BIT Numer Math
DOI 10.1007/s10543-009-0215-2

On the convergence of splitting methods for linear evolutionary Schrödinger equations involving an unbounded potential

Christof Neuhauser · Mechthild Thalhammer

Received: 10 March 2008 / Accepted: 3 December 2008

Abstract In this paper, we study the convergence behaviour of high-order exponential operator splitting methods for the time integration of linear Schrödinger equations

$$\mathrm{i}\,\partial_t \psi(x,t) = -\tfrac{1}{2}\,\Delta\,\psi(x,t) + V(x)\,\psi(x,t)\,, \quad x \in \mathbb{R}^d\,,\ t \geq 0\,,$$

involving unbounded potentials; in particular, our analysis applies to potentials V defined by polynomials. We deduce a global error estimate which implies that any time-splitting method retains its classical convergence order for linear Schrödinger equations, provided that the exact solution of the considered problem fulfills suitable regularity requirements. Numerical examples illustrate the theoretical result.

Keywords Linear Schrödinger equations · Unbounded potential · Splitting methods · Convergence

Mathematics Subject Classification (2000) 65L05 · 65M12 · 65J10

1 Introduction

In the present paper, our concern is to study the convergence behaviour of high-order time-splitting methods for linear Schrödinger equations

$$\mathrm{i}\,\partial_t \psi(x,t) = -\tfrac{1}{2}\,\Delta\,\psi(x,t) + V(x)\,\psi(x,t)\,, \quad x \in \mathbb{R}^d\,,\ t \geq 0\,, \tag{1.1}$$

Communicated by Timo Eirola.

C. Neuhauser · M. Thalhammer (✉)
Institut für Mathematik, Leopold-Franzens Universität Innsbruck, 6020 Innsbruck, Austria
e-mail: Mechthild.Thalhammer@uibk.ac.at

C. Neuhauser
e-mail: Christof.Neuhauser@uibk.ac.at

Published online: 21 February 2009

involving *unbounded* real-valued potentials $V:\mathbb{R}^d\to\mathbb{R}$; in particular, our analysis applies to potentials that comprise a polynomial part and in addition a sufficiently often differentiable function with bounded derivatives. For the theoretical study of time discretisations for (1.1), as standard, the partial differential equation (1.1) is written as a linear evolution equation for $u(t)=\psi(\cdot,t)$

$$u'(t)=A\,u(t)+B\,u(t)\,,\quad t\geq 0\,,\qquad u(0)\text{ given,} \tag{1.2}$$

involving unbounded linear operators $A:D(A)\to X$ and $B:D(B)\to X$ on the underlying function space X. A second-order approximation to the value of the exact solution at time $h>0$ is obtained by the Strang splitting [20, 23]

$$u_1=\mathrm{e}^{\frac{1}{2}hB}\,\mathrm{e}^{hA}\,\mathrm{e}^{\frac{1}{2}hB}u_0\approx u(h)=\mathrm{e}^{h(A+B)}\,u(0)\,; \tag{1.3}$$

example methods of higher-order are found in [12, 17], see also Sect. 2.

The main result of the present work, deduced in Sect. 3, is a convergence estimate for exponential operator splitting methods of arbitrarily high order when applied to linear evolutionary problems of the form (1.2). We employ an abstract analytical framework that includes linear Schrödinger equations (1.1) and further evolution equations of parabolic type. Extending techniques previously exploited in [13, 15, 22], we show that any splitting method retains its classical convergence order, provided that the exact solution of (1.2) satisfies suitable regularity requirements. For simplicity, we restrict ourselves to equidistant time grids; however, it is straightforward to extend our convergence result to variable stepsizes, see also Remark 3.8. Applications to linear Schrödinger equations are the contents of Sect. 4. In particular, we discuss polynomial potentials and illustrate our theoretical error estimate by numerical examples.

The intention of the present work is to give insight in the convergence behaviour of high-order exponential operator splitting methods and makes a contribution to a better understanding of efficient space and time discretisation methods for nonlinear Schrödinger equations; an application of particular interest which arises in quantum physics is the phenomenon of Bose–Einstein condensation, modelled by a system of coupled Gross–Pitaevskii equations, see [2–5, 8–10, 18, 24], e.g.

Henceforth, we denote by C a generic constant with possibly different values at different occurrences.

2 Splitting methods for linear evolution equations

In this section, we introduce exponential operator splitting methods for the time integration of evolutionary equations (1.2) involving (unbounded) linear operators A and B. We employ the following general form of a splitting method that includes the example methods given in literature; for a detailed treatment of composition and splitting methods, we refer to [12, 17].

Splitting methods rely on the fact that the initial value problems

$$v'(t)=A\,v(t)\,,\quad t\geq 0\,,\qquad v(0)\text{ given,} \tag{2.1a}$$

Table 1 Exponential operator splitting methods of order p involving s compositions

Method		Order	#com.
McLachlan	McLachlan [12, V.3.1, (3.3), pp. 138–139]	$p=2$	$s=3$
Strang	Strang (1.3)	$p=2$	$s=2$
BM4-1	Blanes & Moan [6, Table 2, PRKS_6]	$p=4$	$s=7$
BM4-2	Blanes & Moan [6, Table 3, SRKN_6^b]	$p=4$	$s=7$
M4	McLachlan [12, V.3.1, (3.6), pp. 140]	$p=4$	$s=6$
S4	Suzuki [12, II.4, (4.5), pp. 41]	$p=4$	$s=6$
Y4	Yoshida [12, II.4, (4.4), pp. 40]	$p=4$	$s=4$
BM6-1	Blanes & Moan [6, Table 2, PRKS_{10}]	$p=6$	$s=11$
BM6-2	Blanes & Moan [6, Table 3, SRKN_{11}^b]	$p=6$	$s=12$
BM6-3	Blanes & Moan [6, Table 3, SRKN_{14}^a]	$p=6$	$s=15$
KL6	Kahan & Li [12, V.3.2, (3.12), pp. 144]	$p=6$	$s=10$
S6	Suzuki [12, II.4, (4.5), pp. 41]	$p=6$	$s=26$
Y6	Yoshida [12, V.3.2, (3.11), pp. 144]	$p=6$	$s=8$

$$w'(t) = B\, w(t)\,, \quad t \geq 0\,, \qquad w(0) \text{ given,} \tag{2.1b}$$

can be solved numerically in an accurate and efficient way. For some initial value $u_0 \approx u(0)$ and a constant time step $h > 0$, approximations u_n to the exact solution values $u(t_n)$ at time $t_n = nh$ are then determined through the recurrence relation

$$\begin{aligned} &u_n = \mathcal{S}\, u_{n-1}\,, \quad n \geq 1\,, \\ &\mathcal{S} = \prod_{j=1}^{s} \mathrm{e}^{hb_j B}\, \mathrm{e}^{ha_j A} = \mathrm{e}^{hb_s B}\, \mathrm{e}^{ha_s A} \cdots \mathrm{e}^{hb_1 B}\, \mathrm{e}^{ha_1 A}\,, \end{aligned} \tag{2.2}$$

involving certain (complex) coefficients $(a_j, b_j)_{j=1}^s$. We emphasise that for $t \neq 0$ the operators e^{tA} and e^{tB} do not commute, in general; throughout, the product in (2.2) is defined downwards.

