) be valid. Then the finite-difference scheme (4.12), (4.9), (4.13), (4.11) is uniquely solvable at least provided that $\mathcal{S}^m$ is a linear operator for any $m\geqslant 1$.*

In particular, the scheme (4.8)-(4.11) is uniquely solvable, and its solution satisfies the equality

$$\max_{m\geqslant 0}\|\Psi^m\|_{\overline{\omega}_{\mathbf{h}}}=\|\Psi^0_{\mathbf{h}}\|_{\overline{\omega}_{\mathbf{h}}}. \tag{4.17}$$

Clearly, this corollary is the 2D counterpart of Corollary 2.2, and also similarly to (2.21), for $F=0$ and $G=0$, the equality holds

$$\|\Psi^M\|^2_{\overline{\omega}_{\mathbf{h}}}-\|\Psi^0_{\mathbf{h}}\|^2_{\overline{\omega}_{\mathbf{h}}}=-\hbar B_{1\infty}\,\mathrm{Im}\sum_{m=1}^{M}\left(\mathcal{S}^m\left\{\Psi_J^1,\ldots,\Psi_J^m\right\},\overline{s}_t\Psi_J^m\right)_{\omega_\delta}\tau_m\quad\text{for any } M\geqslant 1.$$

We introduce the auxiliary mesh eigenvalue problem

$$-\widehat{\partial}_y\overline{\partial}_yE=\lambda E\quad\text{on}\quad\omega_\delta,\quad E|_{k=0,K}=0,\quad E\not\equiv 0.$$

We denote by $\{E_l,\lambda_{l\delta}\}$, $1\leqslant l\leqslant K-1$, the eigenpairs such that the functions $\{E_l\}_{l=1}^{K-1}$ are real-valued and form an orthonormalized basis in $\overset{\circ}{H}(\overline{\omega}_\delta)$; recall that $\lambda_{l\delta}>0$ for all l. Clearly, for any $U\in\overset{\circ}{H}(\overline{\omega}_\delta)$, the expansion holds

$$U=\mathcal{F}^{-1}U^{(\cdot)}:=\sum_{l=1}^{K-1}U^{(l)}E_l,$$

with the coefficients

$$U^{(l)}=(\mathcal{F}U)^{(l)}:=(U,E_l)_{\omega_\delta}\quad\text{for}\quad 1\leqslant l\leqslant K-1.$$

We also recall the identity

$$(U,W)_{\omega_\delta}=\sum_{l=1}^{K-1}U^{(l)}\left(W^{(l)}\right)^*\quad\text{for any}\quad U,W\in\overset{\circ}{H}(\overline{\omega}_\delta). \tag{4.18}$$

In the case of the uniform mesh $\overline{\omega}_\delta$, that is, if $\delta_k=\delta$ for any $1\leqslant k\leqslant K$, the eigenpairs can be represented explicitly by the well-known formulas, for $1\leqslant l\leqslant K-1$

$$(E_l)_k := \sqrt{\frac{2}{Y}}\sin\frac{\pi l y_k}{Y} \quad \text{for} \quad 0\leqslant k\leqslant K, \quad \lambda_{l\delta} := \left(\frac{2}{\delta}\sin\frac{\pi\delta l}{2Y}\right)^2,$$

and the transforms $\mathcal{F}$ and $\mathcal{F}^{-1}$ can be effectively implemented by applying the discrete fast Fourier transform (FFT) with respect to sines.

For implementation of the scheme, it can be convenient to apply the transform $\mathcal{F}$ to the boundary condition (4.10) and thus rewrite this in the equivalent form for the Fourier coefficients $\Psi^{(l)}$, for $1\leqslant l\leqslant K-1$

$$\Psi_{J-1}^{(l),m}+\Psi_{J-1}^{(l),m-1} = (1+a_{0l}-ia_1)\Psi_J^{(l),m}+(1+a_{0l}+ia_1)\Psi_J^{(l),m-1}$$

$$-2h\left(\mathcal{F}\mathcal{S}^m\left\{\Psi_J^1,\dots,\Psi_J^m\right\}\right)^{(l)}, \tag{4.19}$$

where the real parameters a_{0l} and a_1 are given by the formulas

$$a_{0l} := \frac{h^2 V_{\infty l\delta}}{\hbar^2 B_{1\infty}} \quad \text{with} \quad V_{\infty l\delta} := V_\infty + \frac{\hbar^2}{2}B_{2\infty}\lambda_{l\delta}, \quad a_1 = \frac{2h^2}{\tau\hbar B_{1\infty}} > 0, \tag{4.20}$$

compare with formulas (2.22) and (2.23); a_1 is the same as above.

