# ON MAGNUS INTEGRATORS FOR TIME-DEPENDENT SCHRÖDINGER EQUATIONS

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**Abstract.** Numerical methods based on the Magnus expansion are an efficient class of integrators for Schrödinger equations with time-dependent Hamiltonian. Though their derivation assumes an unreasonably small time step size as would be required for a standard explicit integrator, the methods perform well even for much larger step sizes. This favorable behavior is explained, and optimal-order error bounds are derived which require no or only mild restrictions of the step size. In contrast to standard integrators, the error does not depend on higher time derivatives of the solution, which is in general highly oscillatory.

**1. Introduction.** We study numerical integrators for Schrödinger equations with time-dependent Hamiltonian,

$$i\,\frac{d\psi}{dt} = H(t)\psi, \qquad \psi(t_0) = \psi_0. \tag{1.1}$$

The computational Hamiltonian $H(t)$, which is a finite-dimensional hermitian operator, is typically the sum of a discretized negative Laplacian and a time-dependent potential. As the discretization of an unbounded operator, $H(t)$ can be of arbitrarily large norm.

Magnus integrators are an efficient class of numerical methods for such problems [2, 10]. Though the error behavior of these methods is well understood in the case of moderately bounded $H(t)$ [5, 6], no results are so far available when $\|H(t)\|$ becomes large. The present paper gives optimal-order estimates for situations where the product of the time step $h$ with $\|H(t)\|$ can be of arbitrary size. Even more interesting than the error bounds themselves are the mechanisms which lead to these bounds and which make Magnus methods perform so well for Schrödinger equations.

In Section 2 we recall the concepts underlying the construction of Magnus integrators. Section 3 states the main results, which give asymptotically sharp error bounds for various Magnus integrators, in a framework that applies to time-dependent Schrödinger equations without requiring smallness nor bounds of $h\|H(t)\|$. The general procedure for obtaining such estimates is outlined in Section 4, and is carried out in detail in Sections 5 and 6 for methods of order 2 and 4, respectively. Numerical experiments illustrating the theoretical results are given in Section 7. A basic assumption for the results of this paper are commutator bounds. Their validity for a spectral discretization is shown in the Appendix.

Magnus integrators require computing a matrix exponential multiplying a vector in every time step. For the large matrices (or rather, operators of large dimension) arising from the spatial discretization of Schrödinger equations, this can be done efficiently using operator splitting or Chebyshev or Lanczos approximations. These techniques are well documented in the literature and are not considered here. Because of the stable error propagation, errors arising from the approximation of the matrix exponentials could be straightforwardly included in the error analysis.

Throughout the paper, $\|\cdot\|$ is the Euclidean norm or its induced matrix norm, or occasionally the $L^2$ norm of functions.

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**2. Magnus integrators.** For the linear differential equation

$$\dot{y} = A(t)y, \qquad y(0) = y_0, \tag{2.1}$$

with a time-dependent matrix $A(t)$, the approach of Magnus [8] aims at writing the solution as

$$y(t) = \exp\big(\Omega(t)\big)y_0 \tag{2.2}$$

for a suitable matrix $\Omega(t)$. An expression for $\Omega(t)$ is obtained by making the ansatz (2.2) and differentiating. This gives

$$\dot{y}(t) = \operatorname{dexp}_{\Omega(t)}(\dot{\Omega}(t))\, y(t)\ ,$$

where the dexp operator can be expressed as

$$\operatorname{dexp}_{\Omega}(B) = \varphi(\operatorname{ad}_\Omega)(B) = \sum_{k\geq 0} \frac{1}{(k+1)!}\, \operatorname{ad}_\Omega^k(B) \tag{2.3}$$

with $\varphi(z) = (e^z - 1)/z$ and $\operatorname{ad}_\Omega(B) = [\Omega, B] = \Omega B - B\Omega$. Hence, (2.2) solves (2.1) if

$$A(t) = \operatorname{dexp}_{\Omega(t)}\big(\dot{\Omega}(t)\big), \qquad \Omega(0) = 0. \tag{2.4}$$

As long as $\|\Omega(t)\| < \pi$ (which is *not* the situation of interest in this article!), the operator $\operatorname{dexp}_{\Omega(t)}$ is invertible and the series

$$\operatorname{dexp}^{-1}_{\Omega(t)}\big(A(t)\big) = \sum_{k\geq 0} \frac{\beta_k}{k!}\, \operatorname{ad}^k_{\Omega(t)}(A(t)) \tag{2.5}$$

converges. Here $\beta_k$ is the $k$th Bernoulli number appearing in the series $z/(e^z - 1) = \sum_0^\infty (\beta_k/k!)z^k$, which converges for $|z| < 2\pi$. (Note $\|\operatorname{ad}_\Omega(B)\| \leq 2\|\Omega\| \cdot \|B\|$, which shows that (2.5) indeed converges for $\|\Omega(t)\| < \pi$.) This gives an explicit differential equation for $\Omega(t)$:

$$\dot{\Omega} = A(t) - \frac{1}{2}[\Omega, A(t)] + \frac{1}{12}[\Omega, [\Omega, A(t)]] + \dots\ .$$

Picard iteration yields the *Magnus expansion*

$$\begin{aligned}\Omega(t) = \int_0^t A(\tau)d\tau &- \frac{1}{2}\int_0^t [\int_0^\tau A(\sigma)d\sigma, A(\tau)]\, d\tau \\ &+ \frac{1}{4}\int_0^t [\int_0^\tau [\int_0^\sigma A(\mu)d\mu, A(\sigma)]\, d\sigma, A(\tau)]\, d\tau \\ &+ \frac{1}{12}\int_0^t [\int_0^\tau A(\sigma)d\sigma, [\int_0^\tau A(\mu)d\mu, A(\tau)]]\, d\tau + \dots\ .\end{aligned} \tag{2.6}$$

Numerical methods based on this expansion are reviewed by Iserles, Munthe-Kaas, Nørsett and Zanna [5]. They are of the form

$$y_{n+1} = \exp(\Omega_n)y_n \tag{2.7}$$

to give an approximation to $y(t_{n+1})$ at $t_{n+1} = t_n + h$. Here $\Omega_n$ is a suitable approximation of $\Omega(h)$ given by (2.6) with $A(t_n + \tau)$ instead of $A(\tau)$. This approximation first involves truncating the expansion, and second approximating the integrals, e.g., replacing $A(t)$ locally by an interpolation polynomial $\widehat{A}(t)$ for the nodes $t_n + c_j h$, so that the integrals in the Magnus expansion can be computed analytically.

EXAMPLE 1. *The midpoint rule yields a second-order scheme with*

$$\Omega_n = hA(t_n + h/2). \tag{2.8}$$

EXAMPLE 2. *The two-point Gauss quadrature rule has nodes* $c_{1,2} = 1/2 \mp \sqrt{3}/6$ *and weights* $b_{1,2} = 1/2$. *This yields a fourth-order scheme with*

$$\Omega_n = \frac{h}{2}(A_1 + A_2) + \frac{\sqrt{3}h^2}{12}[A_2, A_1], \tag{2.9}$$

*where* $A_j = A(t_n + c_j h)$, $j = 1, 2$.

