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Analysis of a Third-Order Absorbing Boundary Condition for the Schrödinger Equation Discretized in Space

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Abstract—In this paper, we consider the semidiscrete problem obtained when the Schrödinger equation is discretized in space with finite differences and a third-order absorbing boundary condition specific for this discretization, which has been developed recently in the literature, is used. The well posedness of this problem is analyzed, deducing that it is weakly ill posed similarly as when absorbing boundary conditions for the continuous equation are considered. Nevertheless, we show numerically that with the semidiscrete absorbing boundary condition bigger spatial step sizes can be used, which is essential due to the weak ill posedness of the problems.

Keywords—Absorbing boundary conditions, Well posedness, Schrödinger-type equations.

1. INTRODUCTION

Let us consider the Schrödinger-type equation given by

$$\partial_t u = -\frac{i}{c}\left(\partial_x^2 u + Vu\right), \qquad x \in \mathbf{R}, \quad t > 0, \tag{1}$$

with $c > 0$, $V \in \mathbf{R}$, whose importance is well known. In order to obtain a numerical solution of (1), it is essential to consider a finite spatial subdomain $[x_l, x_r]$ and use artificial boundary conditions, which should be adequate so that spurious reflections of the numerical solution at the boundary are as small as possible. One common technique is to use local absorbing boundary conditions (ABC), obtained by approximating the transparent, or reflection free, boundary conditions (TBC).

In [1], ABC for the continuous Schrödinger equation are developed, some of which had already been used in the literature [2]. They are obtained by approximating the TBC for the continuous equation (1) with interpolatory techniques and are denoted by ABC(j_1, j_2) when $j_1 + j_2 + 1$ interpolatory nodes are used. Moreover, $j_1 + j_2 + 1$ is called order of absorption. Although ABC

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for the wave equation had been obtained with similar techniques, giving rise to stable problems, with the Schrödinger equation the situation is quite different. In fact, in [1] it is proved that ABC$(1,0)$ gives rise to a weak ill-posed semidiscrete problem when the spatial step size h goes to zero. Moreover, in a recent paper [3], a general result on the eigenvalues of a class of matrices allows us to prove that the problem for ABC$(1,1)$ is also weakly ill posed. Although, in practice, this bad behaviour of the Schrödinger problem when $h \to 0$ can be compensated with a good discretization in time as it is showed in [1], it is important that a good absorption can be obtained for moderate values of h.

As an alternative, semidiscrete ABC are developed in [4] for a spatial discretization by finite differences of (1), with a similar spirit to that of [5] for the wave equation. This ABC is denoted by SABC(j_1, j_2) and depends on $j_1 + j_2 + 1$ interpolatory nodes. Moreover, an adaptive implementation of these SABC is developed in [6] so that the absorption is optimal. In this paper, we prove that the semidiscrete problem for the third-order SABC$(1,1)$ is weakly ill posed in a similar way to that for ABC$(1,1)$. Nevertheless, since SABC$(1,1)$ is specific of the spatial discretization, in order to obtain a certain absorption, it is possible to consider bigger values of the spatial step size than with ABC$(1,1)$, as it is shown in Section 2. This is essential, not only because of the saving of computational work, but also because of the weak instability of both problems.

The paper is organized as follows. In Section 2, we introduce SABC$(1,1)$ and it is shown numerically that, with this ABC, it is possible to obtain a good absorption with bigger spatial step sizes than those needed for ABC$(1,1)$. The well posedness of the semidiscrete problem obtained for SABC$(1,1)$ is studied in Section 3. For this, the stability of the matrix of the semidiscrete system with SABC$(1,1)$ is proved and a bound for the possible growth of the norm of the solution is obtained. The ϵ-pseudospectrum of the matrix is also analyzed in Section 3.

2. SEMIDISCRETE ABSORBING BOUNDARY CONDITIONS

In order to discretize (1) in space, let us consider a uniform mesh $\{x^j\}_{j\in\mathbf{Z}}$, where $x^j = x_l + jh$, and $h = (x_r - x_l)/N$ and let us denote by $u^j(t)$ an approximation to $u(x^j, t)$. We consider the following finite differences discretization of (1),

$$\frac{d}{dt}\, u^j(t) = \tilde{m}_1(h) u^{j-1}(t) + \tilde{m}_2(h) u^j(t) + \tilde{m}_1(h) u^{j+1}(t), \qquad j \in \mathbf{Z}, \tag{2}$$