Now we consider the Crank-Nicolson scheme on the infinite mesh for the original problem (4.1)–(4.3)

$$i\hbar\overline{\partial}_t\Psi = \mathcal{H}_{\mathbf{h}}\overline{s}_t\Psi + F \quad \text{on} \quad \omega_{\mathbf{h},\infty}\times\omega^\tau, \tag{4.21}$$

$$\Psi^m|_{j=0}=0, \quad \Psi^m|_{k=0,K}=0 \quad \text{for} \quad m\geqslant 1, \tag{4.22}$$

$$\Psi^0 = \Psi_{\mathbf{h}}^0 \quad \text{on} \quad \overline{\omega}_{\mathbf{h},\infty}. \tag{4.23}$$

The given perturbation F is added to the right-hand side of (4.21) once again in order to analyze the stability of the scheme.

Let $H_{\mathbf{h}}$ be a Hilbert space consisting of complex-valued functions W defined on the mesh $\overline{\omega}_{\mathbf{h},\infty}$ such that $W|_{j=0}=0$, $W|_{j=j_0}\in \overset{\circ}{H}(\overline{\omega}_\delta)$ for any $j_0\geqslant 1$ and $\sum_{j=1}^\infty \|W_{jk}\|_{\omega_\delta}^2 < \infty$, equipped with the inner product

$$(U,W)_{H_{\mathbf{h}}} := \sum_{j=1}^{\infty}\sum_{k=1}^{K-1} U_{jk}W_{jk}^* h_{j+1/2}\delta_{k+1/2}.$$

PROPOSITION 4.3. *Let $F^m\in H_{\mathbf{h}}$ for any $m\geqslant 1$ and $\Psi_{\mathbf{h}}^0\in H_{\mathbf{h}}$. Then there exists a unique solution to the scheme (4.21)-(4.23) such that $\Psi^m\in H_{\mathbf{h}}$ for any $m\geqslant 0$, and the following stability bound holds*

$$\max_{0\leqslant m\leqslant M}\|\Psi^m\|_{H_{\mathbf{h}}} \leqslant \|\Psi_{\mathbf{h}}^0\|_{H_{\mathbf{h}}} + \frac{2}{\hbar}\sum_{m=1}^{M}\|F^m\|_{H_{\mathbf{h}}}\tau_m \quad \textit{for any} \quad M\geqslant 1. \tag{4.24}$$

Moreover, in the particular case $F=0$, the mass conservation law holds

$$\|\Psi^m\|_{H_{\mathbf{h}}}^2 = \|\Psi_{\mathbf{h}}^0\|_{H_{\mathbf{h}}}^2 \quad \textit{for any} \quad m\geqslant 1. \tag{4.25}$$

Proof. We extend $\mathcal{H}_{\mathbf{h}}$ to an operator in $H_{\mathbf{h}}$ by setting

$$\overset{\circ}{\mathcal{H}}_{\mathbf{h}} W := \mathcal{H}_{\mathbf{h}} W \quad \text{on} \quad \omega_{\mathbf{h},\infty} \quad \text{and} \quad \overset{\circ}{\mathcal{H}}_{\mathbf{h}} W := 0 \quad \text{on} \quad \overline{\omega}_{\mathbf{h},\infty} \backslash \omega_{\mathbf{h},\infty}.$$

The operator $\overset{\circ}{\mathcal{H}}_{\mathbf{h}}$ is bounded in H_h by taking account of assumption (4.4). Moreover, $\overset{\circ}{\mathcal{H}}_{\mathbf{h}}$ is self-adjoint since, for any $W, U \in H_{\mathbf{h}}$

$$\left(\overset{\circ}{\mathcal{H}}_{\mathbf{h}} W, U\right)_{H_{\mathbf{h}}} = \frac{\hbar^2}{2} \sum_{j=1}^{\infty} \sum_{k=1}^{K} \Big\{ \widetilde{B}_{11} \overline{s}_y \left[(\overline{\partial}_x W) \overline{\partial}_x U^* \right] + \widetilde{B}_{12} (\overline{s}_x \overline{\partial}_y W) \overline{\partial}_x \overline{s}_y U^*$$

$$+ \widetilde{B}_{21} (\overline{\partial}_x \overline{s}_y W) \overline{s}_x \overline{\partial}_y U^* + \widetilde{B}_{22} \overline{s}_x \left[(\overline{\partial}_y W) \overline{\partial}_y U^* \right] \Big\}_{jk} h_j \delta_k + (V_h W, U)_{H_{\mathbf{h}}}, \qquad (4.26)$$

compare with equalities (3.7) and (4.16). The rest of the proof is similar to one for Proposition 3.1. ∎