EXAMPLE 3. *Blanes, Casas, and Ros* [1] *propose a fourth-order scheme, starting from the observation that the Taylor expansion of* $A(t)$ *at* $t_{n+1/2} = t_n + h/2$ *gives for the double integral in* (2.6)

$$\int_0^h \int_0^\tau [A(\sigma), A(\tau)]\, d\sigma d\tau = -\frac{h^3}{12}[A(t_{n+1/2}), \dot{A}(t_{n+1/2})] + O(h^5).$$

*For the numerical scheme, the authors propose to use the symmetric approximation*

$$h^3[A(t_{n+1/2}), \dot{A}(t_{n+1/2})] = h^2[A(t_n), A(t_{n+1})] + O(h^5).$$

*The single integral in* (2.6) *may be approximated by Simpson's rule. The scheme then uses*

$$\Omega_n = \frac{h}{6}\big(A(t_n) + 4A(t_{n+1/2}) + A(t_{n+1})\big) - \frac{h^2}{12}[A(t_n), A(t_{n+1})]. \tag{2.10}$$

For the purpose of this paper, the Magnus series approach is described only for motivation, since we are interested in the case of large $\|hA(t)\|$, for which $\operatorname{dexp}_{\Omega_n}$ need not be invertible and the Magnus expansion need not converge. The results of Iserles and Nørsett [6] on the order of Magnus integrators are for $\|hA(t)\| \to 0$ and are obtained by studying the remainder of the truncated Magnus series (2.6). The constants in those estimates depend on norms of commutators of $A(t)$ for different values of $t$, which all become large with growing $\|A(t)\|$. Therefore, results on the classical order of a method must be taken with caution in the case of the Schrödinger equation, which involves discretizations of unbounded operators. Nevertheless, Magnus integrators work extremely well even with step sizes for which $\|hA(t)\|$ is large. The aim of the present paper is to explain this unexpectedly good behavior.

**3. Statement of results.** In this section we state our assumptions and main results. We write

$$A(t) = -iH(t) = -i\big(U + V(t)\big). \tag{3.1}$$

We assume, once and for all, that the hermitian matrix-valued function $V(t)$ and its time derivatives are bounded by

$$\left\| \frac{d^m}{dt^m} V(t) \right\| \le M_m, \qquad m = 0, 1, 2, \ldots\ . \tag{3.2}$$

The matrix $U$ is assumed symmetric positive definite, with $\|v\| \le \|Uv\|$ for all $v$, but no bound is assumed for $\|U\|$. We set

$$D = U^{1/2}. \tag{3.3}$$

The typical situation is given by a discretization of the spatially continuous case where $U = -\Delta + I$, e.g., with periodic boundary conditions on a cube $Q$, and $V(t)$ is a bounded multiplication operator, i.e., $(V(t)v)(x) = V(x,t)v(x)$ for a real-valued smooth potential $V(x,t)$. In this continuous case we have

$$\|Dv\|^2 = \int_Q |\nabla v|^2 dx + \int_Q v^2 dx,$$

so that $\|Dv\|$ is the familiar $H^1$ Sobolev norm of $v$. In the spatially discretized case, $\|Dv\|$ can be viewed as a discrete Sobolev norm. For a space discretization with minimal grid spacing $\Delta x$, we note $\|U\| \sim \Delta x^{-2}$ and $\|D\| \sim \Delta x^{-1}$.

Our main assumptions are commutator bounds such as

$$\|[U, V(t)]v\| \le K_0 \|Dv\| \quad \text{and} \quad \|[U, \dot{V}(t)]v\| \le K_1 \|Dv\| \tag{3.4}$$

for all $t$ and all vectors $v$. Condition (3.4) is easily verified in the spatially continuous case, with $U = -\Delta + I$ and a smooth potential $V(x,t)$ acting as a multiplication operator. The bound is obtained by noting that in one space dimension, with $' = d/dx$,

$$[U,V]v = -\big((Vv)'' - Vv''\big) = -\big(2V'v' + V''v\big),$$

with the obvious generalization to higher space dimensions. Hence, $[U,V]$ is a *first-order* differential operator, which yields (3.4). For a spectral discretization the bound (3.4) is shown, uniformly in the discretization parameter, in [7, Lemma 3.1].

Since $[A(\tau), A(\sigma)] = [U, V(\sigma) - V(\tau)] = \int_\tau^\sigma [U, \dot{V}(t)]\, dt$, the second bound of (3.4) implies, for all vectors $v$,

$$\|[A(\tau), A(\sigma)]v\| \le K_1 h \, \|Dv\| \qquad \text{for} \quad |\tau - \sigma| \le h. \tag{3.5}$$

THEOREM 3.1. *If $A(t)$ satisfies the commutator bound* (3.5)*, then the error of the exponential midpoint rule* (2.7) *with* (2.8) *is bounded by*

$$\|y_n - y(t_n)\| \le C h^2 \, t_n \max_{0 \le t \le t_n} \|Dy(t)\|.$$

*The constant $C$ depends only on $M_m$ for $m \le 2$ and on $K_1$. In particular, $C$ is independent of $n$, $h$, and $\|D\|$.*

This error bound is to be contrasted with the error bound of the classical implicit midpoint rule $y_{n+1} = y_n + hA(t_{n+1/2})(y_n + y_{n+1})/2$, for which

$$\|y_n - y(t_n)\| \le C h^2 \, t_n \max_{0 \le t \le t_n} \|\frac{d^3}{dt^3} y(t)\|.$$

Since solutions of Schrödinger equations are in general highly oscillatory, the appearance of higher time derivatives is unfavorable. On the other hand, $\|Dy(t)\|^2$ represents essentially the kinetic energy, which is bounded *a priori*.

For methods of order $p$ which contain products of $A(t_n + c_j h)$ with $r$ terms (we have $p = 4$ and $r = 2$ in Examples 2 and 3), we assume that $A$ satisfies, for all $\tau_j$,

$$\|[A(\tau_k), [\dots, [A(\tau_1), \frac{d^m}{dt^m} V(\tau_0)]] \dots]v\| \le K \, \|D^k v\| \qquad \begin{cases} 0 \le m \le p, \\ k+1 \le rp. \end{cases} \tag{3.6}$$

Like (3.5), condition (3.6) is easily verified in the spatially continuous case. For a spectral space discretization of a time-dependent Schrödinger equation, we show in the Appendix that (3.6) is indeed satisfied uniformly in the discretization parameter. Since $[A(\tau_1), A(\tau_0)] = [A(\tau_1), A(\tau_0) - A(\tau_1)] = [A(\tau_1), i\int_{\tau_0}^{\tau_1} \dot V(\tau)d\tau]$, condition (3.6) implies, whenever $|\tau_1 - \tau_0| \le h$,

$$\|[A(\tau_k), [\ldots, [A(\tau_1), A(\tau_0)]] \ldots]v\| \le Kh\,\|D^k v\|, \qquad k+1 \le rp. \tag{3.7}$$

Unlike the case of the exponential midpoint rule in Theorem 3.1, convergence of higher-order methods is obtained only in the spatially discrete case under a step size restriction

$$h\,\|D\| \le c. \tag{3.8}$$

Note that this restriction is milder than the stability condition for explicit integrators, such as Runge-Kutta methods, for which a more stringent condition $h\|D\|^2 \le c$ is required. The classical error bounds for implicit integrators require smallness of $h\|D\|^2$ unless high temporal smoothness is supposed.