with $\tilde{m}_1(h) = -i/ch^2$, $\tilde{m}_2(h) = i(2 - Vh^2)/ch^2$. For this semidiscrete equation, a general class of ABC are obtained in [4]. In particular, the third-order ones, SABC$(1,1)$, are given by

$$\frac{d}{dt}\, u^0 = \tilde{\alpha} u^0 + \tilde{\beta} u^1 + \tilde{\gamma} u^2, \qquad \frac{d}{dt}\, u^N = \tilde{\alpha} u^N + \tilde{\beta} u^{N-1} + \tilde{\gamma} u^{N-2}, \tag{3}$$

where, $\tilde{\alpha}$, $\tilde{\beta}$, and $\tilde{\gamma}$ depend on h and on the interpolatory nodes $s_1, s_2, s_3 \in (0, 4/h^2)$. If $s_1 = s_2 = s_3 = b$ (which is the right choice when the solution travels with a specific velocity), we have

$$\tilde{\alpha} = \frac{-3\sqrt{1-a^2} + i\left(-a + h^2(b - V)\right)}{ch^2}, \tag{4}$$

$$\tilde{\beta} = \frac{6a\sqrt{1-a^2} + 2i\left(-2 + 3a^2\right)}{ch^2}, \tag{5}$$

$$\tilde{\gamma} = \frac{ia\left(3 - 4a^2\right) + \sqrt{1-a^2}\,\left(1 - 4a^2\right)}{ch^2}, \tag{6}$$

with $a = 1 - h^2 b/2$, and where the value of b can be chosen optimal to absorb a specific velocity. Therefore, when we consider the spatial discretization of (1) in the interior domain $[x_l, x_r]$ given by (2) for $j = 1, \dots, N-1$ along with (3), we obtain a first-order system

$$u_h'(t) = M(h) u_h(t), \tag{7}$$

where $u_h(t) = (u^j(t))_{j=0}^N$ and

$$M(h) = \begin{bmatrix} \tilde{\alpha} & \tilde{\beta} & \tilde{\gamma} & 0 & \cdots & 0 \\ \tilde{m}_1 & \tilde{m}_2 & \tilde{m}_1 & 0 & \cdots & 0 \\ \vdots & & \ddots & \ddots & \ddots & \vdots \\ 0 & \cdots & 0 & \tilde{m}_1 & \tilde{m}_2 & \tilde{m}_1 \\ 0 & \cdots & 0 & \tilde{\gamma} & \tilde{\beta} & \tilde{\alpha} \end{bmatrix} \in \mathcal{M}_{(N+1)\times(N+1)}. \tag{8}$$

Finally, in order to obtain the numerical solution of the problem, system (7) must be solved by a time integrator method.

Let us see now the reason why, in practical situations, it is better to use SABC(1,1) than ABC(1,1), the third-order ABC for the continuous problem (see [3]). Let us consider the Fresnel equation,

$$2in_0k_0\partial_t u = \partial_x^2 u + \left(n^2 - n_0^2\right) k_0^2 u,$$

with $n = 1$, $n_0 = \cos(21.8^\circ)$, and $k_0 = 2\pi/0.832$, which is a particular case of the Schrödinger-type equation (1). We are going to take the initial condition $u_0(x) = \exp(-(\bar{x}/10)^2)\exp(-i\cos(\beta)k_0 \tan(15^\circ)\bar{x})$, $x \in [0, L]$, with $\bar{x} = x - L/2$ and $L = 200$, which gives rise to a solution traveling with a velocity $\tan(15^\circ)$. In Figure 1, we observe the results in terms of reflection (L^2 norm of the solution remaining inside the computational window) for SABC(1,1) and ABC(1,1). In all cases, the implicit midpoint rule is used for the integration in time with step size $k = 0.2$ and different values of h for the discretization in space are considered. We see that, while for SABC(1,1) the result is the same for different values of h, for ABC(1,1) the reflection is smaller when h decreases. This is due to the fact that SABC(1,1) is specific for the spatial discretization used, while this is not the case for ABC(1,1). This way, in order to obtain with ABC(1,1) approximately the same absorption as for SABC(1,1) with $h = 2.0d-2$, it is necessary to consider a much smaller step size $h = 1.0d-4$.

