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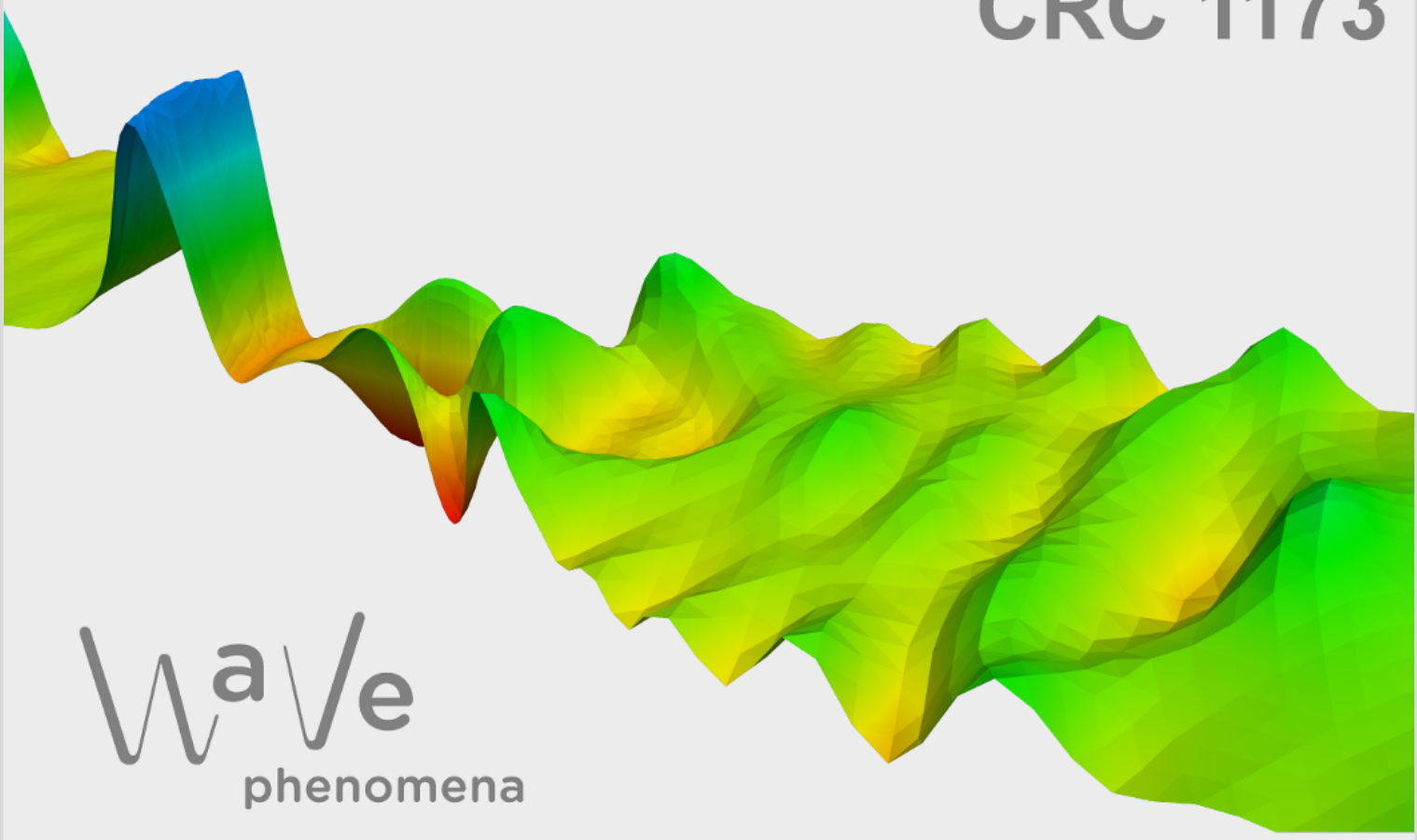

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On the convergence of Lawson methods for semilinear stiff problems

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Since their introduction in 1967, Lawson methods have attracted continuous interest for the time discretization of evolution equations. The popularity of these methods is in some contrast to the fact that they may have a bad convergence behaviour, since they do not satisfy any of the stiff order conditions. The aim of this paper is to explain this discrepancy. It is shown that non-stiff order conditions together with appropriate regularity assumptions imply high-order convergence of Lawson methods. Note, however, that the term regularity here includes the behaviour of the solution at the boundary. For instance, Lawson methods will behave well in the case of periodic boundary conditions, but they will show a dramatic order reduction for, e.g., Dirichlet boundary conditions. The precise regularity assumptions required for high-order convergence are worked out in this paper and related to the corresponding assumptions for splitting schemes. In contrast to previous work the analysis is based on expansions of the exact and the numerical solution along the flow of the homogeneous problem. Numerical examples for the Schrödinger equation are included.

Keywords: exponential integrators; Lawson methods; linear and nonlinear Schrödinger equations; evolution equations; order conditions.

1. Introduction

Exponential integrators are a well-established class of methods for the numerical solution of semilinear stiff differential equations. If the stiff initial value problem stems from a spatial semi-discretization of an evolutionary partial differential equation (PDE), the very form of the domain of the spatial differential operator enters the convergence analysis. The *stiff order conditions*, which guarantee a certain order of convergence independently of the considered problem, must of course be independent of the domain of this operator (which, in general, requires certain boundary conditions). This is the main reason why stiff order conditions for exponential integrators are quite involved (see Hochbruck & Ostermann (2005a) and Luan & Ostermann (2013)).

For particular problems, however, less conditions are required for obtaining a certain order of convergence. (The same is true for ordinary differential equations (ODEs), where linear problems, e.g., require less order conditions for Runge–Kutta methods than nonlinear ones.) It was already observed in Hochbruck & Ostermann (2005b) that periodic boundary conditions do not give any order reduction in exponential integrators of collocation type in contrast to homogeneous Dirichlet boundary conditions,

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which restrict the order of convergence considerably (close to the stage order, depending on the precise situation). Full-order convergence for periodic boundary conditions was also noticed in Kassam & Trefethen (2005) and Besse *et al.* (2015).

A similar behaviour can be observed for Lawson methods which are obtained by a linear variable transformation from (explicit) Runge–Kutta methods (see Lawson (1967) and Section 2 below). These methods are very attractive, since they can be easily constructed from any known Runge–Kutta method. Unfortunately, Lawson methods exhibit a strong order reduction, in general. For particular problems, however, they show full order of convergence (see Cano & González-Pachón (2015), Balac *et al.* (2016), and Montanelli & Bootland (2016)). By construction, Lawson methods do satisfy the order conditions for non-stiff problems. Such conditions will be called *non-stiff* or *conventional order conditions* henceforth. However, Lawson methods *do not* satisfy any of the stiff order conditions, as detailed in Hochbruck & Ostermann (2005a), Hochbruck & Ostermann (2010), and Luan & Ostermann (2013). This fact can result in a dramatic order reduction, even down to order one for parabolic problems with homogeneous Dirichlet boundary conditions.

