Exponential Runge–Kutta methods for the Schrödinger equation

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Abstract

We consider exponential Runge–Kutta methods of collocation type, and use them to solve linear and semi-linear Schrödinger Cauchy problems on the d-dimensional torus. We prove that in both cases (linear and non-linear) and with suitable assumptions, s-stage methods are of order s and we give sufficient conditions to achieve orders $s+1$ and $s+2$. We show and explain the effects of resonant time steps that occur when solving linear Schrödinger problems on a finite time interval with such methods. This work is inspired by [14], where exponential Runge–Kutta methods of collocation type are applied to parabolic Cauchy problems. We compare our results with those obtained for parabolic problems and provide numerical experiments for illustration.

Keywords
Exponential integrators, Runge–Kutta methods, Schrödinger equation.

1 Introduction

Exponential integrators are specific geometric integrators. They have become very popular recently for the numerical integration of first order in time problems (see for example [15], where their multiple discoveries from the 60's are recalled). For example, some specific exponential integrators have been used for solving the non-linear Schrödinger equation (see for example [3] where the numerical analysis is made in one periodical space dimension).

Exponential Runge–Kutta methods are particular exponential integrators. These methods have been derived and analysed for semi-linear *parabolic* Cauchy problems (see for example [14] for collocation methods and [13] for explicit methods).

This article deals with such exponential Runge–Kutta methods applied to the linear and semi-linear Schrödinger equations, namely

$$\begin{aligned} &\partial_t u(t,x) - \iota\Delta u(t,x) = f(t,x) && \text{(linear)} \\ \text{and} \qquad &\partial_t u(t,x) - \iota\Delta u(t,x) = f(t,u) && \text{(semi-linear)}, \end{aligned}$$

considered as Cauchy problems in time (no space discretisation is made). Of course, ι stands for the imaginary unit ($\iota^2 = -1$). The analysis in these cases is different from the one performed for parabolic problems since the spectra of the linear operators are different. We provide a numerical analysis of exponential Runge–Kutta methods of collocation type applied to linear and semi-linear problems on the d-dimensional torus ($d \in \mathbb{N}^*$). We show that s-stage collocation methods are of order s for suitable Sobolev norms. Moreover, we give algebraic sufficient conditions on the collocation points of an s-stage method to achieve orders $s+1$ and $s+2$ when solving Schrödinger Cauchy problems. These results need additional assumptions, for example on the non-linear term of semi-linear problems. These assumptions are fulfilled in many cases of interest, for example in the case of the cubic non-linear Schrödinger equation. We also mention, quantify and explain the effects of resonant time steps that appear when solving linear Schrödinger problems on a finite time interval.

Many other results for the finite-time integration of highly oscillatory (discretisations of) PDEs exist in the literature. For second-order in time problems, like wave equations, we mention the mollified impulse method analysed in [8] and generalised in [16], the Gautschi-type methods analysed in [12] and the analysis carried out in [9] based on a one-step formulation.

This paper is concerned with the numerical integration of Hamiltonian PDEs over a finite time interval. For results on numerical integration of Hamiltonian PDEs over long times, the reader may refer for example to [4, 5, 10] for results on the non-linear wave equation obtained via modulated Fourier expansions and to [7] for results on splitting methods applied to the linear Schrödinger equation with small potential.

Let us mention that many other geometric integrators exist to integrate numerically Schrödinger Cauchy problems. For example, some of them take advantage of the conservation of phase space properties by considering multisymplectic formulations (see for example [2]).

This article is organised as follows: in Section 2 we deal with exponential Runge–Kutta methods of collocation type applied to *linear* Schrödinger Cauchy problems. We first introduce some notation for these methods applied to linear problems. Then we look at order conditions for s-stage methods. We show that these methods are of order at least s and give sufficient conditions to achieve orders $s+1$ and $s+2$. Moreover, we study the effect of resonant time steps on the order constants. In section 3, we look at exponential Runge–Kutta methods of collocation type applied to *semi-linear* Schrödinger Cauchy problems. We set up some notation for these methods applied to non-linear problems. We prove, with suitable assumptions, that s-stage methods provide unique numerical solutions and are of order at least s. Moreover, we give sufficient order conditions for s-stage methods to be of order $s+1$ and $s+2$. We conclude the article with numerical experiments and some comments.