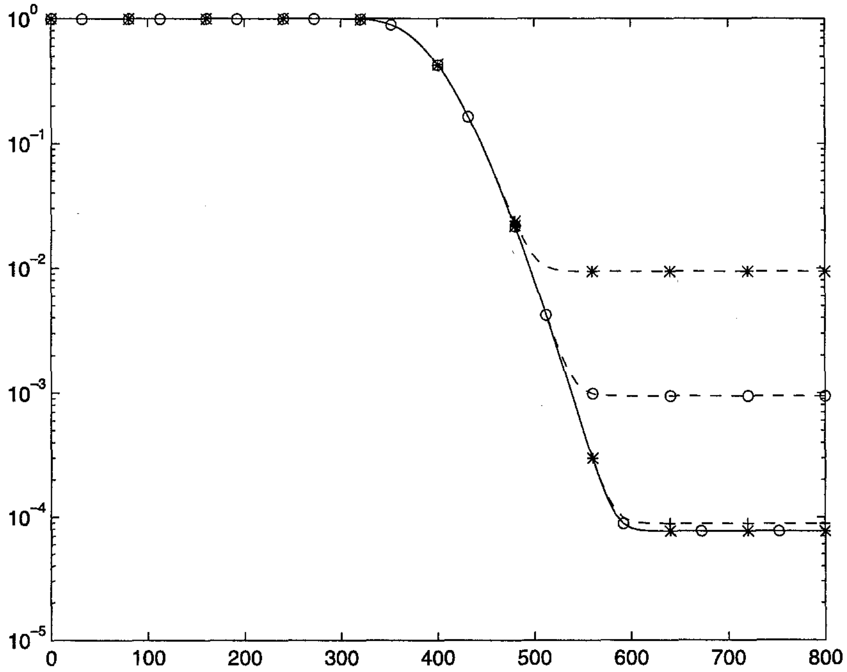


Figure 1. Reflection as a function of time. ABC(1,1): $--*$ $h = 2.0d-2$, $--\circ$ $h = 2.0d-3$, $--+$ $h = 1.0d-4$; SABC(1,1): $—*$ $h = 2.0d-2$, $—\circ$ $h = 2.0d-3$, $—+$ $h = 1.0d-4$.

In view of the advantages of SABC(1,1), let us study the well posedness of (7). It is well known that $\|u_h(t)\|^2 \le \exp(2\mu_2(M(h))t)\|u_h(0)\|^2$, where μ_2 denotes the logarithmic norm. Nevertheless, as it happens for ABC(1,1) (see [3]), $\mu_2(M(h))$ is positive and $O(1/h^2)$, so this bound would allow a catastrophic behaviour for $\|u_h(t)\|$. However, we are going to show that this bound overestimates the growth of $\|u_h(t)\|$ and, that in fact, the problem for SABC(1,1) is weakly ill posed in a similar way to that for ABC(1,1).

3. WELL POSEDNESS OF THE PROBLEM FOR SABC(1,1)

The first objective of this section is to study the stability of matrix (8). For this, let $M_{N+1}(h) \in \mathcal{M}_{(N+1)\times(N+1)}$ be a matrix with the structure of (8) and coefficients $\alpha(h), \beta(h), \gamma(h)-i, i(2-\delta(h))$ (instead of $\tilde{\alpha}, \tilde{\beta}, \tilde{\gamma}, \tilde{m}_1, \tilde{m}_2$, respectively), and let us consider the polynomials

$$\begin{aligned}
S_1^r(x) &= \left(-1+\gamma_i^2-\gamma_r^2\right)x^2 + 2\left(-\epsilon-\gamma_i-\beta_i\gamma_i+\beta_r\gamma_r\right)x \\
&\quad + \alpha_r^2+\beta_i^2-\beta_r^2-\epsilon^2-2\epsilon\gamma_i-\gamma_i^2-2\alpha_r\gamma_r+\gamma_r^2, \\
S_2^r(x) &= \left(-\gamma_i^2+\gamma_r^2\right)x^3 + \left(2\gamma_i+2\beta_i\gamma_i-2\beta_r\gamma_r\right)x^2 \\
&\quad + \left(-2\beta_i-\beta_i^2+\beta_r^2+2\epsilon\gamma_i+2\gamma_i^2+2\alpha_r\gamma_r-2\gamma_r^2\right)x \\
&\quad - 2\alpha_r\beta_r-2\beta_i\epsilon-2\beta_i\gamma_i+2\beta_r\gamma_r, \\
S_1^i(x) &= -\gamma_i\gamma_r x^2 + \left(-\alpha_r+\beta_r\gamma_i+\gamma_r+\beta_i\gamma_r\right)x - \beta_i\beta_r-\alpha_r\epsilon-\alpha_r\gamma_i+\epsilon\gamma_r+\gamma_i\gamma_r, \\
S_2^i(x) &= \gamma_i\gamma_r x^3 + \left(-\beta_r\gamma_i-\gamma_r-\beta_i\gamma_r\right)x^2 \\
&\quad + \left(\beta_r+\beta_i\beta_r+\alpha_r\gamma_i-\epsilon\gamma_r-2\gamma_i\gamma_r\right)x - \alpha_r\beta_i+\beta_r\epsilon+\beta_r\gamma_i+\beta_i\gamma_r,
\end{aligned} \tag{9}$$