THEOREM 3.2. *If the commutator bounds* (3.6) *hold with* $p = 4$ *and* $r = 2$, *then the fourth-order Magnus methods of Examples* 2 *and* 3 *satisfy the error bound*

$$\|y_n - y(t_n)\| \le Ch^4\, t_n \max_{0\le t\le t_n} \|D^3 y(t)\|$$

*for time steps h restricted by* (3.8). *The constant C depends only on* $M_m$ *for* $m \le 4$, *on K, and on c. In particular, C is independent of n, h, and* $\|D\|$ *as long as* $h\|D\| \le c$.

In the following section we describe a general procedure for deriving error bounds which may be taken as a recipe to study Magnus methods of arbitrary order $p$. We will follow this procedure for the exponential midpoint rule in Section 5 and for fourth-order methods in Section 6. However, we do not consider higher order methods here. They require an extension of the arguments for the fourth-order methods which is cumbersome to formulate and is probably best done systematically using trees.

**4. General procedure for deriving error bounds.** The convergence analysis is done in two steps. In the first step we study the error which results from truncating the Magnus expansion; in the second step, we discuss the error resulting from approximating the integrals by quadrature. (In the estimates of this and the following sections, $C$ is a generic constant which assumes different values on different occurrences.)

Truncation of the Magnus expansion amounts to using a suitable, in particular skew hermitian, $\widetilde\Omega$ instead of $\Omega$ in (2.2), i.e.

$$\widetilde y(t) = \exp\bigl(\widetilde\Omega(t)\bigr) y_0.$$

By differentiating, we obtain the approximate solution $\widetilde y(t)$ as the solution of the perturbed problem

$$\dot{\widetilde y}(t) = \widetilde A(t)\widetilde y(t) \qquad \text{with} \qquad \widetilde A(t) = \operatorname{dexp}_{\widetilde\Omega(t)}\bigl(\dot{\widetilde\Omega}(t)\bigr) \tag{4.1}$$

with initial value $\widetilde y(0) = y_0$. Note that $\widetilde A(t)$ is again skew hermitian. As the following lemma shows, a bound on $\widetilde A - A$ immediately gives a local error bound.

LEMMA 4.1. *Let $y$ be a solution of* (2.1), $\widetilde{y}$ *a solution of* (4.1). *With $E = \widetilde{A} - A$, the error satisfies*

$$\| \widetilde{y}(t) - y(t) \| \leq \int_0^t \|E(\tau)y(\tau)\| d\tau.$$

*Proof.* We write (2.1) as $\dot{y} = A(t)y = \widetilde{A}(t)y - E(t)y$ and subtract (4.1). This shows that the error $\widetilde{\varepsilon} = \widetilde{y} - y$ satisfies

$$\dot{\widetilde{\varepsilon}} = \widetilde{A}(t)\widetilde{\varepsilon} + E(t)y, \qquad \widetilde{\varepsilon}(0) = 0.$$

Since $\widetilde{A}$ is skew hermitian, taking the inner product with $\widetilde{\varepsilon}$ on both sides leads to

$$\langle \dot{\widetilde{\varepsilon}}, \widetilde{\varepsilon} \rangle = \langle E\, y, \widetilde{\varepsilon} \rangle \leq \|E\, y\| \, \|\widetilde{\varepsilon}\|.$$

On the other hand, $\langle \dot{\widetilde{\varepsilon}}, \widetilde{\varepsilon} \rangle = \frac{1}{2}\frac{d}{dt}\|\widetilde{\varepsilon}\|^2 = \frac{d}{dt}\|\widetilde{\varepsilon}\| \cdot \|\widetilde{\varepsilon}\|$. Integrating the inequality proves the lemma. □

A crucial step in obtaining a bound on $E = \widetilde{A} - A$ is truncating the dexp series (2.3) and providing a bound for the remainder. We define the remainder function $r_p$, for $p \geq 1$, via

$$\frac{e^z - 1}{z} = 1 + \frac{1}{2}z + \ldots + \frac{1}{(p-1)!}\, z^{p-2} + \frac{1}{p!}\, z^{p-1} r_p(z), \tag{4.2}$$

so that

$$\operatorname{dexp}_{\Omega}(B) = B + \frac{1}{2}[\Omega, B] + \ldots + \frac{1}{(p-1)!}\operatorname{ad}_{\Omega}^{p-2}(B) + \frac{1}{p!}\, r_p(\operatorname{ad}_{\Omega})\Big(\operatorname{ad}_{\Omega}^{p-1}(B)\Big). \tag{4.3}$$

For our analysis, a bound of the type

$$\|r_p(\operatorname{ad}_{\widetilde{\Omega}(t)})\Big(\operatorname{ad}_{\widetilde{\Omega}(t)}^{p-1}(\dot{\widetilde{\Omega}}(t))\Big)v\| \leq Ch^p \,\|D^{p-1}v\| \;, \qquad 0 \leq t \leq h, \tag{4.4}$$

is required. We will prove this bound for $p = 2$ and $p = 4$ in Sections 5 and 6 below. In the case of $p = 4$, it turns out that the bound requires time steps $h$ with (3.8), while for $p = 2$, no restriction on $h$ is necessary.

Next we incorporate the error resulting from approximating the integrals. In the $n$th time step, we take $\widetilde{\Omega}(h)$ corresponding to the truncated Magnus series for $A(t_n + t)$ instead of $A(t)$, which we denote by $\widetilde{\Omega}_n$. By the quadrature approximation, $\widetilde{\Omega}_n$ is replaced by $\Omega_n$ with which the actual computations are done. This approximation typically satisfies

$$\|\big(\widetilde{\Omega}_n - \Omega_n\big)v\| \leq Ch^{p+1}\|D^{r-1}v\| \tag{4.5}$$

where $p$ is the order of the quadrature rule and products with $r$ terms appear in the method. This bound is obvious for the exponential midpoint rule ($p = 2$, $r = 1$), where the bound is independent of $D$. For the fourth-order schemes ($p = 4$, $r = 2$) we will show in detail that (4.5) holds and that this leads to the local error bound

$$\| \exp(\widetilde{\Omega}_n)v - \exp(\Omega_n)v\| \leq Ch^{p+1}\|D^{r-1}v\|, \tag{4.6}$$

cf. Lemma 6.5 below. From (4.5), this is obvious for $r = 1$.