So far, the derivation of (stiff) order conditions for exponential integrators was based on standard Taylor expansions of the exact and the numerical solution. There, the main assumption on the problem is that the exact solution and its composition with the nonlinearity are both sufficiently smooth in time (see Hochbruck & Ostermann (2005a) and Luan & Ostermann (2013)). Any additional regularity in space is not of immediate benefit in this analysis. This is in contrast to splitting methods, where spatial regularity usually shows up in form of commutator bounds (see, e.g., Jahnke & Lubich (2000)).

In this paper, we study the convergence behaviour of Lawson methods for semilinear problems. One of the main contributions of this paper is a different expansion of the solution based on the variation-of-constants formula. This expansion can be derived in a systematic way using trees as in Hairer *et al.* (1993) and Luan & Ostermann (2013). The expansion of the exact solution is carried out in terms of elementary integrals, that of the numerical solution in terms of elementary quadrature rules. We show that conventional, non-stiff order conditions together with (problem-dependent) assumptions on the exact solution give full order of convergence. This involves regularity of the solution in *space and time*. Our main result for Lawson methods is stated in Theorems 4.9 and 4.10. We prove that Lawson methods converge with order p, if the order of the underlying Runge–Kutta methods is at least p and the solution satisfies appropriate regularity assumptions. These conditions are studied in detail for methods of orders one and two, respectively, and they are related to the corresponding conditions that arise in the analysis of splitting methods. In particular, this is worked out for the nonlinear Schrödinger equation. Our error analysis also reveals a different behaviour between the first-order Lawson method and the exponential Euler method, which is visible in numerical experiments.

The outline of the paper is as follows. In Section 2, we recall the construction of Lawson methods. The expansion of the numerical and the exact solution in terms of elementary integrals is given in Section 3. There, we also introduce the analytic (finite dimensional) framework which typically occurs when discretizing a semilinear parabolic or hyperbolic PDEs in space. Order conditions and convergence results are given in Section 4. The resulting regularity assumptions are discussed in Section 5. These assumptions are related to the corresponding conditions for splitting methods. Numerical examples that illustrate the required regularity assumptions and the proven convergence behaviour are also presented.

2. Lawson methods

Consider a semilinear system of stiff differential equations

$$u'(t) = Au(t) + g\big(t, u(t)\big), \qquad u(0) = u_0, \tag{2.1}$$

where the stiffness stems from the linear part of the equation, i.e., the matrix A. The precise assumptions on A and g will be given in Section 3. For the numerical solution of (2.1), Lawson (1967) considered the following change of variables:

$$w(t) = \mathrm{e}^{-tA} u(t).$$

Inserting the new variables into (2.1) gives the transformed differential equation

$$w'(t) = \mathrm{e}^{-tA} g\big(t, \mathrm{e}^{tA} w(t)\big), \qquad w(0) = u_0. \tag{2.2}$$

For the solution of this problem, an s-stage explicit Runge–Kutta method with coefficients b_i, c_i, a_{ij} is considered. The method is assumed to satisfy the simplifying assumptions $c_1 = 0$ and

$$\sum_{j=1}^{i-1} a_{ij} = c_i, \qquad i = 2, \dots, s. \tag{2.3}$$

Transforming the Runge–Kutta discretization of (2.2) back to the original variables yields the corresponding Lawson method for (2.1)

$$U_{ni} = \mathrm{e}^{c_i hA} u_n + h \sum_{j=1}^{i-1} a_{ij} \mathrm{e}^{(c_i - c_j)hA} g(t_n + c_j h, U_{nj}), \qquad i = 1, \dots, s, \tag{2.4a}$$

$$u_{n+1} = \mathrm{e}^{hA} u_n + h \sum_{i=1}^{s} b_i \mathrm{e}^{(1-c_i)hA} g(t_n + c_i h, U_{ni}). \tag{2.4b}$$

Here, u_n is the numerical approximation to the exact solution $u(t)$ at time $t = t_n = nh$, and h is the step size. Note that this method makes explicit use of the action of the matrix exponential function. Depending on the properties of A, the nodes $c_1, \dots, c_s$ have to fulfill particular assumptions, see Assumption 3.1 in the next section. Because of these actions of the matrix exponential, Lawson methods form a particular class of exponential integrators. For a recent review on such integrators, we refer to Hochbruck & Ostermann (2010).

For a non-stiff ordinary differential equation (2.1), it is obvious that the order of the Runge–Kutta method applied to (2.2) coincides with that of the corresponding Lawson method applied to (2.1). It is the aim of this paper to show that this is also true in the stiff situation, if appropriate regularity assumptions hold (we will explain the meaning of regularity in the context of discretized PDEs in Section 5).

3. Expansion of the exact and the numerical solution

By adding $t' = 1$ to (2.1), the differential equation is transformed to autonomous form. It is well known that Runge–Kutta methods of order at least one satisfying (2.3) are invariant under this transformation. Therefore, we restrict ourselves henceforth to the autonomous problem

$$u'(t) = Au(t) + g\big(u(t)\big), \qquad u(0) = u_0. \tag{3.1}$$

Our main assumptions on A and g are as follows.

ASSUMPTION 3.1 Let A belong to a family of matrices $\mathscr{F}$ satisfying

$$\left\|\mathrm{e}^{tA}\right\| \leqslant C_{\mathscr{F}} \tag{3.2}$$

with a moderate constant $C_{\mathscr{F}}$, uniformly for all t. It is sufficient to require (3.2) for $t \geqslant 0$ if the nodes c_i of the considered explicit Runge–Kutta method are ordered as $0 = c_1 \leqslant c_2 \leqslant \ldots \leqslant c_s \leqslant 1$.

This assumption is typically satisfied in situations where (3.1) stems from a spatial discretization of a semilinear parabolic or hyperbolic partial differential equation. The important fact here is that the constant $C_{\mathscr{F}}$ is independent of the spatial mesh width for finite difference and finite element methods, and independent of the number of ansatz functions in spectral methods. Hence the set $\mathscr{F}$ contains all matrices resulting from any of these discretizations on arbitrarily refined meshes.

ASSUMPTION 3.2 The nonlinearity g is sufficiently smooth in a neighborhood of the solution of (3.1).

We illustrate our assumptions with the following example.