with $\alpha_r = \Re(\alpha)$, $\alpha_i = \Im(\alpha)$, $\beta_r = \Re(\beta)$, $\beta_i = \Im(\beta)$, $\gamma_r = \Re(\gamma)$, $\gamma_i = \Im(\gamma)$, and $\epsilon = 2-\delta-\alpha_i$, where the dependence on h has been omitted in the notation.

In [3], the following theorem for the stability of the general matrix $M_{N+1}(h)$ is proved.

THEOREM 3.1. *Let us suppose that*

$$\alpha(h) = -i+\alpha_1 h+i\alpha_2 h^2+\alpha_3 h^3+h^4\alpha_4(h), \qquad \text{with } \alpha_1<0, \tag{10}$$

$$\beta(h) = 2i-2\alpha_1 h+i\beta_2 h^2+\beta_3 h^3+h^4\beta_4(h), \tag{11}$$

$$\gamma(h) = -i+\alpha_1 h+i\gamma_2 h^2+\gamma_3 h^3+h^4\gamma_4(h), \tag{12}$$

$$\delta(h) = h^2\delta_1+h^3 i\delta_2+h^4\delta_3(h) \in \mathbf{R}, \tag{13}$$

$$A = \beta_2+2\gamma_2>0, \qquad B=\alpha_3+\beta_3+\gamma_3-\delta_2>0, \qquad \alpha_1 A+B\neq 0, \tag{14}$$

$$0=\alpha_2+\beta_2+\gamma_2+\delta_1, \qquad \alpha_1(N-2)A-2\Re(\beta_3+2\gamma_3)+NB<0, \tag{15}$$

$$0 > 4\left(\frac{\Im\left(\alpha_4(0)+\beta_4(0)+i\delta_3(0)+\gamma_4(0)\right)}{B}-\frac{\Re(\gamma_2)}{\alpha_1}\right)+\frac{2(N-1)\alpha_1 A+B}{\alpha_1^2}. \tag{16}$$

Let X_j, $j=1,\dots,5$, be the roots of the equation

$$S_1^r(X)S_2^i(X)-S_1^i(X)S_2^r(X)=0, \tag{17}$$

where $S_k^r(x)$, $S_k^i(x)$, $k=1,2$, are given by (9) and assume that for $0<h<h_0$, $X_j \notin (-2,2)$, $j=1,\dots,5$. Let us assume that for each $j\in\{1,\dots,5\}$, one of the following properties is satisfied for $0<h<h_0$:

$$S_1^l(X_j)=0 \qquad \text{and} \qquad S_2^l(X_j)\neq 0, \tag{18}$$

$$S_1^l(X_j)\neq 0 \qquad \text{and} \qquad X_j<\min\left\{-2,-1-\frac{S_2^l(X_j)}{S_1^l(X_j)}\right\}, \tag{19}$$

$$S_1^l(X_j)\neq 0 \qquad \text{and} \qquad X_j>\max\left\{2,1-\frac{S_2^l(X_j)}{S_1^l(X_j)}\right\}, \tag{20}$$

for $l=r$ or $l=i$. Then, for every $h\in(0,h_0)$, all the eigenvalues of $M_{N+1}(h)$ have negative real part.

With the help of Theorem 1, we are going to prove the following result.