A widely used symmetric second-order scheme, the so-called Strang [20] or symmetric Lie–Trotter [23] splitting, can be cast into the form (2.2) for $s = 2$ and

$$\begin{aligned} &a_1 = \tfrac{1}{2} = a_2\,, \qquad b_1 = 1\,, \qquad b_2 = 0\,, \quad \text{or} \\ &a_1 = 0\,, \qquad a_2 = 1\,, \qquad b_1 = \tfrac{1}{2} = b_2\,, \end{aligned} \tag{2.3a}$$

respectively; in both cases, the order conditions

$$a_1 + a_2 = 1\,, \qquad b_1 + b_2 = 1\,, \qquad b_1 a_1 + b_2 = \tfrac{1}{2}\,, \tag{2.3b}$$

are fulfilled. Fourth- and sixth-order symplectic partitioned Runge–Kutta and Runge–Kutta–Nyström methods were proposed in Blanes and Moan [6]; for further example methods, we refer to [12, 14, 16, 17, 21, 25], see also Table 1.

3 Convergence analysis

In the following, we deduce a global error estimate for exponential operator splitting methods of the form (2.2) when applied to linear evolution equations (1.2). Henceforth, we denote by $(X, \|\cdot\|_X)$ a (complex) Banach space with corresponding operator norm $\|\cdot\|_{X\leftarrow X}$. Our hypotheses on the (closed and densely defined) linear operators $A : D(A) \subset X \to X$ and $B : D(B) \subset X \to X$ are as follows, see Engel and Nagel [11] for a detailed treatment of one-parameter (semi)groups.

Hypothesis 3.1 The linear operators $A : D(A) \to X$ and $B : D(B) \to X$ generate $\mathcal{C}_0$-groups $(\mathrm{e}^{tA})_{t\in\mathbb{R}}$ and $(\mathrm{e}^{tB})_{t\in\mathbb{R}}$, respectively, such that

$$\left\|\mathrm{e}^{tA}\right\|_{X\leftarrow X} \leq \mathrm{e}^{\alpha|t|}\,, \qquad \left\|\mathrm{e}^{tB}\right\|_{X\leftarrow X} \leq \mathrm{e}^{\beta|t|}\,, \quad t\in\mathbb{R}\,,$$

for constants $\alpha, \beta \geq 0$.

For evolution equations of parabolic type we employ a more general assumption instead.

Hypothesis 3.2 The linear operators $A : D(A) \to X$ and $B : D(B) \to X$ generate $\mathcal{C}_0$-semigroups $(\mathrm{e}^{tA})_{t\geq 0}$ and $(\mathrm{e}^{tB})_{t\geq 0}$, respectively, such that

$$\left\|\mathrm{e}^{tA}\right\|_{X\leftarrow X} \leq \mathrm{e}^{\alpha t}\,, \qquad \left\|\mathrm{e}^{tB}\right\|_{X\leftarrow X} \leq \mathrm{e}^{\beta t}\,, \quad t\geq 0\,,$$

for constants $\alpha, \beta \geq 0$.

With the help of Hypothesis 3.1, it is straightforward to deduce the following stability result for high-order splitting methods (2.2).

Lemma 3.3 *Suppose that the method coefficients of the exponential operator splitting method* (2.2) *are real and that the assumptions of Hypothesis* 3.1 *hold. Then, the splitting operator $\mathcal{S}$ fulfills the bound*

$$\left\|\mathcal{S}^n\right\|_{X\leftarrow X} \leq \mathrm{e}^{C\,t_n}\,, \quad n\geq 0\,,$$

with constant $C = \alpha\,(|a_1| + \cdots + |a_s|) + \beta\,(|b_1| + \cdots + |b_s|)\,.$

Remark 3.4 The statement of Lemma 3.3 remains valid under Hypothesis 3.2 (replacing Hypothesis 3.1), provided that the method coefficients of the exponential operator splitting method (2.2) are non-negative (but possibly complex).

In order to derive a global error estimate for exponential operator splitting methods (2.2) when applied to abstract evolution equations (1.2), we make use of a *Lady Windermere argument*; that is, we employ the identity

$$u_n - u(t_n) = \mathcal{S}^n\big(u_0 - u(0)\big) - \sum_{j=0}^{n-1} \mathcal{S}^{n-j-1}\,d_{j+1}\,, \quad n\geq 0\,, \tag{3.1a}$$

where $d_{j+1} = u(t_{j+1}) - \mathcal{S}\, u(t_j)$. Estimating (3.1a) with the help of Lemma 3.3 further yields

$$\big\|u_n - u(t_n)\big\|_X \le C \left(\big\|u_0 - u(0)\big\|_X + \sum_{j=0}^{n-1} \big\|d_{j+1}\big\|_X \right), \quad n \ge 0. \tag{3.1b}$$

It remains to deduce a bound for the defect; for this purpose, we employ the following hypothesis. As standard, the iterated commutators are defined through

$$\mathrm{ad}_A^{j+1}(B) = \big[A, \mathrm{ad}_A^j(B)\big] = A\, \mathrm{ad}_A^j(B) - \mathrm{ad}_A^j(B) A\,, \quad j \ge 0\,, \tag{3.2}$$

where $\mathrm{ad}_A^0(B) = B$, see Hairer et al. [12, Chap. III.4.1].

Hypothesis 3.5 Let p denote the (classical) order of the exponential operator splitting method (2.2). Suppose that the estimate

$$\sum_{k=1}^{p+1} \sum_{\substack{\mu \in \mathbb{N}^k \\ |\mu| = p+1-k}} \left\| \prod_{\ell=1}^{k} \left(\mathrm{ad}_A^{\mu_\ell}(B)\, \mathrm{e}^{\zeta_\ell A} \right) \right\|_{X \leftarrow \mathcal{D}_{p+1}} \le C\,, \quad \zeta = (\zeta_1, \dots, \zeta_{p+1}) \in \mathbb{R}^{p+1}\,,$$

remains valid with a (suitably chosen) normed space $\mathcal{D}_{p+1} \subset X$.

For the sake of brevity, we meanwhile consider the Strang splitting (2.3a) only. In this case, we require Hypothesis 3.5 to be fulfilled for $p = 2$; that is, we employ the assumption

$$\begin{aligned} &\big\|B\, \mathrm{e}^{\zeta_3 A}\, B\, \mathrm{e}^{\zeta_2 A}\, B\, \mathrm{e}^{\zeta_1 A}\big\|_{X \leftarrow \mathcal{D}_3} + \big\|B\, \mathrm{e}^{\zeta_2 A}\, \mathrm{ad}_A(B)\, \mathrm{e}^{\zeta_1 A}\big\|_{X \leftarrow \mathcal{D}_3} \\ &\quad + \big\|\mathrm{ad}_A(B)\, \mathrm{e}^{\zeta_2 A}\, B\, \mathrm{e}^{\zeta_1 A}\big\|_{X \leftarrow \mathcal{D}_3} + \big\|\mathrm{ad}_A^2(B)\, \mathrm{e}^{\zeta_1 A}\big\|_{X \leftarrow \mathcal{D}_3} \le C \end{aligned} \tag{3.3}$$

for $\zeta \in \mathbb{R}^3$. Formally, the exact solution of the evolution equation (1.2) is given by $u(t_{n-1} + h) = \mathrm{e}^{h(A+B)}\, u(t_{n-1})$ for $h \ge 0$; alternatively, the representation by the variation-of-constants formula

$$u(t_{n-1} + h) = \mathrm{e}^{hA}\, u(t_{n-1}) + \int_0^h \mathrm{e}^{(h-\tau)A}\, B\, u(t_{n-1} + \tau)\, \mathrm{d}\tau$$