2 Linear problems

2.1 Notation

We denote by $\mathbb{T}$ the one-dimensional torus $\mathbb{R}/(2\pi\mathbb{Z})$. For all given positive integers d, we denote by $\mathbb{T}^d$ the d-dimensional torus. For $x=(x_1,\ldots,x_d)\in\mathbb{R}^d$ and $y=(y_1,\ldots,y_d)\in\mathbb{R}^d$, we denote by $x.y$ the real number $x_1y_1+\cdots+x_dy_d$ and by $|x|_2$ the non-negative real number $(x_1^2+\cdots+x_d^2)^{1/2}$. For $k\in\mathbb{Z}^d$, we denote by p_k the function on $\mathbb{T}^d$ defined for $x\in\mathbb{T}^d$ by $p_k(x)=e^{\iota k.x}$. $L^2(\mathbb{T}^d)$ (or simply L^2) denotes the set of (classes of) complex functions f on $\mathbb{T}^d$ such that $\int_{\mathbb{T}^d}|f(x)|^2\mathrm{d}x<+\infty$, endowed with the norm $\|f\|_{L^2(\mathbb{T}^d)}=\left((2\pi)^{-d}\int_{\mathbb{T}^d}|f(x)|^2\mathrm{d}x\right)^{1/2}$. An unbounded linear operator A acting on L^2 is said to be diagonal if for all $k\in\mathbb{Z}^d$, p_k is in the domain of A and there exists a $\lambda_k\in\mathbb{C}$ such that $Ap_k=\lambda_k p_k$. For example, the Laplace operator Δ acting on $L^2(\mathbb{T}^d)$ is diagonal since for all $k\in\mathbb{Z}^d$, $\Delta p_k=-|k|_2^2p_k$. Another example is the identity operator on L^2 denoted by Id. For all such A and all functions φ from $\mathbb{C}$ to itself, we denote by $\varphi(A)$ the unbounded diagonal linear operator acting on L^2 whose domain is the set of linear combinations of functions $(p_k)_{k\in\mathbb{Z}^d}$ defined for all $k\in\mathbb{Z}^d$ by

$$\varphi(A)p_k=\varphi(\lambda_k)p_k. \tag{2.1}$$

For all functions $f\in L^2$ and all $k\in\mathbb{Z}^d$, we denote by $\hat{f}_k$ the Fourier coefficient $(2\pi)^{-d}\int_{\mathbb{T}^d}f(x)e^{-\iota k.x}\mathrm{d}x$. For $\alpha\in\mathbb{R}^+$, we denote by $H^\alpha(\mathbb{T}^d)$ (or simply H^α) the space of (classes of) complex functions $f\in L^2(\mathbb{T}^d)$ such that $\sum_{k\in\mathbb{Z}^d\setminus\{0\}}|\hat{f}_k|^2|k|_2^{2\alpha}<+\infty$, endowed with the norm

$$\|f\|_{H^\alpha}=\Big(|\hat{f}_0|^2+\sum_{k\in\mathbb{Z}^d\setminus\{0\}}|\hat{f}_k|^2|k|_2^{2\alpha}\Big)^{1/2}.$$

Note that $L^2=H^0$ with the same norm. With these notations, if φ is a function from $\mathbb{C}$ to $\mathbb{C}$ bounded by $M\geq 0$ on $\iota\mathbb{R}$, then for all $h>0$ and $\alpha\geq 0$, $\varphi(\iota h\Delta)$ is a bounded linear operator from H^α to itself with[1] $\|\varphi(\iota h\Delta)\|_{H^\alpha\to H^\alpha}\leq M$. In

[1]Of course, for all $\alpha\geq 0$ and all linear operators A from H^α to itself, we denote

$$\|A\|_{H^\alpha\to H^\alpha}=\sup_{\substack{v\in H^\alpha\\ v\neq 0}}\frac{\|Av\|_{H^\alpha}}{\|v\|_{H^\alpha}}.$$

particular, we have for all $\alpha \geq 0$, $\|e^{\iota h\Delta}\|_{H^\alpha \to H^\alpha} = 1$.