THEOREM 3.2. *Let us consider the matrix $M(h)$ associated to $SABC(1,1)$, given by (8) with (4)–(6). Then, for every $h \in (0, 2/\sqrt{b})$, all the eigenvalues of $M(h)$ have a negative real part.*

To prove this result, we are going to see that the coefficients of $ch^2M(h)$ (recall that $c > 0$) satisfy the hypotheses of Theorem 1 with $h_0 = 2/\sqrt{b}$. The matrix $ch^2M(h)$ is $M_{N+1}(h)$ with $\alpha = ch^2\tilde{\alpha}$, $\beta = ch^2\tilde{\beta}$, $\gamma = ch^2\tilde{\gamma}$, $\delta = Vh^2$, where $\tilde{\alpha}$, $\tilde{\beta}$, $\tilde{\gamma}$ are given by (4)–(6). In this way, the hypotheses (10)–(13) hold with $\alpha_1 = -3\sqrt{b}$, $\alpha_2 = 3b/2 - V$, $\alpha_3 = (3/8)b^{3/2}$, $\beta_2 = -6b$, $\beta_3 = (-15/4)b^{3/2}$, $\gamma_2 = 9b/2$, $\gamma_3 = (35/8)b^{3/2}$, $\delta_1 = V$, $\delta_2 = 0$, and $\alpha_4(0) = 0$, $\beta_4(0) = 3b^2i/2$, $\gamma_4(0) = -3ib^2$, $\delta_3 \equiv 0$. Therefore, (14) is fulfilled since $A = 3b > 0$, $B = b^{3/2} > 0$, and $\alpha_1 A + B = -8b^{3/2} \neq 0$. Moreover, we have that

$$\alpha_2 + \beta_2 + \gamma_2 + \delta_1 = 0,$$
$$\alpha_1(N-2)A - 2\Re(\beta_3 + 2\gamma_3) + NB = -8b^{3/2}(N-1) < 0,$$
$$4\left(\frac{\Im(\alpha_4(0) + \beta_4(0) + i\delta_3(0) + \gamma_4(0))}{B} - \frac{\Re(\gamma_2)}{\alpha_1}\right) + \frac{2(N-1)(\alpha_1 A + B)}{\alpha_1^2} = \frac{-16\sqrt{b}(N-1)}{9} < 0.$$

On the other hand, we have that

$$\alpha_r = -3\sqrt{1-a^2}, \qquad \alpha_i = -a + 2(1-a)\left(1 - \frac{V}{b}\right), \qquad \beta_r = 6a\sqrt{1-a^2},$$
$$\beta_i = 2\left(-2 + 3a^2\right), \qquad \gamma_r = \sqrt{1-a^2}\left(1 - 4a^2\right), \qquad \gamma_i = a\left(3 - 4a^2\right),$$
$$\delta = Vh^2, \qquad \epsilon = 2 - \delta - \alpha_i = 3a,$$

where $a = 1 - h^2b/2 \in (-1,1)$ (recall that $h \in (0, 2/\sqrt{b})$). Let us suppose first that $a \neq 0$, $\pm 1/2, \pm a_1$ with $a_1 = \sqrt{3}/2$. In this case, the roots of $S_1^r(x)S_2^i(x) - S_1^i(x)S_2^r(x)$ are

$$X_1 = \frac{2(-2+a)}{-1+2a}, \qquad X_2 = \frac{-2(2+a)}{1+2a}, \qquad X_3 = \frac{2\left(a + 2\sqrt{3}\left(1-a^2\right)\right)}{3-4a^2},$$
$$X_4 = \frac{2\left(a - 2\sqrt{3}\left(1-a^2\right)\right)}{3-4a^2}, \qquad X_5 = \frac{-2}{a}.$$

It can be proved with a direct calculus that

$$X_1 > 2, \quad \forall\, a \in \left(-1, \frac{1}{2}\right), \qquad X_1 < -2, \quad \forall\, a \in \left(\frac{1}{2}, 1\right),$$
$$X_2 > 2, \quad \forall\, a \in \left(-1, -\frac{1}{2}\right), \qquad X_2 < -2, \quad \forall\, a \in \left(-\frac{1}{2}, 1\right),$$
$$X_3 > 2, \quad \forall\, a \in (-1, -a_1) \cup (-a_1, a_1), \qquad X_3 < -2, \quad \forall\, a \in (a_1, 1),$$
$$X_4 > 2, \quad \forall\, a \in (-1, -a_1), \qquad X_4 < -2, \quad \forall\, a \in (-a_1, a_1) \cup (a_1, 1),$$
$$X_5 > 2, \quad \forall\, a \in (-1, 0), \qquad X_5 < -2, \quad \forall\, a \in (0, 1).$$