EXAMPLE 3.3 Consider the parabolic initial-boundary value problem

$$w_t = w_{xx} + w(1-w), \qquad 0 < x < 1, \quad 0 < t \leqslant T, \tag{3.3}$$

with initial value $w(0,x) = w_0(x)$ and homogeneous Dirichlet boundary conditions $w(t,0) = w(t,1) = 0$. For $N \in \mathbb{N}$, let $\Delta x = \frac{1}{N+1}$ be the spatial grid size and $x_k = k\Delta x$, $k = 0, \ldots, N+1$ be the grid points. Discretizing the second derivative by standard symmetric finite differences gives the following semilinear problem in the space $X = \mathbb{R}^N$:

$$u' = Au + g(u), \qquad u(0) = \big[w_0(x_1), w_0(x_2), \ldots, w_0(x_N)\big]^{\mathsf{T}}, \tag{3.4}$$

where

$$A = \frac{1}{\Delta x^2}\begin{bmatrix} -2 & 1 & & 0 \\ 1 & \ddots & \ddots & \\ & \ddots & \ddots & 1 \\ 0 & & 1 & -2 \end{bmatrix}, \qquad g(u) = \begin{bmatrix} u_1(1-u_1) \\ u_2(1-u_2) \\ \cdots \\ u_N(1-u_N) \end{bmatrix}.$$

We endow X with the weighted Euclidian norm

$$\|u\| = \sqrt{\tfrac{1}{N}\textstyle\sum_{j=1}^{N} u_j^2}.$$

Then, the above assumptions are satisfied and, in particular, $C_{\mathscr{F}} = 1$ for all $N \in \mathbb{N}$.

Regularity properties of the partial differential equation (3.3) translate into boundedness results, uniformly in N, for the spatially discrete problem (3.4). For example, that the initial value w_0 lies in the domain of the Laplacian (considered with homogeneous Dirichlet boundary conditions) means on the discrete level that Au_0 is bounded uniformly for all matrices A in the family $\mathscr{F}$. In particular, it is independent of the dimension N. This excludes, for instance, any constant vector different from zero. A numerical example is given in Section 5.5 below.

We recall that the solution of (3.1) can be represented in terms of the variation-of-constants formula

$$u(t) = \mathrm{e}^{tA}u_0 + \int_0^t \mathrm{e}^{(t-\sigma)A} g\big(u(\sigma)\big)\,\mathrm{d}\sigma.$$

Applying this formula recursively and expanding the nonlinearity along the flow of the homogeneous problem yields the following expansion of the exact solution

$$\begin{aligned} u(h) &= \mathrm{e}^{hA}u_0 + h\int_0^1 \mathrm{e}^{(1-\sigma)hA} g\Big(\mathrm{e}^{\sigma hA}u_0 + h\int_0^\sigma \mathrm{e}^{(\sigma-\eta)hA} g\big(u(\eta h)\big)\mathrm{d}\eta\Big)\mathrm{d}\sigma \\ &= \mathrm{e}^{hA}u_0 + h\int_0^1 \mathrm{e}^{(1-\sigma)hA} g_\sigma \mathrm{d}\sigma \\ &\quad + h^2\int_0^1 \mathrm{e}^{(1-\sigma)hA} g'_\sigma \int_0^\sigma \mathrm{e}^{(\sigma-\eta)hA} g_\eta \mathrm{d}\eta\mathrm{d}\sigma \\ &\quad + h^3\int_0^1 \mathrm{e}^{(1-\sigma)hA} g'_\sigma \int_0^\sigma \mathrm{e}^{(\sigma-\eta)hA} g'_\eta \int_0^\eta \mathrm{e}^{(\eta-\xi)hA} g_\xi \mathrm{d}\xi\mathrm{d}\eta\mathrm{d}\sigma \\ &\quad + \tfrac{1}{2}h^3\int_0^1 \mathrm{e}^{(1-\sigma)hA} g''_\sigma \Big[\int_0^\sigma \mathrm{e}^{(\sigma-\eta)hA} g_\eta \mathrm{d}\eta, \int_0^\sigma \mathrm{e}^{(\sigma-\xi)hA} g_\xi \mathrm{d}\xi\Big]\mathrm{d}\sigma + \mathscr{O}(h^4), \end{aligned} \tag{3.5}$$

where we have used the short notation

$$g_\eta = g\big(\mathrm{e}^{\eta hA}u_0\big), \qquad g_\eta^{(k)} = g^{(k)}\big(\mathrm{e}^{\eta hA}u_0\big), \qquad k \geqslant 1. \tag{3.6}$$

Note that here and throughout the whole paper, the constant in the Landau symbol $\mathscr{O}$ only depends on $C_{\mathscr{F}}$ and the derivatives of g, but not explicitly on A itself. This expansion differs considerably from the previous work (see, e.g., Hochbruck & Ostermann (2005a); Luan & Ostermann (2013)) where the nonlinearity $g(u(t))$ was expanded with respect to t.

Next we perform a similar expansion of the numerical solution (2.4), which yields (again in the autonomous case)

$$\begin{aligned} u_1 &= \mathrm{e}^{hA}u_0 + h\sum_{i=1}^s b_i \mathrm{e}^{(1-c_i)hA} g_{c_i} \\ &\quad + h^2\sum_{i=1}^s b_i \mathrm{e}^{(1-c_i)hA} g'_{c_i} \sum_{j=1}^{i-1} a_{ij}\mathrm{e}^{(c_i-c_j)hA} g_{c_j} \\ &\quad + h^3\sum_{i=1}^s b_i \mathrm{e}^{(1-c_i)hA} g'_{c_i} \sum_{j=1}^{i-1} a_{ij}\mathrm{e}^{(c_i-c_j)hA} g'_{c_j} \sum_{k=1}^{j-1} a_{jk}\mathrm{e}^{(c_j-c_k)hA} g_{c_k} \\ &\quad + \tfrac{1}{2}h^3\sum_{i=1}^s b_i \mathrm{e}^{(1-c_i)hA} g''_{c_i} \Big[\sum_{j=1}^{i-1} a_{ij}\mathrm{e}^{(c_i-c_j)hA} g_{c_j}, \sum_{k=1}^{i-1} a_{ik}\mathrm{e}^{(c_i-c_k)hA} g_{c_k}\Big] + \mathscr{O}(h^4). \end{aligned} \tag{3.7}$$

As we have used the variation-of-constants formula and its discrete counterpart, respectively, the expansions of the exact and numerical solutions reflect the well-known tree structure of (explicit) Runge–Kutta methods, see (Hairer *et al.*, 1993, Sect. II.2). This allows us to study the local error in the same way as for classical Runge–Kutta methods. Exploiting this fact leads to short and elegant proofs as detailed in the next section. Moreover, a term-by-term comparison of (3.5) and (3.7) reveals that the single terms in (3.7) can be interpreted as multivariate quadrature formulas for the corresponding multivariate integrals in (3.5). Consequently, the orders of these quadrature rules determine the local error of the Lawson method. A similar strategy was used in the analysis of splitting methods by Jahnke & Lubich (2000).

4. Order conditions and convergence

In this section we present a systematic way of deriving general stiff convergence results for Lawson methods based on trees. Here we use the same trees which are well-established for the non-stiff order conditions for Runge–Kutta methods, see (Hairer *et al.*, 1993, Section II.2) and references given there. General stiff order conditions for exponential Runge–Kutta methods have been derived in Luan & Ostermann (2013) and for splitting methods in Hansen & Ostermann (2016).