is valid. A repeated application of the above formula yields the following relation for the exact solution value

$$
\begin{aligned}
& u(t_n) = \big(\mathrm{e}^{hA} + \widehat{I}_1 + \widehat{I}_2 + \widehat{R}_3\big)\, u(t_{n-1})\,, \\
& \widehat{I}_1 = \int_0^h \widehat{g}_1(\tau_1)\,\mathrm{d}\tau_1\,, \qquad \widehat{I}_2 = \int_0^h \int_0^{\tau_1} \widehat{g}_2(\tau_1,\tau_2)\,\mathrm{d}\tau_2\mathrm{d}\tau_1\,, \\
& \widehat{R}_3 = \int_0^h \int_0^{\tau_1} \int_0^{\tau_2} \widehat{f}_2(\tau_1,\tau_2)\,\mathrm{e}^{(\tau_2-\tau_3)A}\,B\,\mathrm{e}^{\tau_3(A+B)}\,\mathrm{d}\tau_3\mathrm{d}\tau_2\mathrm{d}\tau_1\,, \\
& \widehat{f}_1(\tau_1) = \mathrm{e}^{(h-\tau_1)A}\,B\,, \qquad \widehat{f}_2(\tau_1,\tau_2) = \widehat{f}_1(\tau_1)\,\mathrm{e}^{(\tau_1-\tau_2)A}\,B\,, \\
& \widehat{g}_1(\tau_1) = \widehat{f}_1(\tau_1)\,\mathrm{e}^{\tau_1 A}\,, \qquad \widehat{g}_2(\tau_1,\tau_2) = \widehat{f}_2(\tau_1,\tau_2)\,\mathrm{e}^{\tau_2 A}\,.
\end{aligned}
\tag{3.4a}
$$

To obtain a similar expansion for the numerical approximation $\mathcal{S}u(t_{n-1})$, we apply the recurrence relation $\varphi_j(z) = \frac{1}{j!} + z\,\varphi_{j+1}(z)$ which holds true for the exponential functions

$$
\varphi_0(z) = \mathrm{e}^z, \qquad \varphi_j(z) = \tfrac{1}{(j-1)!}\int_0^1 \tau^{j-1}\,\mathrm{e}^{(1-\tau)z}\,\mathrm{d}\tau, \quad j \geq 1,\ z \in \mathbb{C};
$$

we note that $\varphi_j(tB): X \to X$ is a bounded linear operator, see also Hypothesis 3.1 and Hypothesis 3.2. Furthermore, we employ the algebraic identity

$$
\prod_{j=1}^{J} \big(K_j + L_j\big) = \prod_{\ell=1}^{J} K_\ell + \sum_{j=1}^{J} \prod_{\ell=j+1}^{J} K_\ell\, L_j \prod_{\ell=1}^{j-1} \big(K_\ell + L_\ell\big),
$$

valid for arbitrary linear operators K_j, L_j, $1 \leq j \leq J$. A stepwise expansion of the splitting operator $\mathcal{S}$ with the help of the above relations gives

$$
\begin{aligned}
& \mathcal{S}\, u(t_{n-1}) = \big(\mathrm{e}^{hA} + Q_1 + Q_2 + R_3\big)\, u(t_{n-1})\,, \\
& Q_1 = h \sum_{j_1=1}^{2} b_{j_1} \widehat{g}_1(c_{j_1}h)\,, \qquad Q_2 = \tfrac{1}{2} h^2 \sum_{j_1=1}^{2} \sum_{j_2=1}^{j_1} \eta_{j_1 j_2} b_{j_1} b_{j_2} \widehat{g}_2(c_{j_1}h, c_{j_2}h)\,, \\
& R_3 = h^3 \Big(b_1^3 \mathrm{e}^{a_2 hA} B^3 \varphi_3\big(b_1 hB\big)\mathrm{e}^{a_1 hA} + b_1^2 b_2 B \mathrm{e}^{a_2 hA} B^2 \varphi_2\big(b_1 hB\big)\mathrm{e}^{a_1 hA} \\
& \qquad + b_1 b_2^2 B^2 \varphi_2\big(b_2 hB\big)\mathrm{e}^{a_2 hA} B \varphi_1\big(b_1 hB\big)\mathrm{e}^{a_1 hA} + b_2^3 B^3 \varphi_3\big(b_2 hB\big)\mathrm{e}^{hA}\Big)\,,
\end{aligned}
\tag{3.4b}
$$

where $c_1 = a_1$ and $c_2 = a_1 + a_2 = 1$, see (2.3b); moreover, we set $\eta_{11} = \eta_{22} = 1$ and $\eta_{21} = 2$. The above expansions (3.4) imply

$$
d_n = \big(\widehat{S}_1 + \widehat{S}_2 + \widehat{R}_3 - R_3\big)\, u(t_{n-1})\,, \quad \widehat{S}_1 = \widehat{I}_1 - Q_1\,,\ \widehat{S}_2 = \widehat{I}_2 - Q_2\,. \tag{3.4c}
$$

In order to expand $\widehat{S}_1$ and $\widehat{S}_2$ further, we employ Taylor series expansions of the functions $\widehat{g}_1$ and $\widehat{g}_2$ about zero. Due to the fact that the order conditions (2.3b) are fulfilled, we obtain

$$
\begin{aligned}
\widehat{S}_1 &= \sum_{j_1=1}^{2} b_{j_1} \int_0^1 \int_0^h (1-\sigma)\big(\widehat{G}_1(\sigma,\tau_1) - \widehat{G}_1(\sigma, c_{j_1} h)\big)\, \mathrm{d}\tau_1\, \mathrm{d}\sigma\,,\\
\widehat{S}_2 &= \sum_{j_1=1}^{2} \sum_{j_2=1}^{j_1} \eta_{j_1 j_2}\, b_{j_1} b_{j_2}\\
&\quad \times \int_0^1 \int_0^h \int_0^{\tau_1} \big(\widehat{G}_2(\sigma,\tau_1,\tau_2) - \widehat{G}_2(\sigma, c_{j_1} h, c_{j_2} h)\big)\, \mathrm{d}\tau_2 \mathrm{d}\tau_1 \mathrm{d}\sigma\,,\\
\widehat{G}_1(\sigma,\tau_1) &= \tau_1^2\, \partial_{\tau_1^2} \widehat{g}_1(\sigma\tau_1)\,, \qquad \widehat{G}_2(\sigma,\tau_1,\tau_2) = \sum_{\ell=1}^{2} \tau_\ell\, \partial_{\tau_\ell} \widehat{g}_2(\sigma\tau_1, \sigma\tau_2)\,;
\end{aligned}
\tag{3.4d}
$$

the involved partial derivatives of $\widehat{g}_1$ and $\widehat{g}_2$ are equal to

$$
\begin{aligned}
\partial_{\tau_1^2} \widehat{g}_1(\tau_1) &= \mathrm{e}^{(h-\tau_1)A}\, \mathrm{ad}_A^2(B)\, \mathrm{e}^{\tau_1 A}\,,\\
\partial_{\tau_1} \widehat{g}_2(\tau_1,\tau_2) &= -\, \mathrm{e}^{(h-\tau_1)A}\, \mathrm{ad}_A(B)\, \mathrm{e}^{(\tau_1-\tau_2)A} B\, \mathrm{e}^{\tau_2 A}\,,\\
\partial_{\tau_2} \widehat{g}_2(\tau_1,\tau_2) &= -\, \mathrm{e}^{(h-\tau_1)A} B\, \mathrm{e}^{(\tau_1-\tau_2)A}\, \mathrm{ad}_A(B)\, \mathrm{e}^{\tau_2 A}\,.
\end{aligned}
\tag{3.4e}
$$

Estimating (3.4c) by means of (3.3) finally yields the local error estimate

$$
\big\| d_n \big\|_X \le C\, h^{p+1} \max_{t_{n-1} \le t \le t_n} \big\| u(t) \big\|_{\mathcal{D}_{p+1}} \tag{3.5}
$$

with $p = 2$ for the Strang splitting scheme (2.3a).