On the other hand, we have that

$$S_1^i(X_1) = 0, \qquad S_2^i(X_1) = \frac{32(1+2a)\left(1-a^2\right)^{7/2}}{(-1+2a)^2} \neq 0,$$

and then, (18) with $l = i$ holds for X_1. Similarly,

$$S_1^i(X_2) = 0, \qquad S_2^i(X_2) = \frac{-32(-1+2a)\left(1-a^2\right)^{7/2}}{(1+2a)^2} \neq 0,$$

and X_2 satisfies (18) with $l = i$. For the root X_3, we have that

$$S_1^i(X_3) = \frac{128a\left(1-a^2\right)^{5/2}(a+a_1)^2}{3-4a^2} \neq 0.$$

Let us see that (19) or (20) is satisfied. For $a \in (-1,-a_1) \cup (-a_1,a_1)$, $X_3 > 2$ and $\psi^i(X_3) = (1+a)g_1(a)/g_2(a)$ with

$$\begin{aligned}
g_1(a) &= 9 - 6\sqrt{3} - 36a + 18\sqrt{3}\,a + 36a^2 - 24\sqrt{3}\,a^2 - 16a^3 + 8\sqrt{3}\,a^3, \\
g_2(a) &= -9 - 12\sqrt{3}\,a + 16\sqrt{3}\,a^3 + 16a^4.
\end{aligned}$$

It can be checked that $g_1(a) > 0$ and $g_2(a) > 0$ for $a \in (-1,-a_1)$ and that $g_1(a) < 0$ and $g_2(a) < 0$ for $a \in (-a_1,a_1)$. Therefore, $\psi^i(X_3) > 0$ for $a \in (-1,-a_1) \cup (-a_1,a_1)$ and (20) holds. If $a \in (a_1,1)$, $X_3 < -2$, and $\varphi^i(X_3) = -(1-a)g_3(a)/g_2(a)$ with

$$g_3(a) = 9 + 6\sqrt{3} + 36a + 18\sqrt{3}\,a + 36a^2 + 24\sqrt{3}\,a^2 + 16a^3 + 8\sqrt{3}\,a^3 > 0,$$

for all $a \in (a_1,1)$. Moreover, since $g_2(a) > 0$ for $a \in (a_1,1)$, we have that $\varphi^i(X_3) < 0$ and (19) is satisfied with $l = i$.

Similarly, we have that

$$S_1^i(X_4) = \frac{128a\left(1-a^2\right)^{5/2}(a-a_1)^2}{3-4a^2} \neq 0.$$

If $a \in (-1,-a_1)$, $X_4 > 2$, and it can be seen that

$$\psi^i(X_4) = \frac{(1+a)\left(9+6\sqrt{3}-36a-18\sqrt{3}\,a+36a^2+24\sqrt{3}\,a^2-16a^3-8\sqrt{3}\,a^3\right)}{-9+12\sqrt{3}\,a-16\sqrt{3}\,a^3+16a^4} > 0,$$

so (20) is fulfilled with $l = i$. If $a \in (-a_1,a_1) \cup (a_1,1)$, $X_4 < -2$, and

$$\varphi^i(X_4) = \frac{-(1-a)\left(9-6\sqrt{3}+36a-18\sqrt{3}\,a+36a^2-24\sqrt{3}\,a^2+16a^3-8\sqrt{3}\,a^3\right)}{-9+12\sqrt{3}\,a-16\sqrt{3}\,a^3+16a^4} < 0,$$

and then (19) holds with $l = i$. Finally,

$$S_1^i(X_5) = \frac{16\left(1-a^2\right)^{5/2}\left(a^2-a_1^2\right)}{a} \neq 0.$$