By $\mathscr{T}$ we denote the set of unlabeled trees (Hairer *et al.*, 1993, Section II.2). We recall that trees are defined recursively by

(1) $\bullet \in \mathscr{T}$,

(2) if $\tau_1,\dots,\tau_k \in \mathscr{T}$, then $[\tau_1,\dots,\tau_k] \in \mathscr{T}$.

Here, $[\tau_1,\dots,\tau_k]$ (a k tuple without ordering) denotes the tree which is obtained by concatenating the roots of the trees $\tau_1,\dots,\tau_k$ via k branches with a new node. This node becomes the root of the tree $[\tau_1,\dots,\tau_k]$.

For $\tau \in \mathscr{T}$ the elementary differential $D(\tau)$ of a smooth function g is defined recursively. For $\tau = \bullet$ we have $D(\bullet)(w) = g\big(w\big)$ and for $\tau = [\tau_1,\dots,\tau_k]$ we have

$$D(\tau)(w) = g^{(k)}\big(w\big)\big[D(\tau_1)(w),\dots,D(\tau_k)(w)\big].$$

By $\rho(\tau)$ we denote the order of the tree τ which is defined as the number of nodes of $\tau \in \mathscr{T}$.

Motivated by the expansion (3.5) of the exact solution we define elementary integrals.

DEFINITION 4.1 For $\tau \in \mathscr{T}$ and $0 \leqslant \zeta \leqslant 1$ we define the *elementary integral* $G_\zeta(\tau)$ recursively in the following way.

(1) For $\tau = \bullet$ we set

$$G_\zeta(\bullet)(w) = \int_0^\zeta \mathrm{e}^{(\zeta-\sigma)hA} g\big(\mathrm{e}^{\sigma hA} w\big)\mathrm{d}\sigma.$$

(2) For $\tau = [\tau_1,\dots,\tau_k]$ we set

$$G_\zeta(\tau)(w) = \int_0^\zeta \mathrm{e}^{(\zeta-\sigma)hA} g^{(k)}\big(\mathrm{e}^{\sigma hA} w\big)\big[G_\sigma(\tau_1)(w),\dots,G_\sigma(\tau_k)(w)\big]\mathrm{d}\sigma.$$

Moreover, we also need the integrand of such an elementary integral which is defined as follows.

DEFINITION 4.2 For $\tau \in \mathscr{T}$ we set $G(\tau) = G_1(\tau)$. The integrand of $G(\tau)(w)$ is denoted by $\Psi(\tau)(\cdot, w)$.

Note that $G(\tau)$ is a $\rho(\tau)$-fold multivariate integral and thus $\Psi(\tau)$ is a function of $\rho(\tau)$ variables. For example, $\bullet\!\!\swarrow = [\bullet]$ and

$$\Psi(\bullet\!\!\swarrow)(\sigma_1,\sigma_2,w) = \mathrm{e}^{(1-\sigma_1)hA} g'_{\sigma_1}(w)\mathrm{e}^{(\sigma_1-\sigma_2)hA} g_{\sigma_2}(w).$$

Our assumptions on g and A ensure that the integrand $\Psi(\tau)$ is bounded.

The following theorem shows how the expansion (3.5) can be expressed in terms of elementary integrals.

THEOREM 4.3 The solution of (3.1) formally satisfies

$$u(h) = \mathrm{e}^{hA}u_0 + \sum_{\tau\in\mathscr{T}} h^{\rho(\tau)}\alpha(\tau)G(\tau)(u_0) \tag{4.1}$$

with certain coefficients $\alpha(\tau)$ which are independent of the differential equation (3.1). If g is sufficiently smooth, we have

$$u(h) = \mathrm{e}^{hA}u_0 + \sum_{\substack{\tau\in\mathscr{T}\\ \rho(\tau)\leqslant k}} h^{\rho(\tau)}\alpha(\tau)G(\tau)(u_0) + \mathscr{O}(h^{k+1}). \tag{4.2}$$

Proof. The theorem follows immediately by observing that we have the following isomorphism:

$$\tau \simeq D(\tau) \simeq G(\tau).$$

The remainder in (4.2) is bounded if g is sufficiently smooth. □

Now we proceed analogously for the numerical solution starting with the definition of elementary quadrature formulas.

DEFINITION 4.4 For $\tau \in \mathscr{T}$ we define the *elementary quadrature formula* $\widehat{G}(\tau)$ recursively in the following way.

(1) For $\tau = \bullet$ we set

$$\widehat{G}(\bullet)(w) = \sum_{i=1}^{s} b_i \mathrm{e}^{(1-c_i)hA} g\big(\mathrm{e}^{c_i hA}w\big),$$
$$\widehat{G}_i(\bullet)(w) = \sum_{j=1}^{i-1} a_{ij} \mathrm{e}^{(c_i-c_j)hA} g\big(\mathrm{e}^{c_j hA}w\big).$$

(2) For $\tau = [\tau_1,\dots,\tau_k]$ we set

$$\widehat{G}(\tau)(w) = \sum_{i=1}^{s} b_i \mathrm{e}^{(1-c_i)hA} g^{(k)}\big(\mathrm{e}^{c_i hA}w\big)\big[\widehat{G}_i(\tau_1)(w),\dots,\widehat{G}_i(\tau_k)(w)\big],$$
$$\widehat{G}_i(\tau)(w) = \sum_{j=1}^{i-1} a_{ij} \mathrm{e}^{(c_i-c_j)hA} g^{(k)}\big(\mathrm{e}^{c_j hA}w\big)\big[\widehat{G}_j(\tau_1)(w),\dots,\widehat{G}_j(\tau_k)(w)\big].$$

As usual, the value of any empty sum is defined as zero.

This definition allows us to express the expansion (3.7) of the numerical solution in terms of elementary quadrature rules.

THEOREM 4.5 The numerical solution of (3.1) formally satisfies

$$u_1 = \mathrm{e}^{hA}u_0 + \sum_{\tau\in\mathscr{T}} h^{\rho(\tau)}\alpha(\tau)\widehat{G}(\tau)(u_0)$$

with the same coefficients $\alpha(\tau)$ as for the exact solution in Theorem 4.3. If g is sufficiently smooth, we have

$$u_1 = \mathrm{e}^{hA}u_0 + \sum_{\substack{\tau\in\mathscr{T}\\ \rho(\tau)\leqslant k}} h^{\rho(\tau)}\alpha(\tau)\widehat{G}(\tau)(u_0) + \mathscr{O}(h^{k+1}).$$

Proof. The proof follows from the observation that the numerical solution (2.4) is of the same structure as the exact solution if one replaces all integrals in the iterated variation-of-constants formula by quadrature formulas.