Following Thalhammer [22], the above considerations generalise to arbitrary splitting methods of the form (2.2); estimating (3.1b) with the help of (3.5) we thus obtain the convergence result stated below. We note that the derivation of Theorem 3.6 is not effected by exchanging the roles of A and B in (2.2). Concerning the (classical) order conditions for higher-order splitting methods, we refer to Hairer et al. [12], e.g., see also Thalhammer [22].

Theorem 3.6 *Suppose that the coefficients $a_j, b_j \in \mathbb{R}$, $1 \le j \le s$, of the exponential operator splitting method (2.2) fulfill the classical order conditions for $p \ge 1$. Assume further that the unbounded linear operators A and B satisfy the requirements of Hypothesis 3.1 and 3.5 for a suitably chosen normed space $\mathcal{D}_{p+1} \subset X$. Then, the error estimate*

$$
\big\| u_n - u(t_n) \big\|_X \le C \Big(\big\| u_0 - u(0) \big\|_X + h^p \max_{0 \le t \le t_n} \big\| u(t) \big\|_{\mathcal{D}_{p+1}} \Big)\,, \qquad 0 \le t_n \le T\,,
$$

is valid, provided that the exact solution of the linear evolutionary equation (1.2) remains bounded in $\mathcal{D}_{p+1}$.

Remark 3.7 The statement of Theorem 3.6 remains valid under the assumptions of Hypothesis 3.2 (replacing Hypothesis 3.1), provided that the method coefficients of the exponential operator splitting method (2.2) are non-negative (but possibly complex).

Remark 3.8 It is straightforward to extend the convergence estimate of Theorem 3.6 to non-equidistant time grids $0 = t_0 < t_1 < \cdots < t_N = T$ with associated stepsizes defined by $h_j = t_{j+1} - t_j$ for $0 \le j \le N-1$; in this case, for $0 \le t_n \le T$ the error bound

$$\|u_n - u(t_n)\|_X \le C \Big(\|u_0 - u(0)\|_X + \sum_{j=0}^{n-1} h_j^{p+1} \max_{t_j \le t \le t_{j+1}} \|u(t)\|_{\mathcal{D}_{p+1}} \Big)$$

follows.

4 Applications to linear Schrödinger equations

We next apply the convergence analysis given in Sect. 3 to linear Schrödinger equations (1.1), subject to asymptotic boundary conditions on the unbounded domain and a certain initial condition. We are primarily interested in problems involving *unbounded* real potentials $V : \mathbb{R}^d \to \mathbb{R}$; in particular, in Sect. 4.3, we discuss the case where V comprises a polynomial and in addition a sufficiently often differentiable function with bounded derivatives. For the spatial discretisation of (1.1), we employ the Hermite spectral method. Basic properties of the Hermite basis functions are collected in Sect. 4.1; we refer to Boyd [7] for a detailed description of spectral methods. We note that similar arguments apply to linear Schrödinger equations (1.1) that are subject to periodic boundary conditions and involve a large potential; in this case, Fourier techniques are applicable.

4.1 Hermite basis functions

Henceforth, we let $\mu = (\mu_1, \dots, \mu_d) \in \mathbb{N}^d$ denote a multi-index of non-negative integers and define $|\mu| = \mu_1 + \cdots + \mu_d$. Further, we employ the compact vector notation $x = (x_1, \dots, x_d) \in \mathbb{R}^d$ and set

$$x^\mu = x_1^{\mu_1} \cdots x_d^{\mu_d}, \qquad \partial^\mu = \partial_{x_1^{\mu_1}} \cdots \partial_{x_d^{\mu_d}}, \qquad \partial_{x_j^{\mu_j}} = \frac{\partial^{\mu_j}}{\partial x_j^{\mu_j}}; \tag{4.1}$$

as standard, $\Delta = \partial_{x_1}^2 + \cdots + \partial_{x_d}^2$ denotes the d-dimensional Laplace operator. We denote by $\mathcal{C}_0^\infty(\mathbb{R}^d)$ the space of infinitely many times differentiable functions with compact support. The Lebesgue space $L^2(\mathbb{R}^d) = L^2(\mathbb{R}^d, \mathbb{C})$ of square integrable complex-valued functions is endowed with scalar product and associated norm given by

$$(f \,|\, g)_{L^2} = \int_{\mathbb{R}^d} f(x)\, \overline{g(x)}\, \mathrm{d}x, \qquad \|f\|_{L^2} = \sqrt{(f \,|\, f)_{L^2}}, \quad f, g \in L^2(\mathbb{R}^d).$$

Moreover, the Banach space $L^\infty(\mathbb{R}^d)$ is endowed with the norm

$$\|f\|_{L^\infty} = \operatorname*{ess\,sup}_{x\in\mathbb{R}^d} \big|f(x)\big|.$$

The Sobolev space $H^m(\mathbb{R}^d)$ comprises all functions with partial derivatives up to order $m \geq 0$ contained in $L^2(\mathbb{R}^d)$; the associated norm $\|\cdot\|_{H^m}$ is defined through

$$\|f\|_{H^m}^2 = \sum_{\substack{\mu\in\mathbb{N}^d\\ |\mu|\leq m}} \|\partial^\mu f\|_{L^2}^2, \quad f \in H^m(\mathbb{R}^d).$$

Detailed information on Sobolev spaces is found in the monograph Adams [1].

We let $H_{\mu_j} : \mathbb{R} \to \mathbb{R} : x_j \mapsto H_{\mu_j}(x_j)$ denote the Hermite polynomial of degree $\mu_j \geq 0$ that is normalised with respect to the weights $w_j(x_j) = \exp(-(\gamma_j\, x_j)^2)$. Then, for $\mu \in \mathbb{N}^d$ the Hermite function $\mathcal{H}_\mu : \mathbb{R}^d \to \mathbb{R} : x \mapsto \mathcal{H}_\mu(x)$ is defined by

$$\mathcal{H}_\mu(x) = \prod_{j=1}^{d} \mathcal{H}_{\mu_j}(x_j), \quad \mathcal{H}_{\mu_j}(x_j) = H_{\mu_j}(x_j)\, \mathrm{e}^{-\frac{1}{2}(\gamma_j\, x_j)^2}. \tag{4.2a}$$