Following [14], we set for all $k \in \mathbb{N}^*$

$$\forall z \in \mathbb{C}^*, \qquad \varphi_k(z) = \frac{1}{z^k}\Big(e^z - \sum_{p=0}^{k-1} \frac{z^p}{p!}\Big), \tag{2.2}$$

and $\varphi_k(0) = \frac{1}{k!}$. We also set $\varphi_0 = \exp$. Note that for all $k \in \mathbb{N}$, φ_k is holomorphic on $\mathbb{C}$, and is bounded on $\iota\mathbb{R}$. For all unbounded linear diagonal operator A and all $h > 0$, we have

$$\forall k \in \mathbb{N}, \qquad \varphi_{k+1}(-hA) = \frac{1}{h^{k+1}} \int_0^h e^{-(h-\tau)A} \frac{\tau^k}{k!} \mathrm{d}\tau. \tag{2.3}$$

In order to compute numerical solutions of the following Cauchy problem

$$\begin{array}{rcll} \partial_t u(t,x) + A\, u(t,x) & = & f(t,x) & (t,x) \in [0,T] \times \mathbb{T}^d \\ u(0,x) & = & u_0(x) & x \in \mathbb{T}^d, \end{array} \tag{2.4}$$

where $T > 0$, $A = -\iota\Delta$, u_0 and f are given, we consider the following numerical methods, called *exponential Runge–Kutta methods of collocation type*; we refer to [14] for a derivation of such methods for semi-linear problems based on the variation-of-constants formula:

$$\forall n \in \{0,\ldots,N\}, \qquad \left\{ \begin{array}{rcl} t_n & = & nh \\ u_{n+1} & = & e^{-hA} u_n + h \displaystyle\sum_{i=1}^{s} b_i(-hA) f(t_n + c_i h), \end{array} \right. \tag{2.5}$$

where $h > 0$, $s \in \mathbb{N}^*$, $(c_1,\ldots,c_s) \in [0,1]^s$ are given and $N = \lfloor T/h \rfloor$. We assume that for all $(i,j) \in \{1,\ldots,s\}^2$, $c_i \neq c_j$ if $i \neq j$. The operators $b_i(-hA)$ are defined by

$$\forall i \in \{1,\ldots,n\}, \qquad b_i(-hA) = \frac{1}{h} \int_0^h e^{-(h-\tau)A} l_i(\tau) \mathrm{d}\tau, \tag{2.6}$$

where for all $i \in \{1,\ldots,s\}$, l_i is the i-th Lagrange polynomial with respect to the points $(c_j h)_{j \in \{1,\ldots,s\}}$:

$$\forall i \in \{1,\ldots,s\}, \qquad l_i(\tau) = \prod_{j=1, j\neq i}^{s} \frac{\frac{\tau}{h} - c_j}{c_i - c_j}. \tag{2.7}$$

Note that for all $i \in \{1,\ldots,s\}$, $b_i \in \mathrm{span}(\varphi_0,\ldots,\varphi_{s-1})$. We therefore derive that b_i is holomorphic on $\mathbb{C}$ and is bounded on $\iota\mathbb{R}$.

In the case $A = 0$, the linear PDE (2.4) reduces to the collection of linear ODEs for $x \in \mathbb{T}^d$

$$\frac{\mathrm{d}u}{\mathrm{d}t}(t,x) = f(t,x) \qquad\qquad t \in [0,T],$$

with initial conditions $u(0,x) = u_0(x)$. Moreover, the exponential Runge–Kutta method (2.5) reduces to a classical Runge–Kutta method called the *underlying Runge–Kutta method* with coefficients $(b_i(0))_{i\in\{1,\dots,s\}}$ since for all $i \in \{1,\dots,s\}$, $b_i(-hA) = b_i(0)\mathrm{Id}$.

2.2 Order of exponential Runge–Kutta methods for linear problems

2.2.1 An s-stage method is of order s

Our first result shows that an s-stage exponential Runge–Kutta method of collocation type (2.5) applied to a linear Schrödinger problem (2.4) is of order at least s, provided that the right hand side of (2.4) is sufficiently smooth with respect to the time, when considered as an $L^2(\mathbb{T}^d)$-valued function. This somehow natural result is very similar to the one obtained in the context of parabolic linear equations in [14] (see Theorem 1). However, note that in the case of the linear Schrödinger equation, the order constant C does not depend on T.