Hence we obtain an isomorphism

$$\tau \simeq D(\tau) \simeq G(\tau) \simeq \widehat{G}(\tau).$$

The truncated expansion follows by the assumption on the smoothness of g. □

As usual, we say that the Lawson method is of (stiff) order p if the local error satisfies

$$\|u(h) - u_1\| \leqslant Ch^{p+1}$$

uniformly for all matrices of the family $\mathscr{F}$, meaning that the constant C depends on the constant $C_{\mathscr{F}}$ defined in (3.2) but not on A itself.

THEOREM 4.6 The Lawson method (2.4) is of order p if

$$\widehat{G}(\tau)(u_0) - G(\tau)(u_0) = \mathscr{O}(h^{p+1-\rho(\tau)}), \qquad \text{for all } \tau \in \mathscr{T}, \quad \rho(\tau) \leqslant p.$$

Proof. This follows immediately from Theorems 4.3 and 4.5. □

EXAMPLE 4.7 The above derivation can be easily generalized to exponential integrators using fixed linearization

$$U_i = \mathrm{e}^{c_i hA} u_0 + h \sum_{j=1}^{i-1} a_{ij}(hA) g(U_j), \qquad i = 1, \dots, s,$$

$$u_1 = \mathrm{e}^{hA} u_0 + h \sum_{i=1}^{s} b_i(hA) g(U_i),$$

cf. Hochbruck & Ostermann (2010). If one replaces $b_i \mathrm{e}^{(1-c_i)hA}$ by $b_i(hA)$ and $a_{ij}\mathrm{e}^{(c_i-c_j)hA}$ by $a_{ij}(hA)$ in Definition 4.4, Theorems 4.5 and 4.6 also hold for general exponential Runge–Kutta methods. If the stiff order conditions derived in Hochbruck & Ostermann (2005a) and Luan & Ostermann (2013) are satisfied up to order p, then $\widehat{G}(\tau)(u_0) - G(\tau)(u_0) = \mathscr{O}(h^{p+1-\rho(\tau)})$ for all $\tau \in \mathscr{T}$, $\rho(\tau) \leqslant p$.

EXAMPLE 4.8 For the exponential Euler method, where $s = 1$, $c_1 = 0$, and $b_1(z) = \varphi_1(z)$, we have

$$\widehat{G}(\tau)(u) - G(\tau)(u) = \int_0^1 \mathrm{e}^{(1-\sigma)hA} \big(g(u) - g_\sigma\big) \mathrm{d}\sigma.$$

The condition for order one requires that $\|g(u) - g_\sigma(u)\| \leqslant Ch$. In the linear case, where $g(w) = Bw$, this can be written as

$$h^{-1}\big(g(u) - g_\sigma(u)\big) = h^{-1}B\big(I - \mathrm{e}^{\sigma hA}\big)u = -B\varphi_1(\sigma hA)\sigma Au. \tag{4.3}$$

Hence the condition is fulfilled if Au is uniformly bounded and, in particular, independent of $\|A\|$.

It might be interesting to compare (4.3) to the condition given in (Hochbruck & Ostermann, 2010, Lemma 2.13) which was proved by a Taylor series expansion of $g\big(u(t)\big)$. For linear problems, it reads

$$\|B(Au + Bu)\| \leqslant C. \tag{4.4}$$

Hence both results require the same regularity, namely that Au is uniformly bounded. Note, however, that (4.4) does not involve the φ_1 function. The latter decays like $1/z$ as $z \to \infty$ in the closed left half-plane.

The following theorem provides a sufficient condition for Lawson methods being of (stiff) order p.

THEOREM 4.9 Let

$$\Psi(\tau)\big(\cdot,u(t)\big) \in C^{p-\rho(\tau),1}\big([0,1]^{\rho(\tau)},X\big) \qquad \text{for all } \tau \in \mathscr{T} \text{ with } \rho(\tau) \leqslant p, \tag{4.5}$$

where $u(t) \in X$ is the solution of (3.1), $0 \leqslant t \leqslant T$. If the underlying Runge–Kutta method is of (conventional) order p, then the Lawson method (2.4) is of (stiff) order p.

Proof. Let $\rho = \rho(\tau)$. We expand $\Psi(\tau)$ into a Taylor polynomial of degree $p+1-\rho$. By assumption on $\Psi(\tau)$, the coefficients and the remainder of this Taylor polynomial are bounded. The multivariate quadrature formula $\widehat{G}(\tau)$ is exact for all polynomials of degree $p+1-\rho$. This can be seen from considering a non-stiff ordinary differential equation, for which it is known that the method is of order p. This proves the theorem. □

This result now allows us to prove an error bound for Lawson methods which is uniform for all problems (3.1) with $A \in \mathscr{F}$.

THEOREM 4.10 Let u be the solution of (3.1) and let the assumptions of Theorem 4.9 be satisfied. If the underlying Runge–Kutta method is of (conventional) order p, then there exists $h_0 > 0$ such that for all $0 < h \leqslant h_0$ sufficiently small,

$$\|u(t_n) - u_n\| \leqslant Ch^p, \qquad t_n = nh \leqslant T,$$

where C and h_0 are independent of n, h, and A.

Proof. We define a norm by

$$\|v\|_\star = \sup_{t\in\mathbb{R}} \left\|\mathrm{e}^{tA}v\right\|.$$

This norm is equivalent to $\|\cdot\|$ and we have

$$\left\|\mathrm{e}^{tA}\right\| \leqslant 1, \qquad \text{for all } t \in \mathbb{R}. \tag{4.6}$$

By assumption, g is locally Lipschitz continuous. Then (4.6) shows that the Lawson method is locally Lipschitz with respect to the initial value with a Lipschitz constant of size $1+\mathscr{O}(h)$. This implies the required stability.

The error bound follows in a standard way using Lady Windermere's fan. □

5. Regularity conditions and applications

It remains to discuss the regularity conditions (4.5) and to give some applications. We first examine the conditions for orders one and two, respectively. The extension to higher orders is a tedious but straightforward exercise. It turns out that these regularity conditions can all be expressed in terms of commutators, very much like in the case of splitting methods.

In order to obtain simple sufficient conditions, we replace the space $C^{k,1}(\Omega,X)$ in condition (4.5) by the subspace of $k+1$ times partially differentiable functions with uniformly bounded partial derivatives on Ω in the following discussion. This is also justified by the fact that Lipschitz continuous functions are almost everywhere differentiable (Rademacher's theorem).