The functions $(\mathcal{H}_\mu)$ form an orthonormal basis of the function space $L^2(\mathbb{R}^d)$; thus, for any $v \in L^2(\mathbb{R}^d)$ the representation

$$v = \sum_{\mu\in\mathbb{N}^d} v_\mu\, \mathcal{H}_\mu, \quad v_\mu = \big(v \,\big|\, \mathcal{H}_\mu\big)_{L^2}, \tag{4.2b}$$

follows. Furthermore, the eigenvalue relation

$$\tfrac{1}{2}\big(-\Delta + V_H\big)\,\mathcal{H}_\mu = \lambda_\mu\, \mathcal{H}_\mu, \quad \lambda_\mu = \sum_{j=1}^{d} \gamma_j^2\, \big(\mu_j + \tfrac{1}{2}\big), \tag{4.2c}$$

holds; here, we denote by $V_H : \mathbb{R}^d \to \mathbb{R}$ a scaled harmonic potential

$$V_H(x) = \sum_{j=1}^{d} \gamma_j^4\, x_j^2 \tag{4.2d}$$

involving positive weights $\gamma_j > 0$, $1 \leq j \leq d$. We note that the values of H_{μ_j} are computed through the recurrence relation

$$\begin{aligned} &H_0(x_j) = \sqrt[4]{\frac{\gamma_j^2}{\pi}}, \qquad H_1(x_j) = \sqrt{2}\,\gamma_j\, x_j\, H_0(x_j),\\ &H_{\mu_j}(x_j) = \frac{1}{\sqrt{\mu_j}}\big(\sqrt{2}\,\gamma_j\, x_j\, H_{\mu_j-1}(x_j) - \sqrt{\mu_j - 1}\, H_{\mu_j-2}(x_j)\big), \quad \mu_j \geq 2; \end{aligned} \tag{4.3a}$$

as a consequence, for the derivative of $\mathcal{H}_{\mu_j}$ the identity

$$\partial_{x_j} \mathcal{H}_{\mu_j} = -\frac{\gamma_j}{\sqrt{2}} \big(\sqrt{\mu_j + 1}\, \mathcal{H}_{\mu_j+1} - \sqrt{\mu_j}\, \mathcal{H}_{\mu_j-1}\big), \quad \mu_j \ge 1\,, \tag{4.3b}$$

is valid.

4.2 Splitting methods for Schrödinger equations

In this section, we relate linear Schrödinger equations of the form (1.1) to abstract evolution equations (1.2) and discuss the validity of Hypothesis 3.1; as underlying function space, we consider the Hilbert space $L^2(\mathbb{R}^d)$. Besides, we comment on the numerical solution of (1.1) by exponential operator splitting Hermite spectral methods.

Regarding the spatial discretisation, the unbounded linear operators A and B are constructed as follows. Let $\widetilde{A} : \mathcal{C}_0^\infty(\mathbb{R}^d) \to L^2(\mathbb{R}^d)$ be defined by

$$\big(\widetilde{A}v\big)(x) = \tfrac{1}{2}\big(-\Delta\, v(x) + V_H(x)\, v(x)\big)$$

for $v \in \mathcal{C}_0^\infty(\mathbb{R}^d)$. The Friedrich's extension $\widetilde{A}_F$ of $\widetilde{A}$ is a selfadjoint operator, see Reed and Simon [19], e.g.; consequently, by Stone's Theorem, see Engel and Nagel [11], e.g., the operator $A = -\mathrm{i}\,\widetilde{A}_F : D(A) = D(\widetilde{A}_F) \to L^2(\mathbb{R}^d)$ generates a unitary group $(\mathrm{e}^{tA})_{t\in\mathbb{R}}$ on $L^2(\mathbb{R}^d)$. We note that the domain of A can be characterised as

$$D(A) = \Big\{ v \in L^2(\mathbb{R}^d) : \sum_{\mu\in\mathbb{N}^d} \lambda_\mu^2\, |v_\mu|^2 < \infty \Big\}\,,$$

see (4.2). Moreover, we define the multiplication operator $\widetilde{B}$ through

$$\big(\widetilde{B}v\big)(x) = W(x)\, v(x) = \big(V(x) - \tfrac{1}{2}\, V_H(x)\big)\, v(x)\,;$$

under suitable assumptions on $W = V - \frac{1}{2}\, V_H$, the operator $\widetilde{B} : \mathcal{C}_0^\infty(\mathbb{R}^d) \to L^2(\mathbb{R}^d)$ is well-defined, positive, and symmetric. Thus, similarly to before, its Friedrich's extension $\widetilde{B}_F : D(\widetilde{B}_F) \to L^2(\mathbb{R}^d)$ is a selfadjoint operator; again, by Stone's Theorem, it is ensured that $B = -\mathrm{i}\,\widetilde{B}_F : D(B) = D(\widetilde{B}_F) \to L^2(\mathbb{R}^d)$ generates a unitary group $(\mathrm{e}^{tA})_{t\in\mathbb{R}}$ on $L^2(\mathbb{R}^d)$. Altogether, it follows

$$\big\|\mathrm{e}^{tA}\big\|_{L^2\leftarrow L^2} = 1\,, \qquad \big\|\mathrm{e}^{tB}\big\|_{L^2\leftarrow L^2} = 1\,, \quad t \ge 0\,; \tag{4.4}$$

that is, Hypothesis 3.1 is fulfilled with $\alpha = 0$ and $\beta = 0$. Furthermore, we conclude that the splitting operator $\mathcal{S}$, defined in (2.2), is a unitary operator on $L^2(\mathbb{R}^d)$; more precisely, the relations in (4.4) imply the stability result

$$\big\|\mathcal{S}^n\, u_0\big\|_{L^2} = \big\|u_0\big\|_{L^2}\,, \quad n \ge 0\,, \tag{4.5}$$

for any initial value $u_0 \in L^2(\mathbb{R}^d)$, see also Lemma 3.3.

The practical realisation of exponential operator splitting methods (2.2) for linear Schrödinger equations (1.1) relies on the following approach. On the one hand, the numerical solution of (2.1a) is based on a spectral decomposition of the initial value into Hermite basis functions

$$v(t) = \mathrm{e}^{tA}\, v(0) = \sum_{\mu \in \mathbb{N}^d} v_\mu\, \mathrm{e}^{-\mathrm{i}\, t \lambda_\mu}\, \mathcal{H}_\mu\,, \quad t \geq 0\,, \qquad v(0) = \sum_{\mu \in \mathbb{N}^d} v_\mu\, \mathcal{H}_\mu\,, \tag{4.6a}$$

see (4.2); on the other hand, a rapid componentwise multiplication yields an approximation to the solution $w(t) = \psi(\cdot, t)$ of (2.1b)

$$\psi(x,t) = \mathrm{e}^{-\mathrm{i}\, t\, W(x)}\, \psi(x,0)\,, \quad t \geq 0\,. \tag{4.6b}$$

For details on the implementation, we refer to Caliari et al. [8] and references given therein.

4.3 Potentials defined by polynomials

In this section, we study the special case where the unbounded linear operator

$$B = B_1 + B_2 \tag{4.7}$$

comprises a polynomial part B_1 and in addition an operator B_2 that is defined through a sufficiently often differentiable function with bounded derivatives. As in Sect. 3, in the derivation, we restrict ourselves to the consideration of the Strang splitting method (2.3a); that is, we characterise the normed space $\mathcal{D}_3$ in assumption (3.3). Similar though more tedious calculations then yield the stated result for a general splitting method.