COROLLARY 4.4. *Bound (4.24) implies the uniform-norm bound*

$$\sup_{m \geqslant 0} \max_{j \geqslant 0, 0 \leqslant k \leqslant K} \left| \Psi_{jk}^m \right| \leqslant \frac{1}{\sqrt{h_{\min} \delta_{\min}}} \left(\|\Psi_{\mathbf{h}}^0\|_{H_{\mathbf{h}}} + \frac{2}{\hbar} \sum_{m=1}^{\infty} \|F^m\|_{H_{\mathbf{h}}} \tau_m \right).$$

COROLLARY 4.5. *Let $F^m = 0$ and $\Psi^0 = 0$ on $\omega_{\mathbf{h},\infty} \backslash \omega_{\mathbf{h}}$ for $m \geqslant 1$. If the solution to the scheme (3.1)-(3.3) such that $\Psi^m \in H_{\mathbf{h}}$, for any $m \geqslant 0$, satisfies relation (4.7) with some operator $\mathcal{S}$, then we have, for any $M \geqslant 1$*

$$\hbar B_{1\infty} \operatorname{Im} \sum_{m=1}^{M} \left(\mathcal{S}^m \left\{ \Psi_J^1, \ldots, \Psi_J^m \right\}, \overline{s}_t \Psi_J^m \right)_{\omega_\delta} \tau_m$$

$$= \|\Psi^M\|_{\omega_{\mathbf{h},\infty} \backslash \omega_{\mathbf{h}}}^2 := \frac{h}{2} \|\Psi_J^M\|_{\omega_\delta}^2 + \sum_{j=J+1}^{\infty} \|\Psi_j^M\|_{\omega_\delta}^2 h \geqslant 0.$$

Clearly, Corollaries 4.4 and 4.5 are counterparts of Corollaries 3.2 and 3.3, and also the identity holds

$$\|W\|_{H_{\mathbf{h}}}^2 = \|W\|_{\overline{\omega}_{\mathbf{h}}}^2 + \|W\|_{\omega_{\mathbf{h},\infty} \backslash \omega_{\mathbf{h}}}^2 \quad \text{for any} \quad W \in H_{\mathbf{h}}.$$

To construct the discrete 2D TBC, we consider the auxiliary finite-difference problem on the uniform in x part of the infinite mesh

$$i\hbar \overline{\partial}_t \Psi = \mathcal{H}_{\mathbf{h},\infty} \overline{s}_t \Psi \quad \text{on} \quad (\omega_{\mathbf{h},\infty} \backslash \omega_{\mathbf{h}}) \times \omega^\tau,$$

$$\Psi|_{j=J-1} \quad \text{is given}, \quad \sup_{m \geqslant 1} \max_{0 \leqslant k \leqslant K} |\Psi_{(J-1)k}^m| < \infty,$$

$$\Psi^m|_{k=0,K} = 0 \quad \text{on} \quad \omega_{h,\infty} \backslash \omega_h \quad \text{for} \quad m \geqslant 1,$$

$$\sup_{j \geqslant J-1, 0 \leqslant k \leqslant K, m \geqslant 0} |\Psi_{jk}^m| < \infty,$$

$$\Psi_{jk}^0 = 0 \quad \text{for} \quad j \geqslant J-1, \quad 0 \leqslant k \leqslant K,$$

which involves the limiting 2D mesh Hamiltonian operator

$$\mathcal{H}_{\mathbf{h},\infty}W := -\frac{\hbar^2}{2}\left(B_{1\infty}\widehat{\partial}_x\overline{\partial}_x W + B_{2\infty}\widehat{\partial}_y\overline{\partial}_y W\right) + V_\infty W \quad \text{on} \quad \omega_{\mathbf{h},\infty}\backslash\omega_{\mathbf{h}}.$$

Hereafter we assume that the time mesh $\overline{\omega}^\tau$ is uniform as well.