5.1 *Condition for order one*

Since $p = \rho(\tau) = 1$, we only have to consider the tree $\tau = \bullet$ in (4.5). Differentiating

$$\Psi(\bullet)(\sigma, w) = \mathrm{e}^{(1-\sigma)hA} g_\sigma(w)$$

with respect to σ yields

$$\begin{aligned} \partial_\sigma \Psi(\bullet)(\sigma, w) &= h\mathrm{e}^{(1-\sigma)hA}\Big(g'_\sigma(w)A\mathrm{e}^{\sigma hA}w - Ag_\sigma(w)\Big) \\ &= h\mathrm{e}^{(1-\sigma)hA}[g,A]\big(\mathrm{e}^{\sigma hA}w\big), \end{aligned} \tag{5.1}$$

where $[g,A]$ denotes the Lie commutator of g and A, defined as

$$[g,A](w) = g'(w)Aw - Ag(w).$$

From this calculation, we conclude the following result. If the bound

$$\sup_{0\leqslant\sigma\leqslant 1}\ \sup_{0\leqslant t\leqslant T}\ \Big\|\mathrm{e}^{(1-\sigma)hA}[g,A]\big(\mathrm{e}^{\sigma hA}u(t)\big)\Big\| \leqslant C \tag{5.2}$$

holds with a constant C that is allowed to depend on $C_{\mathscr{F}}$, but *not* on $\|A\|$, then a Lawson method of non-stiff order *one* has also *stiff* order *one*.

5.2 *Conditions for order two*

Stiff order two is achieved if we require the following two regularity conditions

$$\Psi(\bullet)(\cdot, u(t)) \in C^{1,1}([0,1], X) \qquad \text{and} \qquad \Psi(\swarrow\!\!\bullet)(\cdot, u(t)) \in C^{0,1}([0,1]^2, X).$$

Again, we work with a slightly stronger regularity assumption on Ψ. We commence with the first condition. Differentiating (5.1) once more with respect to σ yields

$$\begin{aligned} \partial_\sigma^2 \Psi(\bullet)(\sigma, w) = h^2\mathrm{e}^{(1-\sigma)hA}\Big(&-2Ag'_\sigma(w)A\mathrm{e}^{\sigma hA}w + A^2 g_\sigma(w) \\ &+ g''_\sigma(A\mathrm{e}^{\sigma hA}w, \mathrm{e}^{\sigma hA}Aw) + g'_\sigma(w)A^2\mathrm{e}^{\sigma hA}w\Big), \end{aligned}$$

which again can be expressed with the help of a commutator,

$$\partial_\sigma^2 \Psi(\bullet)(\sigma, w) = h^2\mathrm{e}^{(1-\sigma)hA}\big[A,[A,g]\big]\big(\mathrm{e}^{\sigma hA}w\big).$$

This calculation shows that the bound

$$\sup_{0\leqslant\sigma\leqslant 1}\ \sup_{0\leqslant t\leqslant T}\ \Big\|\mathrm{e}^{(1-\sigma)hA}\big[A,[A,g]\big]\big(\mathrm{e}^{\sigma hA}u(t)\big)\Big\| \leqslant C \tag{5.3}$$

should hold with a constant C that is independent of $\|A\|$.

Next, we move to the second condition. Differentiating

$$\Psi(\swarrow\!\!\bullet)(\sigma_1, \sigma_2, w) = \mathrm{e}^{(1-\sigma_1)hA} g'_{\sigma_1}(w)\mathrm{e}^{(\sigma_1-\sigma_2)hA} g_{\sigma_2}(w)$$

with respect to σ_1 and σ_2 yields

$$\begin{aligned}\partial_{\sigma_1}\Psi(\bullet\!\!\!\!\bullet)(\sigma_1,\sigma_2,w) &= h\mathrm{e}^{(1-\sigma_1)hA}\Big(-Ag'_{\sigma_1}(w)\mathrm{e}^{(\sigma_1-\sigma_2)hA}g_{\sigma_2}(w)\\ &\qquad + g''_{\sigma_1}(w)\big(\mathrm{e}^{\sigma_1 hA}Aw,\mathrm{e}^{(\sigma_1-\sigma_2)hA}g_{\sigma_2}(w)\big) + g'_{\sigma_1}(w)\mathrm{e}^{(\sigma_1-\sigma_2)hA}Ag_{\sigma_2}(w)\Big)\\ &= h\mathrm{e}^{(1-\sigma_1)hA}[g',A]\big(\mathrm{e}^{\sigma_1 hA}w\big)\cdot\mathrm{e}^{(\sigma_1-\sigma_2)hA}g_{\sigma_2}(w)\end{aligned}$$

and

$$\begin{aligned}\partial_{\sigma_2}\Psi(\bullet\!\!\!\!\bullet)(\sigma_1,\sigma_2,w) &= h\mathrm{e}^{(1-\sigma_1)hA}g'_{\sigma_1}(w)\mathrm{e}^{(\sigma_1-\sigma_2)hA}\Big(-Ag_{\sigma_2}(w)+g'_{\sigma_2}A\mathrm{e}^{\sigma_2 hA}w\Big)\\ &= h\mathrm{e}^{(1-\sigma_1)hA}g'_{\sigma_1}(w)\mathrm{e}^{(\sigma_1-\sigma_2)hA}[g,A]\big(\mathrm{e}^{\sigma_2 hA}w\big),\end{aligned}$$

respectively. From these two relations, we infer that the bounds

$$\sup_{0\leqslant\sigma\leqslant 1}\sup_{0\leqslant t\leqslant T}\Big\|\mathrm{e}^{(1-\sigma_1)hA}[g',A]\big(\mathrm{e}^{\sigma_1 hA}u(t)\big)\cdot\mathrm{e}^{(\sigma_1-\sigma_2)hA}g_{\sigma_2}(u(t))\Big\|\leqslant C, \tag{5.4a}$$

$$\sup_{0\leqslant\sigma\leqslant 1}\sup_{0\leqslant t\leqslant T}\Big\|\mathrm{e}^{(1-\sigma_1)hA}g'_{\sigma_1}(u(t))\mathrm{e}^{(\sigma_1-\sigma_2)hA}[g,A]\big(\mathrm{e}^{\sigma_2 hA}u(t)\big)\Big\|\leqslant C \tag{5.4b}$$

should hold with a constant C that is independent of $\|A\|$.

From the above calculations, we conclude the following result. If the conditions (5.2), (5.3), and (5.4) hold with a constant C that does not depend on $\|A\|$, then a Lawson method of non-stiff order *two* has also *stiff* order *two*.