Putting both steps together, the exact solution $y$ of (2.1) satisfies

$$y(t_{n+1}) = \exp(\Omega_n)y(t_n) + \varepsilon_n, \tag{4.7}$$

with $\varepsilon_n = y(t_{n+1}) - \exp\big(\widetilde{\Omega}_n\big)y(t_n) + \exp\big(\widetilde{\Omega}_n\big)y(t_n) - \exp(\Omega_n)y(t_n)$. By Lemma 4.1 and (4.6), this gives

$$\|\varepsilon_n\| \le \int_{t_n}^{t_{n+1}} \|E(\tau)y(\tau)\|d\tau + Ch^{p+1}\|D^{r-1}y(t_n)\|.$$

Subtracting (2.7) from (4.7) leads to the error recursion for $e_n = y_n - y(t_n)$:

$$e_{n+1} = \exp(\Omega_n)e_n + \varepsilon_n \ ,$$

and thus

$$\|e_n\| \le \sum_{j=0}^{n-1} \|\varepsilon_j\|. \tag{4.8}$$

In summary, error bounds for general Magnus methods are obtained as follows: We have to provide a bound on $E(t)y(t)$, which basically means to prove (4.4), and we have to show that the approximation $\Omega_n$ satisfies (4.6).

**5. Error bounds for the exponential midpoint rule.** In this section we prove Theorem 3.1. The simplest possible Magnus type method is obtained by truncating the Magnus expansion after the first term, i.e., by setting

$$\widetilde{\Omega}(t) = \int_0^t A(\tau)\, d\tau, \qquad 0 \le t \le h.$$

Following the approach described in Section 4, we know that $\widetilde{y}(t) = \exp\big(\widetilde{\Omega}(t)\big)y_0$ solves (4.1) with

$$\widetilde{A}(t) = \operatorname{dexp}_{\widetilde{\Omega}(t)}\big(\dot{\widetilde{\Omega}}(t)\big) = A(t) + \frac{1}{2}r_2(\operatorname{ad}_{\widetilde{\Omega}(t)})\left(\operatorname{ad}_{\widetilde{\Omega}(t)}(\dot{\widetilde{\Omega}}(t))\right) =: A(t) + E_2(t) \tag{5.1}$$

where the representation (4.3) for the dexp operator war used. The remainder $r_2$ was defined in (4.2).

Lemma 5.1. *$r_2$ satisfies (4.4) with $p = 2$, where the constant $C$ depends only on $M_0$ of (3.2) and $K_1$ of (3.5).*

*Proof.* We fix an arbitrary $t$ with $0 \le t \le h$. After an orthogonal similarity transform, we may assume that $\Omega := \widetilde{\Omega}(t)$ is diagonal, $\Omega = \operatorname{diag}(\omega_k)$ with purely imaginary eigenvalues $\omega_k$, and we define $B = \dot{\widetilde{\Omega}}(t)$. Denoting by $\bullet$ the entrywise product of matrices, we can write

$$\operatorname{ad}_\Omega(B) = \Omega B - B\Omega = Z \bullet B,$$

where $Z = \big(\omega_k - \omega_\ell\big)_{k,\ell}$. This yields

$$u := r_p(\operatorname{ad}_\Omega)\Big(\operatorname{ad}_\Omega^{p-1}(B)\Big)v = \Big(R \bullet \operatorname{ad}_\Omega^{p-1}(B)\Big)v,$$

where $R = \big(r_p(\omega_k - \omega_\ell)\big)_{k,\ell}$. We now follow the proof of Lemma 2.2 of [4]. Note that for real $x$, $r_p(ix) = 1 + O(x)$, $x \to 0$ and $r_p(ix) = O(x^{-1})$, $|x| \to \infty$ and hence

$r_p, r_p' \in L^2(i\mathbb{R})$. As can be seen, e.g., from formula (2.13) in [4], $r_p$ has a Fourier transform $\widehat{r}_p \in L^1(\mathbb{R})$,

$$r_p(ix) = \int_{\mathbb{R}} e^{i\xi x} \widehat{r}_p(\xi)\, d\xi \ ,$$

with $\|\widehat{r}_p\|_{L^1(\mathbb{R})} \le 2\pi \|r_p\|_{L^2(i\mathbb{R})}^{1/2} \|r_p'\|_{L^2(i\mathbb{R})}^{1/2}$. Consequently, $u$ can be written as

$$u = \int_{\mathbb{R}} \widehat{r}_p(\xi) \exp(\xi\Omega)\, \mathrm{ad}_\Omega^{p-1}\big(B\big) \exp(-\xi\Omega)\, v\, d\xi,$$

so that

$$\|u\| \le \|\widehat{r}_p\|_{L^1(\mathbb{R})} \sup_{\xi\in\mathbb{R}} \|\mathrm{ad}_\Omega^{p-1}\big(B\big) \exp(-\xi\Omega) v\|. \tag{5.2}$$

So far, this holds for general $p$. From now on we set $p = 2$. Using

$$\mathrm{ad}_\Omega(B) = \mathrm{ad}_{\widetilde{\Omega}(t)}(\dot{\widetilde{\Omega}}(t)) = [\widetilde{\Omega}(t), \dot{\widetilde{\Omega}}(t)] = \int_0^t [A(\tau), A(t)]\, d\tau$$

and (3.5), we obtain for all vectors $w$

$$\|\mathrm{ad}_\Omega(B) w\| \le K_1 h^2 \|Dw\|.$$

Hence we have

$$\|u\| \le C h^2 \sup_{\xi\in\mathbb{R}} \|D \exp(-\xi\Omega) v\|. \tag{5.3}$$

We now use the splitting (3.1) and write

$$\frac{i}{h}\Omega = U + \frac{1}{h}\int_0^h V(\tau) d\tau =: U + \widetilde{V}.$$

We choose $\alpha \ge 0$ such that $U + \widetilde{V} + \alpha I$ is symmetric and positive definite. To keep the notation simple, we omit the constants and denote by $\sim$ equivalent norms. Because of the boundedness of $\widetilde{V}$ and (3.3) we have for all vectors $w$

$$\|Dw\| = \sqrt{w^* U w} \sim \sqrt{w^*(U + \widetilde{V} + \alpha I) w} = \|\left(\tfrac{i}{h}\Omega + \alpha I\right)^{1/2} w\|.$$

We use this norm equivalence to bound the last factor in (5.3):

$$\begin{aligned} \|D \exp(-\xi\Omega) v\| &\sim \|\left(\tfrac{i}{h}\Omega + \alpha I\right)^{1/2} \exp(-\xi\Omega) v\| \\ &= \|\exp(-\xi\Omega) \left(\tfrac{i}{h}\Omega + \alpha I\right)^{1/2} v\| \\ &= \|\left(\tfrac{i}{h}\Omega + \alpha I\right)^{1/2} v\| \\ &\sim \|Dv\|. \end{aligned}$$