Regarding (3.3), we remark that the iterated commutator $\mathrm{ad}_A^k(B)$ defined by (3.2) is a differential operator of order k. More precisely, it holds

$$\mathrm{ad}_A(B)\, v = \sum_{j=1}^{d} \Big(\partial_{x_j} W\, \partial_{x_j} + \tfrac{1}{2}\, \partial_{x_j^2} W \Big)\, v\,, \tag{4.8a}$$

$$\mathrm{ad}_A^2(B)\, v = \mathrm{i} \sum_{j,\ell=1}^{d} \Big(\partial_{x_j x_\ell} W\, \partial_{x_j x_\ell} + \partial_{x_j x_\ell^2} W\, \partial_{x_j} + \tfrac{1}{4}\, \partial_{x_j^2 x_\ell^2} W + \tfrac{1}{d}\, \partial_{x_j} V_H\, \partial_{x_j} W \Big)\, v\,, \tag{4.8b}$$

where $\partial_{x_j} V_H(x) = 2\, \gamma_j^4\, x_j$, see (4.2d).

The following considerations rely on the fact that the Hermite functions $(\mathcal{H}_\mu)$ form an orthonormal basis of the function space $L^2(\mathbb{R}^d)$; thus, for any $v \in L^2(\mathbb{R}^d)$ the representation

$$v = \sum_{\mu \in \mathbb{N}^d} v_\mu \mathcal{H}_\mu \tag{4.9}$$

is valid, see also (4.2).

As a first step, we study the unbounded linear operators P_κ and Q_κ that are defined through

$$\big(P_\kappa\, v\big)(x) = x^\kappa\, v(x)\,, \qquad \big(Q_\kappa\, v\big)(x) = \partial^\kappa v(x)\,, \quad \kappa \in \mathbb{N}^d\,, \tag{4.10}$$

see (4.1); the following auxiliary result implies that P_κ and Q_κ are well-defined on the normed space

$$D_\kappa = \Big\{ v \in L^2(\mathbb{R}^d) : \|v\|_{D_\kappa} < \infty \Big\}, \quad \|v\|_{D_\kappa}^2 = \sum_{\mu \in \mathbb{N}^d} (\mu+\kappa)^\kappa \, |v_\mu|^2 ; \tag{4.11}$$

here, we set $(\mu+\kappa)^\kappa = (\mu_1+\kappa_1)^{\kappa_1} \cdots (\mu_d+\kappa_d)^{\kappa_d}$.

Lemma 4.1 (i) *The functions $x \mapsto x^\kappa \mathcal{H}_\mu(x)$ and $\partial^\kappa \mathcal{H}_\mu$ can be represented by a finite linear combination of Hermite basis functions; more precisely, the identities*

$$\big(P_\kappa \mathcal{H}_\mu\big)(x) = \sum_{\substack{\nu \in \mathbb{Z}^d \\ |\nu_j| \le \kappa_j}} c_{\mu+\nu} \, \mathcal{H}_{\mu+\nu}(x) , \qquad \big(Q_\kappa \mathcal{H}_\mu\big)(x) = \sum_{\substack{\nu \in \mathbb{Z}^d \\ |\nu_j| \le \kappa_j}} d_{\mu+\nu} \, \mathcal{H}_{\mu+\nu}(x) ,$$

hold with real coefficients $(c_{\mu+\nu})$ and $(d_{\mu+\nu})$ that fulfill the bound

$$c_{\mu+\nu}^2 + d_{\mu+\nu}^2 \le C \, (\mu+\kappa)^\kappa$$

for a constant $C > 0$ that depends on κ.

(ii) *The linear operator $\mathrm{e}^{tA} : D_\kappa \to D_\kappa$ is unitary, that is, the relation*

$$\big\| \, \mathrm{e}^{tA} \big\|_{D_\kappa \leftarrow D_\kappa} = 1$$

is valid for all $t \ge 0$.

(iii) *For any $\eta \in \mathbb{N}^k$ the following estimate*

$$\big\| P_\kappa \big\|_{D_\eta \leftarrow D_{\eta+\kappa}} + \big\| Q_\kappa \big\|_{D_\eta \leftarrow D_{\eta+\kappa}} \le C \tag{4.12}$$

remains valid with a constant C that depends on κ.

Proof (i) On the one hand, we repeatedly apply the relation

$$x_j \, \mathcal{H}_{\mu_j}(x_j) = \frac{1}{\gamma_j} \left(\sqrt{\frac{\mu_j+1}{2}} \, \mathcal{H}_{\mu_j+1}(x_j) + \sqrt{\frac{\mu_j}{2}} \, \mathcal{H}_{\mu_j-1}(x_j) \right)$$

that is a direct consequence of (4.2a) and the recurrence formula (4.3); this yields

$$x_j^{\kappa_j} \mathcal{H}_{\mu_j}(x_j) = \sum_{\substack{\ell \in \mathbb{Z} \\ |\ell| \le \kappa_j}} \widetilde{c}_{\mu_j \ell} \, \mathcal{H}_{\mu_j+\ell}(x_j) , \quad \widetilde{c}_{\mu_j \ell}^{\,2} \le C \, (\mu_j+\kappa_j)^{\kappa_j} ,$$

with constant C depending on κ_j. Thus, we finally obtain

$$x^\kappa \, \mathcal{H}_\mu(x) = \prod_{j=1}^d \Big(x_j^{\kappa_j} \mathcal{H}_{\mu_j}(x_j) \Big) = \sum_{\substack{\nu \in \mathbb{Z}^d \\ |\nu_j| \le \kappa_j}} c_{\mu+\nu} \, \mathcal{H}_{\mu+\nu} ,$$

with coefficients $c_{\mu+\nu}^2$ that satisfy the bound $c_{\mu+\nu}^2 \le C\,(\mu+\kappa)^\kappa$ for some constant C depending on κ. Using that the relation

$$\partial_{x_j} \mathcal{H}_{\mu_j}(x_j) = \gamma_j \Bigg(-\sqrt{\frac{\mu_j+1}{2}}\, \mathcal{H}_{\mu_j+1}(x_j) + \sqrt{\frac{\mu_j}{2}}\, \mathcal{H}_{\mu_j-1}(x_j) \Bigg)$$

holds, see also (4.3b), similar considerations yield the statement for $\partial^\kappa \mathcal{H}_\mu$.

(ii) Due to the fact that A possesses the purely imaginary eigenvalues $(-\mathrm{i}\,\lambda_\mu)$, see also (4.2c), the identity

$$\big\| \mathrm{e}^{tA}\, v \big\|_{D_\kappa}^2 = \Big\| \sum_{\mu\in\mathbb{N}^d} v_\mu\, \mathrm{e}^{-\mathrm{i}\,t\lambda_\mu} \mathcal{H}_\mu \Big\|_{D_\kappa}^2 = \sum_{\mu\in\mathbb{N}^d} (\mu+\kappa)^\kappa\, \big|v_\mu\big|^2 = \|v\|_{D_\kappa}^2$$

remains true for all $t \ge 0$.