5.3 *Specialisation to linear problems*

For the linear evolution equation

$$u' = Au + Bu, \qquad u(0) = u_0$$

with bounded operator B on X, the above conditions (5.2), (5.3), and (5.4) simplify a bit. A first-order Lawson method is of *stiff* order one if

$$\sup_{0\leqslant\sigma\leqslant 1}\sup_{0\leqslant t\leqslant T}\Big\|\mathrm{e}^{(1-\sigma)hA}[B,A]\mathrm{e}^{\sigma hA}u(t)\Big\|\leqslant C. \tag{5.5a}$$

For second order, the conditions read

$$\sup_{0\leqslant\sigma\leqslant 1}\sup_{0\leqslant t\leqslant T}\Big\|\mathrm{e}^{(1-\sigma)hA}[A,[A,B]]\mathrm{e}^{\sigma hA}u(t)\Big\|\leqslant C, \tag{5.5b}$$

$$\sup_{0\leqslant\sigma_2\leqslant\sigma_1\leqslant 1}\sup_{0\leqslant t\leqslant T}\Big\|\mathrm{e}^{(1-\sigma_1)hA}[B,A]\mathrm{e}^{(\sigma_1-\sigma_2)hA}B\mathrm{e}^{\sigma_2 hA}u(t)\Big\|\leqslant C, \tag{5.5c}$$

$$\sup_{0\leqslant\sigma_2\leqslant\sigma_1\leqslant 1}\sup_{0\leqslant t\leqslant T}\Big\|\mathrm{e}^{(1-\sigma_1)hA}B\mathrm{e}^{(\sigma_1-\sigma_2)hA}[B,A]\mathrm{e}^{\sigma_2 hA}u(t)\Big\|\leqslant C. \tag{5.5d}$$

We recall that such conditions also arise in the analysis of splitting methods, cf. Jahnke & Lubich (2000).

The above analysis can easily be generalized to higher order, since for linear problems, only long trees have to be considered. For all other trees which start with at least two branches at the root, the integrand Ψ vanishes.

5.4 *Nonlinear Schrödinger equations*

For the time discretization of nonlinear Schrödinger equations

$$u_t = \mathrm{i}\big(\Delta u + f(|u|^2)u\big), \tag{5.6}$$

split-step methods are commonly viewed as the method of choice. In recent years, however, exponential integrators have been considered as a viable alternative for the solution of (5.6). For instance, Besse *et al.* (2015) studied exponential integrators in the context of Bose–Einstein condensates; Cano & González-Pachón (2015) and Balac *et al.* (2016) reported favourable results for Lawson integrators of the form as discussed in this paper. Rigorous convergence results, however, are still missing for these methods.

As an application of our analysis, we will use the above regularity conditions (5.2), (5.3), and (5.4) to verify second-order convergence of Lawson methods. In contrast to the rest of the paper, we refrain from any particular space discretization and argue in an abstract Hilbert space framework. Note, however, that our reasoning carries over to spatial discretizations (by spectral methods, e.g.) without any difficulty.

For this purpose, we consider (5.6) with periodic boundary conditions on the d dimensional torus and smooth potential. Then it is well known (see, e.g., (Kato, 1995, Thm. 4.1)) that the problem is well posed in H^s for $s > d/2$. The regularity of an initial value $u_0 \in H^s$ is thus preserved along the solution. Henceforth we choose $s > d/2$.

Second-order Strang splitting for (5.6) with $f(u) = \pm u$ was rigorously analysed in Lubich (2008). There it was shown that commutator relations similar to our conditions (5.2), (5.3), and (5.4) play a crucial role in the convergence proof for Strang splitting. The analysis given here shows that Lawson methods converge under the same regularity assumptions as splitting schemes. This will be worked out now in detail for first and second-order methods.

Let $A = \mathrm{i}\Delta$ and $g(u) = \mathrm{i}\beta|u|^2u$, i.e. $f = \beta I$. The first commutator $[A,g]$ then takes the form

$$\begin{aligned}
[A,g](u) &= Ag(u) - g'(u)Au \\
&= -\beta\nabla\cdot\big(2u\bar{u}\nabla u + u^2\nabla\bar{u}\big) + 2\beta u\bar{u}\Delta u - \beta u^2\Delta\bar{u} \\
&= -2\beta\big(\bar{u}\nabla u\cdot\nabla u + 2u\nabla u\cdot\nabla\bar{u} + u^2\Delta\bar{u}\big).
\end{aligned}$$

This explicit representation shows that the commutator is clearly bounded in H^s for $u \in H^{s+2}$. For Lawson methods, a first-order convergence bound in H^s thus requires H^{s+2} regularity of the exact solution, which is the same regularity as required for the first-order Lie splitting.

For second-order methods, one has to estimate the double commutator $[A,[A,g]]$. A simple calculation shows that a bound in H^s requires H^{s+4} regularity of the exact solution. Up to here, the situation is exactly the same as for second-order Strang splitting (see Lubich (2008)). The additional commutator $[A,g']$ can be expressed as

$$[A,g'](u)w = Ag'(u)w - g''(u)(Au,w).$$

A simple calculation shows that this commutator can again be bounded in H^s for $u,w \in H^{s+2}$. We thus conclude that Lawson methods require the same regularity for second-order convergence as Strang splitting.

5.5 *Numerical examples*

We consider the linear Schrödinger equation

$$u_t = iu_{xx} + if(x)u, \qquad x \in [-\pi,\pi], \quad u(0,\cdot) = u_0, \tag{5.7}$$

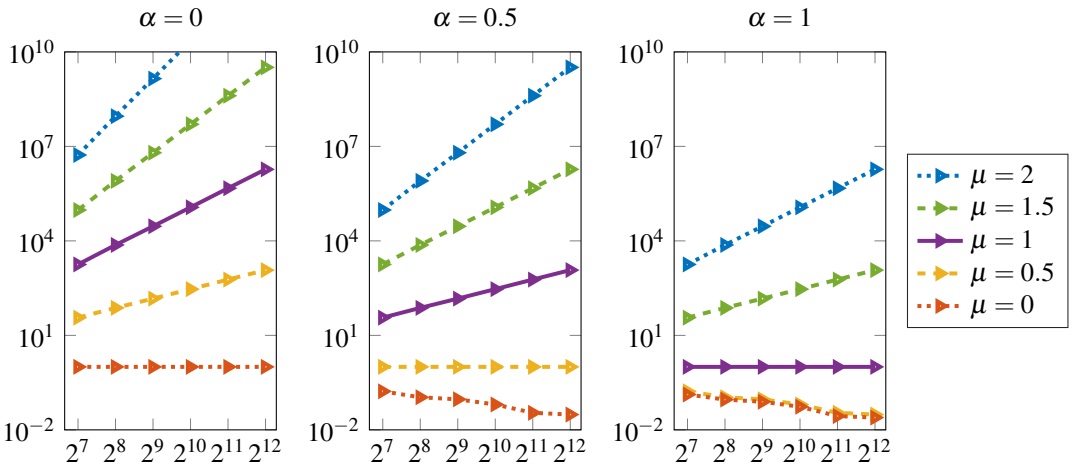

FIG. 1. Illustration of discrete regularity: $\|A^\mu u_0\|$ is plotted over the number N of Fourier modes, where u_0 is chosen as in (5.9).

with periodic boundary conditions and discretize it using a Fourier spectral method on an equidistant grid. In Fourier space, the matrix A is given by

$$A = -iD^2, \qquad \text{where} \qquad D = \operatorname{diag}(-\tfrac{N}{2}+1, -\tfrac{N}{2}+2, \dots, \tfrac{N}{2}).$$

For the function f we consider two different examples:

$$f(x) = \sin x, \tag{5.8a}$$
$$f(x) = (x/\pi)^2. \tag{5.8b}$$

Let us first explain what regularity means in the ODE context, where the operator stems from a spatial discretization. For each $N = 2^7, \dots, 2^{12}$ we choose a vector $r \in \mathbb{C}^N$ of Fourier coefficients such that $r_{N/2} = 0$ and where the remaining $N-1$ entries contain random numbers uniformly distributed in the unit disc. Then we normalize r such that its inverse discrete Fourier transform has unit norm (in the discrete L^2-norm). As an initial value we then set

$$(u_0)_{N/2} = 0, \qquad (u_0)_j = (D^{-2\alpha} r)_j, \quad j \in \{1, \dots, N\} \setminus \{N/2\}. \tag{5.9}$$

We are interested in the case $\alpha \geqslant 0$, since in the continuous case this resembles the situation of an initial function u_0 belonging to the Sobolev space $H^{2\alpha}([-\pi, \pi])$. Hence, larger values of $|\alpha|$ yield more regular initial values.