Inserting this into (5.3) proves the lemma. □

By definition (5.1) of $E_2$, this immediately yields the bound

$$\|E_2(t) y(t)\| \le C h^2 \|Dy(t)\|, \qquad 0 \le t \le h.$$

Applying Lemma 4.1 gives

$$\|\widetilde{\varepsilon}(t)\| \le Ch^3 \max_{0\le\tau\le h} \|Dy(\tau)\|. \tag{5.4}$$

The midpoint rule uses the approximation

$$\widetilde{\Omega}_n = \int_0^h A(t_n+\tau)d\tau \approx hA(t_{n+1/2}) =: \Omega_n$$

in the scheme (2.7). The midpoint rule is of order two, and since $\|\ddot{A}(t)\| \le M_2$, the quadrature error is bounded by

$$\|\widetilde{\Omega}_n - \Omega_n\| \le \frac{1}{24} M_2 h^3.$$

The identity

$$\exp(\widetilde{\Omega}_n) - \exp(\Omega_n) = \int_0^1 \exp\bigl((1-s)\Omega_n\bigr)\bigl(\widetilde{\Omega}_n - \Omega_n\bigr)\exp\bigl(s\widetilde{\Omega}_n\bigr)\,ds$$

then yields

$$\|\exp(\widetilde{\Omega}_n) - \exp(\Omega_n)\| \le \frac{1}{24} M_2 h^3. \tag{5.5}$$

Combining (5.4) and (5.5) yields for the defects $\varepsilon_j$ of (4.7)

$$\|\varepsilon_j\| \le Ch^3 \max_{t_j\le\tau\le t_{j+1}} \|Dy(\tau)\|.$$

By (4.8), this gives

$$\|e_n\| \le Ch^2\, t_n \max_{0\le t\le t_n} \|Dy(t)\|,$$

which is just the statement of Theorem 3.1.

**6. Error bounds for fourth order Magnus methods.** This section gives the proof of Theorem 3.2. A Magnus method of classical order four is constructed by setting

$$\dot{\widetilde{\Omega}}(t) = A(t_n+t) - \frac{1}{2}\int_0^t [A(t_n+\tau), A(t_n+t)]\,d\tau, \qquad \widetilde{\Omega}(t_n) = 0 \tag{6.1}$$

for $0 \le t \le h$. To study the local error we simplify the notation and consider the case $n = 0$. Then integrating yields

$$\widetilde{\Omega}(t) = \int_0^t A(\tau)\,d\tau - \frac{1}{2}\int_0^t \int_0^\tau [A(\sigma), A(\tau)]\,d\sigma d\tau, \qquad 0 \le t \le h. \tag{6.2}$$

In this case, $\widetilde{y}(t) = \exp\bigl(\widetilde{\Omega}(t)\bigr)y_0$ solves (4.1) with (partly omitting the argument $t$)

$$\widetilde{A}(t) = \dot{\widetilde{\Omega}}(t) + \frac{1}{2}[\widetilde{\Omega}, \dot{\widetilde{\Omega}}] + \frac{1}{6}[\widetilde{\Omega}, [\widetilde{\Omega}, \dot{\widetilde{\Omega}}]] + \frac{1}{24} r_4(\mathrm{ad}_{\widetilde{\Omega}})\left(\mathrm{ad}^3_{\widetilde{\Omega}}(\dot{\widetilde{\Omega}})\right). \tag{6.3}$$

Lemma 6.1. *If $h\|D\| \le c$, then $r_4$ defined in (4.2) satisfies (4.4) with $p = 4$, where the constant $C$ depends only on $K$, $M_0$, and $c$.*

*Proof.* The first part of the proof is identical to the proof of Lemma 5.1. We therefore start with the bound (5.2) and turn to estimate $\mathrm{ad}_{\Omega}^3(B)w = \mathrm{ad}_{\Omega(t)}^3(\dot{\widetilde{\Omega}}(t))w$ for $\widetilde{\Omega}(t)$ of (6.2). Using the commutator bound (3.7) (and previously the Jacobi identity, if necessary) for terms such as, e.g.,

$$\Big\|[\int_0^t A(\tau)d\tau, [\int_0^t A(\tau)d\tau, [\int_0^t \int_0^\tau [A(\sigma), A(\tau)]\, d\sigma d\tau, A(t)]]]w\Big\| \le Kh^5 \|D^4 w\|,$$

it is shown under the restriction $h\|D\| \le c$ that for all $w$,

$$\|\mathrm{ad}_{\Omega(t)}^3(\dot{\widetilde{\Omega}}(t))w\| \le Ch^4 \|D^3 w\|, \qquad 0 \le t \le h.$$

Inserted in (5.2), this bound yields

$$\|r_4(\mathrm{ad}_{\widetilde{\Omega}(t)})\Big(\mathrm{ad}_{\Omega(t)}^3(\dot{\widetilde{\Omega}}(t))\Big)v\| \le Ch^4 \sup_{\xi\in\mathbb{R}} \|D^3 \exp(-\xi\Omega)v\|. \tag{6.4}$$

It remains to show that the supremum can be bounded by $C\|D^3 v\|$. We use the splitting (3.1) and write

$$\frac{i}{h}\Omega = U + \frac{1}{h}\int_0^h V(\tau)d\tau - \frac{i}{2h}\int_0^h \int_0^\tau [A(\sigma), A(\tau)]\, d\sigma d\tau =: U + \widetilde{V}.$$

By the assumptions, $\widetilde{V} = V(0) + O(h)$ is a hermitian bounded operator, and thus there exists $\alpha \ge 0$ such that $U + \widetilde{V} + \alpha I$ is positive definite. Our next aim is to show that for all $w$,

$$\|D^4 w\| = \|U^2 w\| \sim \|\left(\tfrac{i}{h}\Omega + \alpha I\right)^2 w\|. \tag{6.5}$$

We have

$$(U + \widetilde{V} + \alpha I)^2 - U^2 = 2(\widetilde{V} + \alpha I)U + [U, \widetilde{V} + \alpha I] + (\widetilde{V} + \alpha I)^2.$$

The first and the last term on the right-hand side yield bounds

$$\|2(\widetilde{V} + \alpha I)Uw\| + \|(\widetilde{V} + \alpha I)^2 w\| \le C\|D^2 w\| + C\|w\|. \tag{6.6}$$

Bounds for the second term are obtained from assumption (3.7). By definition of $\widetilde{V}$ and writing $U = iA(\tau) - V(\tau)$, we have

$$\begin{aligned}
[U, \widetilde{V}] =& \Big[U, \frac{1}{h}\int_0^h V(\tau)d\tau - \frac{i}{2h}\int_0^h \int_0^\tau [A(\sigma), A(\tau)]\, d\sigma d\tau\Big] \\
=& \frac{i}{h}\int_0^h [A(\tau), V(\tau)]\, d\tau \\
&+ \frac{1}{2h}\int_0^h \int_0^\tau [A(0), [A(\sigma), A(\tau)]]\, d\sigma d\tau \\
&+ \frac{i}{2h}\int_0^h \int_0^\tau [V(0), [A(\sigma), A(\tau)]]\, d\sigma d\tau.
\end{aligned}$$