(iii) In the following, we derive the bound for $\|P_\kappa\|_{D_\eta \leftarrow D_{\eta+\kappa}}$; similar arguments then show the estimate involving Q_κ. Suppose v to be given by a finite linear combination of the form (4.9); by means of statement (i) we obtain

$$\big(P_\kappa\, v\big)(x) = x^\kappa\, v(x) = \sum_{\mu\in\mathbb{N}^d} v_\mu\, x^\kappa\, \mathcal{H}_\mu(x) = \sum_{\substack{\nu\in\mathbb{Z}^d\\ |\nu_j|\le\kappa_j}} \sum_{\mu\in\mathbb{N}^d} c_{\mu+\nu}\, v_\mu\, \mathcal{H}_{\mu+\nu}(x)\,.$$

Furthermore, due to the fact that the relation

$$\Big\| \sum_{\mu\in\mathbb{N}^d} c_{\mu+\nu}\, v_\mu\, \mathcal{H}_{\mu+\nu} \Big\|_{D_\eta}^2 \le C \sum_{\mu\in\mathbb{N}^d} (\mu+\eta)^\eta\, (\mu+\kappa)^\kappa\, |v_\mu|^2 \le C\, \|v\|_{D_{\eta+\kappa}}^2$$

is valid with a constant C depending on κ, the estimate

$$\big\| P_\kappa\, v \big\|_{D_\eta} \le \sum_{\substack{\mu\in\mathbb{N}^d\\ |\nu_j|\le\kappa_j}} \Big\| \sum_{\mu\in\mathbb{N}^d} c_{\mu+\nu}\, v_\mu\, \mathcal{H}_{\mu+\nu} \Big\|_{L^2} \le C\, \|v\|_{D_\kappa} \tag{4.13}$$

follows. A standard limiting process finally yields the desired result for any v of the form (4.9). □

We are now ready to characterise the normed space $\mathcal{D}_3$ in (3.3) for linear operators that are defined by a polynomial; namely, for a finite set $K \subset \mathbb{N}^d$ and real coefficients $(\omega_\kappa)_{\kappa\in K}$ we set

$$B_1 = -\,\mathrm{i}\, W_1\,, \qquad W_1 = \sum_{\kappa\in K} \omega_\kappa\, P_\kappa\,. \tag{4.14a}$$

With the help of Lemma 4.1, we obtain the following estimate

$$\big\| B_1 v \big\|_{D_\eta} \le C\, \|v\|_{D_{\eta+\widehat{\kappa}}}\,, \quad \widehat{\kappa}\in\mathbb{N}^d\,,\ \widehat{\kappa}_j = \max_{\kappa\in K} \kappa_j\,, \tag{4.14b}$$

involving a constant $C > 0$ that depends on $(\omega_\kappa)_{\kappa \in K}$ and $\kappa \in K$. Moreover, the relations in (4.8) and the bound (4.12) for the differential operator Q_κ imply

$$\left\| B_1 \,\mathrm{e}^{\zeta_3 A}\, B_1 \,\mathrm{e}^{\zeta_2 A}\, B_1 \,\mathrm{e}^{\zeta_1 A}\, v \right\|_{L^2} \leq C \, \|v\|_{D_{3\widehat{\kappa}}} ,$$

$$\left\| B_1 \,\mathrm{e}^{\zeta_2 A}\, \mathrm{ad}_A(B_1)\, \mathrm{e}^{\zeta_1 A}\, v \right\|_{L^2} + \left\| \mathrm{ad}_A(B_1)\, \mathrm{e}^{\zeta_2 A}\, B_1 \,\mathrm{e}^{\zeta_1 A}\, v \right\|_{L^2} \leq C \, \|v\|_{D_{2\widehat{\kappa}}} ,$$

$$\left\| \mathrm{ad}_A^2(B)\, \mathrm{e}^{\zeta_1 A}\, v \right\|_{L^2} \leq C \, \|v\|_{D_{\widehat{\kappa}}} ,$$

for any $\zeta \in \mathbb{R}^3$; in the present situation, the above estimates allow to choose $\mathcal{D}_3 = D_{3\widehat{\kappa}}$. In case that B involves an additional bounded function, the following result holds true; we omit the details.

Theorem 4.2 *Suppose that the exponential operator splitting method* (2.2) *has* (*classical*) *order p. Assume further that the unbounded linear operator* (4.7) *comprises a polynomial part of the form* (4.14a) *and that $B_2 = \mathrm{i}\, W_2$ is defined by a real-valued function W_2 such that* $\max\left\{ \|\partial^\mu W_2\|_{L^\infty} : |\mu| \leq 2p \right\}$ *remains bounded. Then, Hypothesis* 3.5 *is satisfied for $\mathcal{D}_{p+1} = D_{(p+1)\widehat{\kappa}}$, see also* (4.11) *and* (4.14b).

4.4 Illustrations

In this section, we illustrate our theoretical convergence result by numerical examples for the two-dimensional linear Schrödinger equation

$$\mathrm{i}\, \partial_t \psi(x,t) = \left(-\tfrac{1}{2}\, \Delta + \tfrac{1}{2}\, x_1^2 + x_2^2 + W(x) \right) \psi(x,t) , \quad x \in \mathbb{R}^2 ,\ t \geq 0 ; \tag{4.15}$$

we consider in particular the following unbounded potentials

$$W(x) = x_1^2 + 2\, x_2^2 , \tag{4.16a}$$

$$W(x) = x_1^2 + 2\, x_2^2 + \tfrac{3}{2}\, \cos(3\, x_1) + \tfrac{3}{2}\, \cos(3\, x_2) , \tag{4.16b}$$

$$W(x) = x_1 - \tfrac{3}{2}\, x_2 , \tag{4.16c}$$

$$W(x) = \tfrac{1}{20} \left(x_1^4 + 2\, x_2^4 \right) . \tag{4.16d}$$

For the first (somewhat artificial) problem (4.15)–(4.16a) the exact solution is computable in an easy manner by a suitable choice of the weights in the Hermite functions; we thus have at hand a reliable reference solution. The solution of the modified equation (4.15)–(4.16b) comprising an additional bounded part is illustrated in Fig. 1.

Obviously, it holds $\widehat{\kappa} = (2,2)$ for (4.16a) and (4.16b), $\widehat{\kappa} = (1,1)$ for (4.16c), and $\widehat{\kappa} = (4,4)$ for (4.16d), see (4.14b). To ensure that the exact solution of the problem fulfills the requirements of Theorem 3.6, see also Hypothesis 3.5 and Theorem 4.2, we choose $\psi(x,0) = \frac{1}{\sqrt{\pi}} \exp(-\frac{1}{2}(x_1^2 + x_2^2))$ as initial value for (4.16a)–(4.16c). On the other hand, for (4.16d), we evolve the corresponding ground state solution, computed by minimisation techniques, see also [8, 9].

The linear Schrödinger equation (4.15) is discretised in space by the Hermite pseudospectral method with 128 basis functions in each coordinate direction; in our implementation, we use Hermite polynomials, normalised with respect to the weight

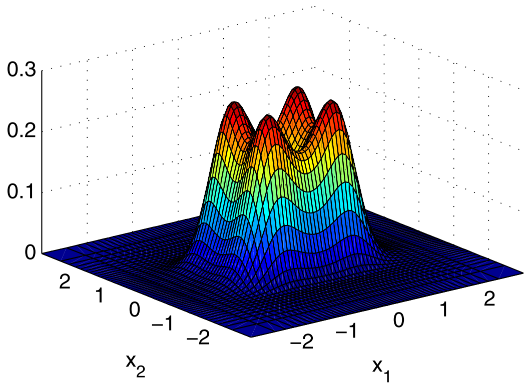

Fig. 1 Numerical solution of the linear Schrödinger equation (4.15) involving the unbounded potential (4.16b). Value of $|\psi(x_1, x_2, T)|^2$ at time $T = 8.98$ versus (x_1, x_2)

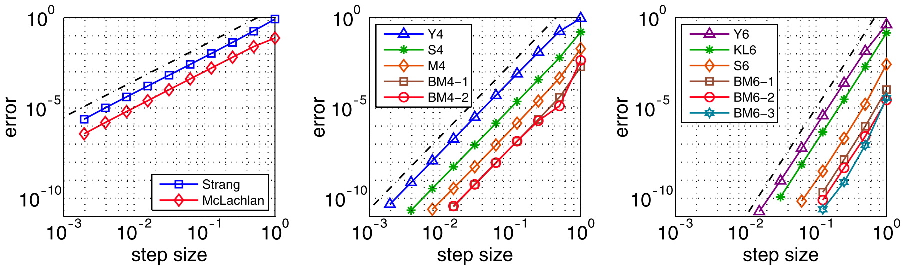

Fig. 2 Temporal orders of various time-splitting Hermite spectral methods when applied to the linear Schrödinger equation (4.15) involving the unbounded potential (4.16a). Error versus stepsize

$w_j(x_j) = \exp(-c_j^2 x_j^2)$ for some $c_j \in \mathbb{R}$, so that the corresponding Hermite functions are eigenfunctions of the operator $-\frac{1}{2}\Delta + x_1^2 + 2x_2^2$.