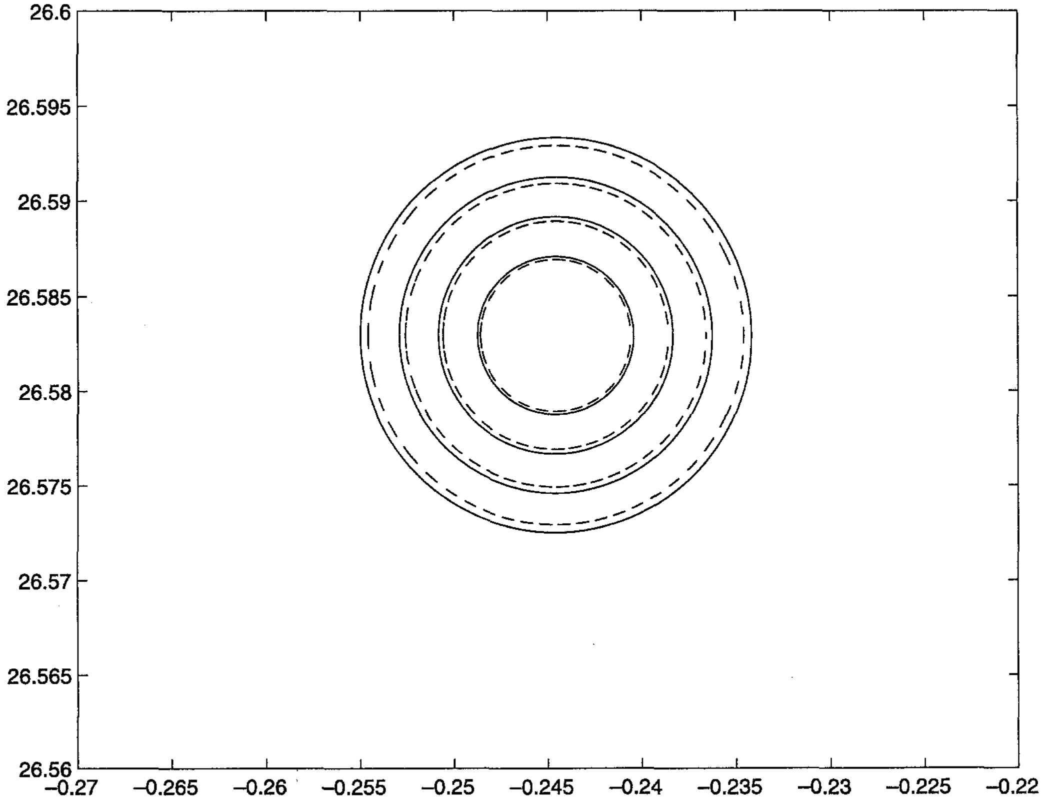
If $a \in (-1,0)$, (20) with $l = i$ is satisfied since $X_5 > 2$ and $\psi^i(X_5) = -1 - 1/a > 0$. If $a \in (0,1)$, $X_5 < -2$, and $\varphi^i(X_5) = 1 - 1/a < 0$ so (19) holds with $l = i$.

It only remains to check that in the particular cases $a = 0, \pm 1/2, \pm a_1$, the roots of (17) satisfy (18), (19), or (20). Let us suppose $a = 0$ (for $a = \pm 1/2, \pm a_1$ the proof is similar). Then, the roots of (17) are $X_a = -4 < -2, X_b = 4 > 2, X_c = -4/\sqrt{3} < -2, X_d = 4/\sqrt{3} > 2$. Since $S_1^i(X_a) = S_1^i(X_b) = 0$ and $S_2^i(X_a) = S_2^i(X_b) = 32 \neq 0$, X_a, and X_b satisfy (18) with $l = i$. On the other hand, $S_1^r(X_c) = S_1^r(X_d) = 64/3 \neq 0$ and $\varphi^r(X_c) = 1 - 2/\sqrt{3} < 0$, $\psi^r(X_d) = -1 + 2/\sqrt{3} > 0$, so X_c, X_d satisfy (19) and (20) with $l = r$, respectively. ∎

REMARK. Notice that the hypothesis $h \in (0, 2/\sqrt{b})$ is not a restriction since the interpolatory nodes are chosen equal to a value $b \in (0, 4/h^2)$ (see [4] for details).