By the commutator bounds (3.6) and (3.7) and the Jacobi identity, we obtain for $h\|D\| \le c$

$$\|[U,\widetilde{V}]w\| \le K\|Dw\| + \tfrac{1}{2}Kh^2\|D^2w\| + Kh\|D^2w\| \le C\|Dw\|. \tag{6.7}$$

Together with (6.6) this proves (6.5). Moreover, the estimates (6.6) and (6.7) show that

$$\|\big((U+\widetilde{V}+\alpha I)^2 - U^2\big)U^{-1}w\| \le C\|w\|.$$

So we can apply Lemma 6.2 below with $\mu = 1/2$ and $\theta = 3/4$, to show that (6.5) implies

$$\|D^3w\| = \|U^{3/2}w\| \sim \|\left(\tfrac{i}{h}\Omega + \alpha I\right)^{3/2} w\|.$$

As at the end of the proof of Lemma 5.1, we then obtain

$$\|D^3 \exp(-\xi\Omega)v\| \le C\|D^3v\|$$

with a constant independent of $\xi$. Inserting this bound in (6.4) completes the proof. $\square$

LEMMA 6.2. *Suppose $S, T$ are hermitian positive definite operators such that $\|(S-T)S^{-\mu}\| \le M$ holds with $0 \le \mu < 1$. If*

$$\|Sv\| \le \|Tv\| \qquad \textit{for all } v,$$

*then, for $0 < \theta < 1$,*

$$\|S^\theta v\| \le C\|T^\theta v\| \qquad \textit{for all } v,$$

*where $C$ depends only on $M$ and $\mu$.*

*Proof.* This is a reformulation of Theorem 1.4.6 in [3]. $\square$

We are now in the position to prove a bound of $\widetilde{A}(t) - A(t)$.

LEMMA 6.3. *For $\widetilde{A}(t)$ defined in (6.3) and time steps $h$ with $h\|D\| \le c$, the error $E_4(t) := \widetilde{A}(t) - A(t)$ is bounded, for all vectors $v$, by*

$$\|E_4(t)v\| \le Ch^4\|D^3v\|, \qquad 0 \le t \le h. \tag{6.8}$$

*The constant $C$ depends only on $K$, $M_0$, $M_1$, and $c$.*

*Proof.* We insert (6.1) and (6.2) into (6.3):

$$\begin{aligned}
E_4(t) = &-\frac{1}{12}\int_0^t\int_0^t\int_0^t [A(\mu),[A(\tau),[A(\sigma),A(t)]]]\,d\sigma d\tau d\mu \\
&-\frac{1}{12}\int_0^t\int_0^t\int_0^\tau [A(\mu),[[A(\sigma),A(\tau)],A(t)]]\,d\sigma d\tau d\mu \\
&+\frac{1}{24}\int_0^t\int_0^\mu\int_0^t [[A(\sigma),A(\mu)],[A(\tau),A(t)]] d\tau d\sigma d\mu + R(t) \\
&+\frac{1}{24} r_4(\mathrm{ad}_{\widetilde{\Omega}})\left(\mathrm{ad}^3_{\widetilde{\Omega}}(\dot{\widetilde{\Omega}})\right)
\end{aligned}$$

Here, $R(t)v$ contains integrals of commutators which, by (3.7), are bounded by

$$C\big(h^5\|D^4v\| + h^6\|D^5v\|\big) \le C'h^4\|D^3v\|$$

for $h\|D\| \le c$. The constant $C$ only depends on $K$. Then, by (3.7),

$$\|E_4(t)v\| \le Ch^4\|D^3v\| + \frac{1}{24}\|r_4(\mathrm{ad}_{\widetilde{\Omega}})\left(\mathrm{ad}^3_{\widetilde{\Omega}}(\dot{\widetilde{\Omega}})\right)v\|.$$

The bound (6.8) now follows from Lemma 6.1. □

Lemma 4.1 shows that $\widetilde{\varepsilon} = \widetilde{y} - y$ is bounded by

$$\|\widetilde{\varepsilon}(t)\| \le Ch^5 \max_{0\le\tau\le h} \|D^3y(\tau)\|, \qquad 0 \le t \le h.$$

Since we want to have a fourth order scheme, we use a quadrature formula $(b_i, c_i)_{i=1}^s$ of order $p \ge 4$. In (6.2) we replace $A$ by its interpolation polynomial $\widehat{A}$ in the nodes $t_n + c_jh$. The integrals can then be evaluated exactly. The quadrature error for $n = 0$ is given by

$$\begin{aligned} \widetilde{\Omega}_0 - \Omega_0 = &\int_0^h A(\tau)d\tau - \int_0^h \widehat{A}(\tau)d\tau \\ &- \left(\frac{1}{2}\int_0^h\int_0^\tau [A(\sigma), A(\tau)]d\sigma d\tau - \frac{1}{2}\int_0^h\int_0^\tau [\widehat{A}(\sigma), \widehat{A}(\tau)]d\sigma d\tau\right), \end{aligned} \tag{6.9}$$

and similarly for the general $n$th step with $A(t_n + \tau)$ instead of $A(\tau)$.

Lemma 6.4. *The quadrature error in the nth step satisfies*

$$\|(\widetilde{\Omega}_n - \Omega_n)v\| \le Ch^{p+1}\|Dv\|. \tag{6.10}$$

*The constant $C$ depends only on $M_m$ for $m \le p$ and $K_1$.*

*Proof.* For ease of notation we let $n = 0$. The error of the single integral in the representation of $\widetilde{\Omega}_n - \Omega_n$ is $O(h^{p+1})$. Assume that we use a quadrature rule with $s$ nodes. For estimating the error of the double integral we define the interpolation error

$$J(t) := A(t) - \widehat{A}(t) = h^s \int_0^1 \widehat{\kappa}_s(\theta, \vartheta)A^{(s)}(\theta h)d\theta, \qquad 0 \le t = \vartheta h \le h,$$

where $\widehat{\kappa}_s$ denotes the Peano kernel. The difficulty in the remaining proof comes from the fact that we have only $J(t) = O(h^s)$, but we need an $O(h^p)$ estimate. We use in addition $J(c_ih) = 0$ and $\int_0^h J(t)\,dt = O(h^{p+1})$. For the second term in (6.9) we write

$$\begin{aligned} &\int_0^h\int_0^\tau [A(\sigma), A(\tau)]\,d\sigma d\tau - \int_0^h\int_0^\tau [\widehat{A}(\sigma), \widehat{A}(\tau)]\,d\sigma d\tau \\ &\quad = \int_0^h\int_0^\tau \Big([\widehat{A}(\sigma), J(\tau)] + [J(\sigma), \widehat{A}(\tau)] + [J(\sigma), J(\tau)]\Big)\,d\sigma d\tau. \end{aligned}$$