In Figure 1 we plot $\left\|D^{2\mu} u_0\right\|$ for different values of μ over the number of Fourier modes N. In the continuous case this norm is bounded if $u_0 \in H^{2\mu}$. The three graphs clearly show that $\left\|D^{2\mu} u_0\right\|$ is bounded independently of the number N of Fourier modes only for $\mu \leqslant \alpha$.

Now we fix the spatial discretization and set $N = 2048$. In Figure 2 we show the numerically observed orders of the exponential Euler and the Lawson Euler method for the periodic potential (5.8a) for different values of α such that the corresponding initial function is contained in $H^{2\alpha}$. We observe an order reduction for $\alpha = 0$ for both methods and (almost) order one for $\alpha \geqslant 0.5$.

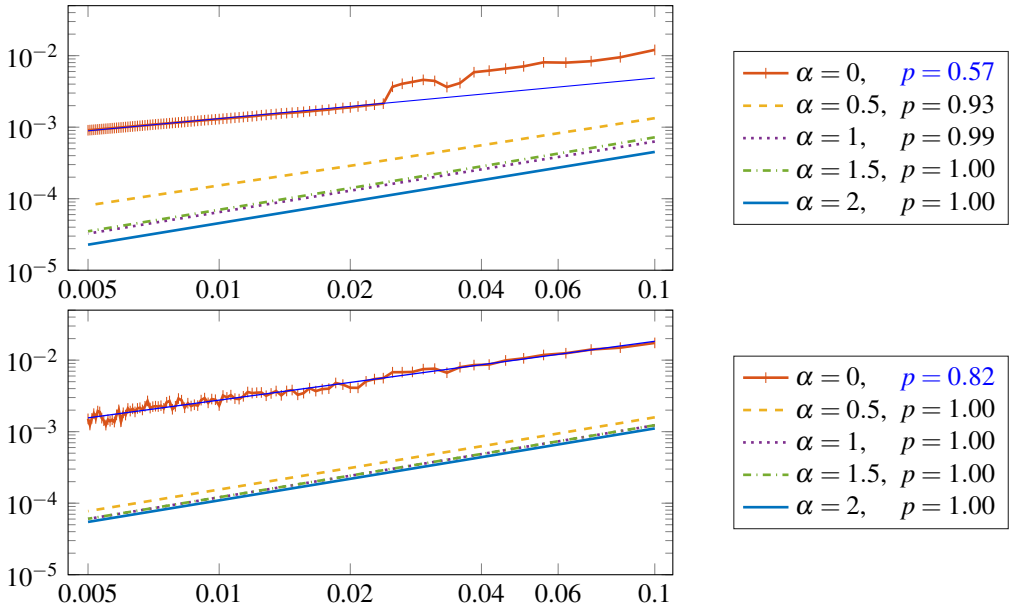

FIG. 2. Discrete $L^\infty((0,1),L^2(\Omega))$ error of the numerical solution of (5.7) with periodic potential (5.8a) for the exponential Euler method (top) and the Lawson Euler method (bottom) for different values of α. The values of p in the legend show the numerically observed orders of the schemes.

For $\alpha = 0$ the error of the exponential Euler method has an irregular behaviour for larger step sizes. To better visualise the order, we added thin lines (blue in the colour version) to all curves related to $\alpha = 0$. The slopes of these lines are also given in the legends (blue in the colour version).

In Figure 3 we present the same experiment for the quadratic potential (5.8b). The situations differs considerably for the exponential Euler methods while the Lawson Euler method still converges with order one for $\alpha \geqslant 0.5$. However, the exponential Euler methods suffers from order reduction for $\alpha < 1.5$ due to the nonsmooth potential f.

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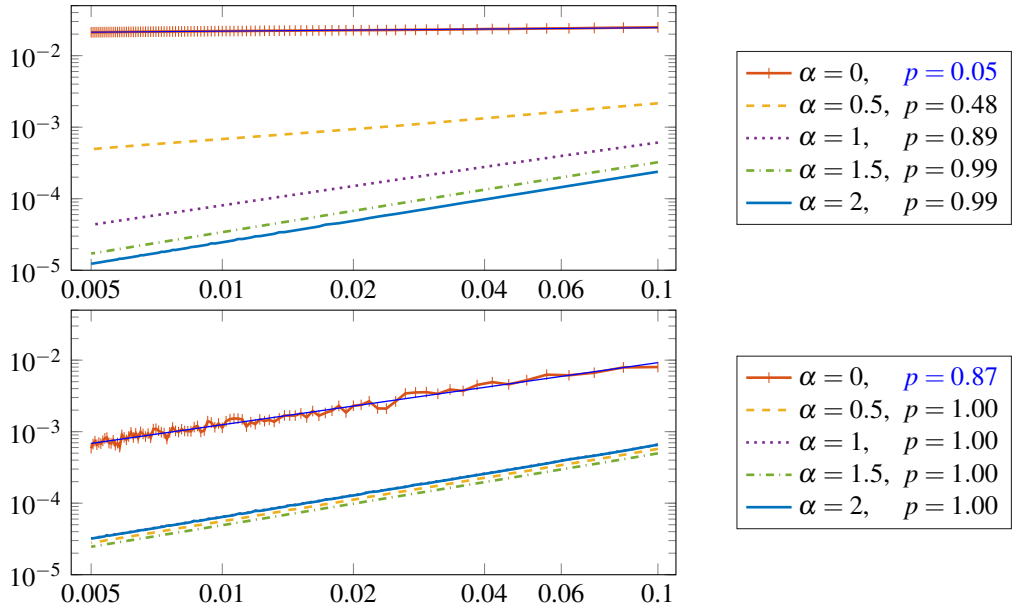

FIG. 3. Discrete $L^\infty((0,1),L^2(\Omega))$ error of the numerical solution of (5.7) with quadratic potential (5.8b) for the exponential Euler method (top) and the Lawson Euler method (bottom) for different values of α. The values of p in the legend show the numerically observed orders of the schemes.

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