For the time integration, we apply several time-splitting methods of orders two, four, and six, proposed in [6, 14, 16, 21, 25], and further the Strang splitting (1.3), see also (2.3a) and Table 1. In the present situation, due to the fact that the additional condition $[B,[B,[B,A]]] = 0$ holds, also the Runge–Kutta–Nyström methods developed by Blanes and Moan [6] are consistent of orders four and six, respectively; however, in this case, exchanging the roles of A and B in (2.2) could lead to an order reduction. For time stepsizes $h = 2^{-j}$, $0 \le j \le 9$, we determine the numerical convergence orders of the integration methods at time $T = 1$; reference solutions are computed with stepsize 2^{-11}.

The numerical results, obtained for the potential (4.16a), are displayed in Fig. 2. We refer to the splitting schemes by the initials of the authors and their orders of convergence, see Table 1.

As expected, all splitting schemes retain their classical temporal convergence orders reflected by the slopes of the dashed-dotted lines. For the potentials (4.16b)–(4.16d), we included the results obtained for the second-order Strang splitting (1.3) and the fourth- and sixth-order Runge–Kutta–Nyström methods BM4-2 and BM6-3, which are favourable in view of their small error constants, see Fig. 3.

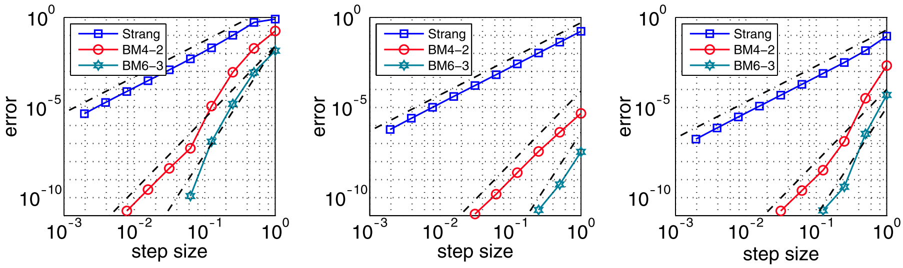

Fig. 3 Temporal orders of second, fourth and sixth-order time-splitting Hermite spectral methods when applied to the linear Schrödinger equation (4.15) involving the unbounded potential (4.16b) (*left*), (4.16c) (*middle*), and (4.16d) (*right*), respectively. Error versus stepsize

References

1. Adams, R.A.: Sobolev Spaces. Academic Press, San Diego (1978)
2. Bao, W., Shen, J.: A fourth-order time-splitting Laguerre–Hermite pseudospectral method for Bose–Einstein condensates. SIAM J. Sci. Comput. **26**(6), 2010–2028 (2005)
3. Bao, W., Jaksch, D., Markowich, P.: Numerical solution of the Gross–Pitaevskii equation for Bose–Einstein condensation. J. Comput. Phys. **187**, 318–342 (2003)
4. Bao, W., Du, Q., Zhang, Y.: Dynamics of rotating Bose–Einstein condensates and its efficient and accurate numerical computation. SIAM J. Appl. Math. **66**(3), 758–786 (2006)
5. Besse, C., Bidégaray, B., Descombes, S.: Order estimates in time of splitting methods for the nonlinear Schrödinger equation. SIAM J. Numer. Anal. **40**(5), 26–40 (2002)
6. Blanes, S., Moan, P.C.: Practical symplectic partitioned Runge–Kutta and Runge–Kutta–Nyström methods. J. Comput. Appl. Math. **142**, 313–330 (2002)
7. Boyd, J.: Chebyshev and Fourier Spectral Methods. Dover, New York (2000)
8. Caliari, M., Neuhauser, Ch., Thalhammer, M.: High-order time-splitting Hermite and Fourier spectral methods for the Gross–Pitaevskii equation. J. Comput. Phys. **228**, 822–832 (2009)
9. Caliari, M., Ostermann, A., Rainer, S., Thalhammer, M.: A minimisation approach for computing the ground state of Gross–Pitaevskii systems. J. Comput. Phys. **228**, 349–360 (2009)
10. Dion, C.M., Cancès, E.: Spectral method for the time-dependent Gross–Pitaevskii equation with a harmonic trap. Phys. Rev. E **67**, 046706 (2003)
11. Engel, K.-J., Nagel, R.: One-Parameter Semigroups for Linear Evolution Equations. Springer, New York (2000)
12. Hairer, E., Lubich, Ch., Wanner, G.: Geometric Numerical Integration. Structure-Preserving Algorithms for Ordinary Differential Equations. Springer, Berlin (2002)
13. Jahnke, T., Lubich, Ch.: Error bounds for exponential operator splittings. BIT **40**(4), 735–744 (2000)
14. Kahan, W., Li, R.-C.: Composition constants for raising the orders of unconventional schemes for ordinary differential equations. Math. Comput. **66**, 1089–1099 (1997)
15. Lubich, Ch.: On splitting methods for Schrödinger–Poisson and cubic nonlinear Schrödinger equations. Math. Comput. **77**, 2141–2153 (2008)
16. McLachlan, R.I.: On the numerical integration of ordinary differential equations by symmetric composition methods. SIAM J. Sci. Comput. **16**, 151–168 (1995)
17. McLachlan, R.I., Quispel, R.: Splitting methods. Acta Numer. **11**, 341–434 (2002)
18. Pérez–García, V.M., Liu, X.: Numerical methods for the simulation of trapped nonlinear Schrödinger equations. J. Appl. Math. Comput. **144**, 215–235 (2003)
19. Reed, M., Simon, B.: Methods of Modern Mathematical Physics. II: Fourier Analysis, Self-Adjointness. Academic Press, New York (1975)
20. Strang, G.: On the construction and comparison of difference schemes. SIAM J. Numer. Anal. **5**, 506–517 (1968)
21. Suzuki, M.: Fractal decomposition of exponential operators with applications to many-body theories and Monte Carlo simulations. Phys. Lett. A **146**, 319–323 (1990)

22. Thalhammer, M.: High-order exponential operator splitting methods for time-dependent Schrödinger equations. SIAM J. Numer. Anal. **46**(4), 2022–2038 (2008)
23. Trotter, H.F.: On the product of semi-groups of operators. Proc. Am. Math. Soc. **10**, 545–551 (1959)
24. Weishäupl, R., Schmeiser, Ch., Markowich, P., Borgna, J.: A Hermite pseudo-spectral method for solving systems of Gross–Pitaevskii equations. Commun. Math. Sci. **5**, 299–312 (2007)
25. Yoshida, H.: Construction of higher order symplectic integrators. Phys. Lett. A **150**, 262–268 (1990)