Approximating the outer integral with the quadrature formula, the first term becomes

$$\int_0^h\int_0^\tau [\widehat{A}(\sigma), J(\tau)]\,d\sigma d\tau = h^{p+1}\int_0^1 \kappa_p(\theta)G^{(p)}(\theta h)\,d\theta,$$

where $\kappa_p$ is the Peano kernel, and

$$G(\tau) = \int_0^\tau [\widehat{A}(\sigma), J(\tau)]\,d\sigma.$$

Using Leibniz' rule, it is seen that the dominant term of $G^{(p)}(\tau)$ is $p\,[\widehat{A}(\tau), J^{(p-1)}(\tau)]$, so that by (3.6), for any vector $v$,

$$\|G^{(p)}(\theta h)v\| \leq C\|Dv\|.$$

This yields

$$\|\int_0^h \int_0^\tau [\widehat{A}(\sigma), J(\tau)]\, d\sigma d\tau\; v\| \leq Ch^{p+1}\|Dv\|. \tag{6.11}$$

For the second term, we use partial integration

$$\int_0^h \int_0^\tau [J(\sigma), \widehat{A}(\tau)]\, d\sigma d\tau = [\int_0^h J(\sigma)d\sigma, \int_0^h \widehat{A}(\mu)d\mu] - \int_0^h \int_0^\tau [J(\tau), \widehat{A}(\sigma)]\, d\sigma d\tau.$$

Here, for the last term, the bound was already given in (6.11). Using the quadrature formula for the integral over $J$, we have for the first term

$$[\int_0^h J(\sigma)d\sigma, \int_0^h \widehat{A}(\mu)d\mu] = h^{p+1}[\int_0^1 \kappa_p(\theta)J^{(p)}(\theta h)d\theta, \int_0^h \widehat{A}(\mu)d\mu].$$

Noting $J^{(p)}(t) = A^{(p)}(t)$ and using (3.6), this gives the bound

$$\|\int_0^h \int_0^\tau [J(\sigma), \widehat{A}(\tau)]\, d\sigma d\tau\; v\| \leq Ch^{p+1}\|Dv\|.$$

With (6.11), this proves (6.10). □

Lemma 6.5. *In the situation of Lemma* 6.4*,*

$$\|\exp(\widetilde{\Omega}_n)v - \exp(\Omega_n)v\| \leq Ch^{p+1}\|Dv\|.$$

*The constant $C$ depends only on $M_m$ for $m \leq p$ and $K_1$.*

*Proof.* The variation-of-constants formula yields

$$\exp\big(\widetilde{\Omega}_n\big)v - \exp(\Omega_n)v = \int_0^1 \exp\big((1-s)\Omega_n\big)\big(\widetilde{\Omega}_n - \Omega_n\big)\exp\big(s\widetilde{\Omega}_n\big)v\, ds.$$

By (6.10) we have

$$\|\big(\widetilde{\Omega}_n - \Omega_n\big)\exp\big(s\widetilde{\Omega}_n\big)v\| \leq Ch^{p+1}\|D\exp\big(s\widetilde{\Omega}_n\big)v\| \leq C'h^{p+1}\|Dv\|,$$

where the last inequality is obtained as in the proof of Lemma 5.1. This gives the stated bound. □

For $p \geq 4$, the local error $\varepsilon_n$ of the scheme (2.7) thus satisfies (4.7) with

$$\|\varepsilon_n\| \leq Ch^5 \max_{t_n \leq t \leq t_{n+1}} \|D^3 y(t)\|.$$

Hence, with (4.8), the global error is bounded by

$$\|e_n\| \leq Ct_n h^4 \max_{0 \leq t \leq t_n} \|D^3 y(t)\|,$$

and Theorem 3.2 is proved.

For the fourth order scheme (2.10), it can be verified that for all $v$,

$$\|(\widetilde{\Omega}_n - \Omega_n)v\| \leq Ch^5\|Dv\|.$$

Thus, (4.5) is again satisfied with $p = 4$ and $r = 2$. The remaining proof is then the same as for methods based on interpolatory quadrature.

**7. Numerical experiments.** To illustrate the theoretical results presented in this paper, we consider the Schrödinger equation

$$i\,\frac{\partial\psi}{\partial t} = -\tfrac{1}{2}\Delta\psi + b(x,t)\psi, \qquad x=(x_1,\dots,x_d)\in\mathbb{R}^d,\ t>0 \tag{7.1}$$

with a smooth ($C^\infty$) potential $b(x,t)$ that is $2\pi$-periodic in every coordinate direction $x_j$. We impose periodic initial conditions $\psi(x,0)=\psi_0(x)$. For ease of notation only, the following discussion is for the one-dimensional case $d=1$.

A standard space discretization is given by the pseudo-spectral method. Here, a trigonometric polynomial

$$\psi^N(x,t) = \sum_{k=-N/2}^{N/2-1} c_k^N(t)\, e^{ikx}$$

is determined such that the equations

$$\begin{aligned} i\dot\psi^N(x_\ell,t) &= -\tfrac{1}{2}\Delta\psi^N(x_\ell,t) + b(x_\ell,t)\psi^N(x_\ell,t)\\ \psi^N(x_\ell,0) &= \psi_0(x_\ell) \end{aligned}$$

are satisfied at the mesh-points $x_\ell = 2\pi\ell/N$ with $\ell = -N/2,\dots,N/2-1$. Setting $c^N(t) = \big(c_k^N(t)\big)$ the vector of Fourier coefficients, this amounts to solving

$$i\dot c^N = -\tfrac{1}{2}\widehat\Delta^N c^N + B^N(t)c^N\ , \tag{7.2}$$

where, in the case of one space dimension,

$$\widehat\Delta^N = -(\widehat D^N)^2 \qquad \text{with} \quad \widehat D^N = \mathrm{diag}\,(ik) \quad (k=-N/2,\dots,N/2-1),$$

and, with $F_N$ denoting the discrete Fourier transform of length $N$,

$$B^N(t) = F_N\,\mathrm{diag}\,\big(b(x_\ell,t)\big)F_N^{-1}.$$

We consider a one-dimensional example with data from [9], slightly modified to make the potential periodic with respect to the space interval $x\in[-\ell,\ell]$ for $\ell=10$:

$$b(x,t) = \tfrac{1}{2}\tfrac{\pi^2}{\ell^2}\big(1-\cos\tfrac{\pi x}{\ell}\big) + \sin^2(t)\tfrac{\pi}{\ell}\sin\tfrac{\pi x}{\ell}.$$

In the left picture of Figure 7.1 we give precision–step size diagrams at $t=1$ for four different initial values, where we used $N=128$ Fourier modes for the spatial discretization. As a smooth initial value, we used the eigenstate of the unforced harmoic oscillator to the lowest energy level, $\Psi(x,0) = e^{-x^2/2}$. The convergence curves of the exponential midpoint and the fourth-order Gauss method corresponding to the smooth initial data are the solid lines marked with circles. For the other three curves, initial data of finite energy is chosen as $c^N(0) = (I - i(\widehat D^N)^j)^{-1}v/\rho$, $j=1,2,3$, where $v$ is a vector of normally distributed random numbers, and $\rho$ is chosen such that $\|c^N(0)\|=1$. For $j=1$, the results are plotted in the dashdotted curve marked with $\times$ symbols, for $j=2$, we have the dashed curved marked with $+$ symbols, and for $j=3$, the curve is dotted marked with diamonds.