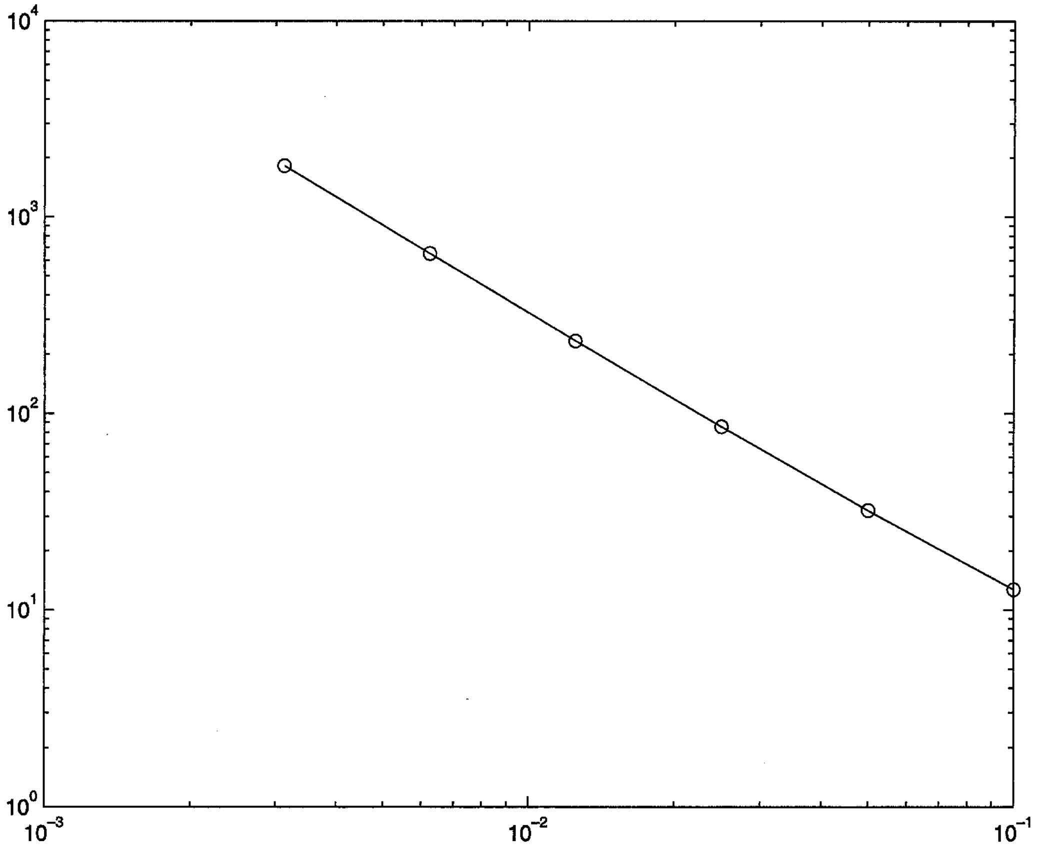
By Theorem 2, we can assure that the solution of (7) goes to zero as $t \to \infty$. Nevertheless, some caution should be taken, since if the character of nonnormality of $M(h)$ were very high, its spectrum would not describe properly the behaviour of $\|u_h(t)\|$. The study of the nonnormality of $M(h)$ can be done by analysing its ϵ-pseudospectrum [7], defined by $\Lambda_\epsilon(M(h)) = \{\mu_\epsilon \in \mathbf{C} : \mu_\epsilon$ is an eigenvalue of $M(h)+E$ for some E with $\|E\| \leq \epsilon\}$, for $\epsilon > 0$. This sets are ϵ-balls centered at the eigenvalues if the matrix is normal. Moreover, for a nonnormal matrix, the difference between its ϵ-pseudospectra and the ϵ-balls around its eigenvalues, indicates the degree of nonnormality of the matrix. We have carried out an analysis of the ϵ-pseudospectra of the matrix associated to SABC(1, 1), checking that its degree of nonnormality is weak. For instance, in Figure 2a, we see for an example, the boundaries of the ϵ-pseudospectra associated to the eigenvalue with biggest real part, which do not differ much of the ϵ-balls about the eigenvalue (dashed line).

However, a more precise analysis can be done in order to obtain a more realistic estimate for $\|u_h(t)\|$ than the bound involving the logarithmic norm. In fact, for the generic case when $M(h)$ is diagonalizable ($M(h) = LDL^{-1}$ with D diagonal), we have $\|u_h(t)\| \leq \kappa_h \|u_h(0)\|$ where κ_h is the condition number of L. A numerical study of κ_h shows (see Figure 2b) that $\kappa_h \approx O(h^{-3/2})$, leading to a bound for $\|u_h(t)\|$ similar to that obtained in [3] for ABC(1, 1). Therefore, we can conclude that, as the weak ill posedness of ABC(1, 1) and SABC(1, 1) is of the same degree, but with SABC(1, 1) higher values for h can be used, SABC(1, 1) should be preferred to ABC(1, 1).



(a) —Boundaries of ϵ-pseudospectra for the eigenvalue of matrix (8) with biggest real part – – ϵ-balls about the eigenvalue. $\epsilon = 1.0d-2, 8.0d-3, 6.0d-3, 4.0d-3$.

Figure 2.



(b) Condition number κ_h as a function of h for an example of matrix $M(h)$.

Figure 2. (cont.)

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