Following an idea from [6], we apply the transform $\mathcal{F}$ to the last problem and decompose this into the equivalent collection of the disjoint 1D problems for the Fourier coefficients $\Psi^{(l)}$, $1\leqslant l\leqslant K-1$

$$i\hbar\overline{\partial}_t\Psi^{(l)} = \mathcal{H}_{h,\infty}\overline{s}_t\Psi^{(l)} + \frac{\hbar^2}{2}B_{2\infty}\lambda_{l\delta}\overline{s}_t\Psi^{(l)} \quad \text{on} \quad (\omega_{h,\infty}\backslash\omega_h)\times\omega^\tau,$$

$$\Psi^{(l)}_{J-1} \text{ is given}, \quad \sup_{m\geqslant 1}|\Psi^{(l),m}_{J-1}|<\infty,$$

$$\sup_{j\geqslant J-1,\, m\geqslant 0}|\Psi^{(l),m}_j|<\infty,$$

$$\Psi^{(l),0}_j = 0 \quad \text{for} \quad j\geqslant J-1.$$

These are the same problems as the above 1D problem (3.12)-(3.15) but with the auxiliary potentials $V_{\infty l\delta}$, see (4.20), replacing V_∞.

By virtue of the 1D discrete TBC in the second form (3.31) we obtain

$$\left(\overset{\circ}{\partial}_x\overline{s}_t\Psi^{(l)}\right)_J = \frac{1}{2h}R_l * \Psi^{(l)}_J,$$

where the sequence R_l is described by the same formulas as R in Proposition 3.7 but with the parameter a_{0l} (see (4.20)) replacing the parameter a_0 (see (2.23)).

Applying the inverse transform $\mathcal{F}^{-1}$, we finally get the 2D discrete TBC of form (4.7)

$$\left(\overset{\circ}{\partial}_x\overline{s}_t\Psi\right)\Big|_{j=J} = \frac{1}{2h}\mathcal{F}^{-1}\left(R_l * \Psi^{(l)}_J\right), \tag{4.27}$$

that is, with

$$\mathcal{S}^m\left\{\Psi^1_J,\dots,\Psi^m_J\right\} = \frac{1}{2h}\mathcal{F}^{-1}\left(R_l * \Psi^{(l)}_J\right)^m \quad \text{for any} \quad m\geqslant 1. \tag{4.28}$$

Thus the system of equations (4.19) takes the form of *disjoint* equations, for $1\leqslant l\leqslant K-1$

$$\Psi^{(l),m}_{J-1} + \Psi^{(l),m-1}_{J-1} = (1+a_{0l}-ia_1)\Psi^{(l),m}_J + (1+a_{0l}+ia_1)\Psi^{(l),m-1}_J - \sum_{q=1}^m R_l^{m-q}\Psi^{(l),q}_J,$$

which are non-local only in time similarly to (2.22) in 1D case. These can be effectively coupled to a chosen iterative (or direct) method to compute Ψ^m.

Proposition 4.6. *For the 2D discrete TBC (4.27), inequality (4.14) holds.*

Proof. We can reduce 2D case to 1D one studied in the previous section. For any $M\geqslant 1$ and for any function Φ defined on $\overline{\omega}_\delta\times\overline{\omega}^\tau$ such that $\Phi^0=0$ and $\Phi|_{k=0,K}=0$, we have

$$\sum_{m=1}^M\left(\mathcal{F}^{-1}\left(R_l*\Phi^{(l)}\right)^m, \overline{s}_t\Phi^m\right)_{\omega_\delta}\tau = \sum_{m=1}^M\sum_{l=1}^{K-1}\left(R_l*\Phi^{(l)}\right)^m\left(\overline{s}_t\Phi^{(l),m}\right)^*\tau,$$

where identity (4.18) has been applied. Consequently by rearranging the sums and applying Proposition 3.6, for operator (4.28) we obtain

$$2h\,\mathrm{Im}\sum_{m=1}^{M}\left(\mathcal{S}^m\left\{\Phi^1,\ldots,\Phi^m\right\},\overline{s}_t\Phi^m\right)_{\omega_\delta}\tau=\sum_{l=1}^{K-1}\mathrm{Im}\sum_{m=1}^{M}\left(R_l*\Phi^{(l)}\right)^m\left(\overline{s}_t\Phi^{(l),m}\right)^*\tau\geqslant 0.$$

Thus the stability condition (4.14) for the 2D discrete TBC is verified. ☐

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