For the right picture of Figure 7.1, we took the smooth initial state $\Psi(x,0) = e^{-x^2/2}$ for all curves but varied the number of Fourier modes from $N=32$ to $N=2048$

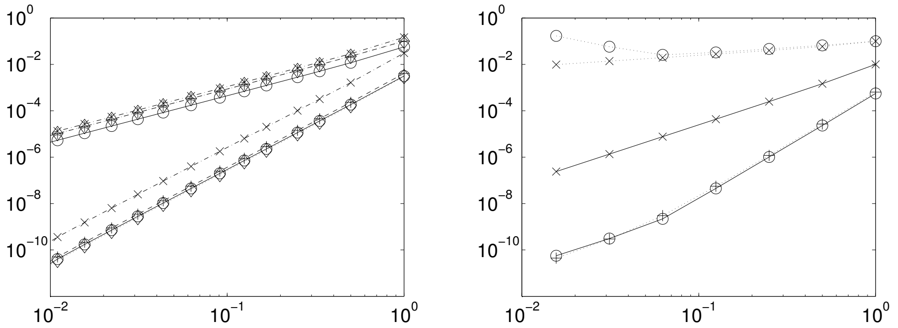


FIG. 7.1. *Error versus step sizes for the laser example: smooth and nonsmooth initial data on the left,* $h\|D\| = const$ *on the right.*

and the time steps such that $Nh = 32$. This corresponds to the situation that $\|hD\| \approx 3.5$, where $D = (-\frac{1}{2}\widehat{\Delta}^N + I)^{1/2}$. The solid line marked with the $\times$ symbol indicates the error of the midpoint rule, the solid line marked with circles is the error for the fourth order Gauss method and the dotted line marked with the $+$ symbols gives the error of the fourth order scheme with $\Omega$ taken from (2.10). The dotted lines in the top of the picture represent the errors of the exponential midpoint and the Gauss method divided by $h^2$ and $h^4$, respectively, up to a constant.

**8. Appendix. Commutator bounds for a spectral discretization.** We consider the pseudo-spectral space discretization (7.2) of the Schrödinger equation (7.1). Equation (7.2) is of the type studied in this paper, with $U = -\big(\widehat{D}^N\big)^2 + I$ and $V(t) = B^N(t) - I$. The matrix $B^N(t)$ is circulant, with $(k,l)$ entry equal to

$$\widehat{b}^N_{k-l}(t) = \sum_{q=-\infty}^{\infty} \widehat{b}_{k-l+qN}(t)$$

by the aliasing formula, where $\widehat{b}_j(t)$ is the $j$th Fourier coefficient of the $2\pi$-periodic (in $x$) function $b(x,t)$. If (and only if) $b(x,t)$ is a $C^\infty$ function of $x$, the Fourier coefficients $\widehat{b}_j(t)$ decay faster than any negative power of $|j|$. It then follows that the entries of the matrix $B^N(t) = (b^N_{k,l})$ are bounded by

$$|b^N_{kl}| \le \begin{cases} \gamma_m(|k-l|+1)^{-m}, & |k-l| \le N/2 \\ \gamma_m(N-|k-l|)^{-m}, & |k-l| > N/2 \end{cases} \qquad (8.1)$$

for $k,l = -N/2,\dots,N/2-1$ with $\gamma_m$ $(m = 1,2,3,\dots)$ independent of $N$.

The commutator bound (3.6) is obtained as a direct consequence of the three lemmas below, for which we need to give a further definition. We say that a sequence of matrices $\mathcal{B} = (B^N)$, with $B^N$ of dimension $N \times N$, belongs to the class $\Gamma^\infty$, if the entries satisfy estimates (8.1) with all $\gamma_m$ independent of $N$. We denote by $\gamma(\mathcal{B}) = (\gamma_1, \gamma_2, \gamma_3, \dots)$ the sequence of smallest possible such numbers.

LEMMA 8.1. *If* $\mathcal{A} = (A^N)$ *and* $\mathcal{B} = (B^N)$ *are in* $\Gamma^\infty$*, then also* $\mathcal{AB} = (A^N B^N)$ *is in* $\Gamma^\infty$*, and* $\gamma(\mathcal{AB})$ *is bounded in terms of* $\gamma(\mathcal{A})$ *and* $\gamma(\mathcal{B})$.

The proof is by direct estimation and is not given here. The following result is shown in the proof of Lemma 3.1 in [7].

LEMMA 8.2. *If $\mathcal{B} = (B^N)$ is in $\Gamma^\infty$, then $[\widehat{\mathcal{D}}^2, \mathcal{B}] = \big([(\widehat{D}^N)^2, B^N]\big)$ is of the form*

$$[\widehat{\mathcal{D}}^2, \mathcal{B}] = \mathcal{M}_0 + \mathcal{M}_1 \widehat{\mathcal{D}} \ ,$$

*where $\mathcal{M}_0$ and $\mathcal{M}_1$ are in $\Gamma^\infty$, with $\gamma(\mathcal{M}_0)$ and $\gamma(\mathcal{M}_1)$ bounded in terms of $\gamma(\mathcal{B})$.*

The next lemma is proved in the same way.

LEMMA 8.3. *If $\mathcal{B} = (B^N)$ is in $\Gamma^\infty$, then $\widehat{\mathcal{D}}\mathcal{B} = (\widehat{D}^N B^N)$ is of the form*

$$\widehat{\mathcal{D}}\mathcal{B} = \mathcal{K}_0 + \mathcal{K}_1 \widehat{\mathcal{D}} \ ,$$

*where $\mathcal{K}_0$ and $\mathcal{K}_1$ are in $\Gamma^\infty$, with $\gamma(\mathcal{K}_0)$ and $\gamma(\mathcal{K}_1)$ bounded in terms of $\gamma(\mathcal{B})$.*

Repeated application of these lemmas shows that

$$[-(\widehat{D}^N)^2 + B^N(\tau_k), [\ldots, [-(\widehat{D}^N)^2 + B^N(\tau_1), \frac{d^m}{dt^m} B^N(\tau_0)]] \ldots] = \sum_{j=0}^{k} M_j^N (\widehat{D}^N)^j$$

with matrices $M_j^N$ bounded independently of $N$ and $\tau_0, \ldots, \tau_k$. This gives the desired commutator bound (3.6).

**Acknowledgment.** We thank Katina Lorenz for stimulating discussions on commutator bounds.

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