Theorem 2.1 *An s-stage exponential Runge–Kutta method of collocation type* (2.5) *applied to a linear problem* (2.4) *such that $f \in C^s([0,T], L^2(\mathbb{T}^d))$ is of global order s in the sense that there exists a positive constant C depending only on $(c_1,\dots,c_s)$ such that for all $h>0$ and all $n \in \{0,\dots,N\}$,*

$$\|u_n - u(t_n)\|_{L^2} \le C\, h^s \int_0^{t_n} \|f^{(s)}(\tau)\|_{L^2}\, \mathrm{d}\tau. \tag{2.8}$$

Proof. Let us denote for all $n \in \{0,\dots,N\}$, $e_n = u_n - u(t_n)$. The variation-of-constants formula for the exact solution u of problem (2.4) reads for $h \in]0,T]$ and $t \in [0, T-h]$,

$$u(t+h) = e^{-hA}u(t) + \int_0^h e^{-(h-s)A} f(t+s)\mathrm{d}s. \tag{2.9}$$

Using Taylor expansions of f in (2.5) and (2.9) and the properties of the Lagrange collocation polynomials (2.7) involved in the functions $(b_i)_{i\in\{1,\dots,s\}}$ (see (2.6)), one has

$$\begin{aligned} e_{n+1} = e^{-hA}e_n &+ \int_0^h e^{-(h-\tau)A} \int_0^\tau \frac{(\tau-\sigma)^{s-1}}{(s-1)!} f^{(s)}(t_n+\sigma)\mathrm{d}\sigma\mathrm{d}\tau \\ &- \sum_{i=1}^s \int_0^h e^{-(h-\tau)A} l_i(\tau)\mathrm{d}\tau \int_0^{c_i h} \frac{(c_i h-\sigma)^{s-1}}{(s-1)!} f^{(s)}(t_n+\sigma)\mathrm{d}\sigma. \end{aligned} \tag{2.10}$$

Recall that $\|e^{-hA}\|_{L^2\to L^2} = 1$. Denoting $\delta_{n+1} = e_{n+1} - e^{-hA}e_n$, we have that for some constant C depending only on $c_1,\dots,c_s$,

$$\|\delta_{n+1}\|_{L^2} \le C\, h^s \int_{t_n}^{t_{n+1}} \|f^{(s)}(\tau)\|_{L^2}\, \mathrm{d}\tau.$$

This inequality and the relation

$$e_n = \sum_{p=0}^{n-1} e^{-phA}\delta_{n-p},$$

complete the proof. ■

Remark 2.2 Notice that for all $r > 0$, estimate (2.8) holds true with the $L^2(\mathbb{T}^d)$-norm replaced by the $H^r(\mathbb{T}^d)$-norm provided that $f \in C^s([0,T], H^r(\mathbb{T}^d))$.

2.2.2 Achieving order $s+1$

If its underlying Runge–Kutta method is of order $s+1$, then the exponential Runge–Kutta method of collocation type (2.5) applied to the linear Schrödinger problem (2.4) also has order $s+1$, provided that we assume that the the right-hand side of (2.4) has higher spatial regularity than just a standard L^2 one (see Theorem 2.4 for a precise statement). This is a difference with the case of parabolic linear equations studied in [14] (see Theorem 2). Let us first recall (see [14], formula (12)) that

Lemma 2.3 *If the underlying Runge–Kutta method is of order $s+1$, then*

$$\sum_{i=1}^{s} c_i^s b_i(0) = \frac{1}{s+1}. \tag{2.11}$$

We are now able to state the first result of this section:

Theorem 2.4 *Assume $r \geq 0$ is given, the underlying Runge–Kutta method is of order $s+1$ and $f \in C^{s+1}([0,T], L^2(\mathbb{T}^d))$ is such that $f^{(s)} \in C^1([0,T], H^{r+2})$. Then, the exponential Runge–Kutta method of collocation type (2.5) applied to the linear problem (2.4) is of order $s+1$ in the sense that there exists a positive constant C depending only on $(c_1, \ldots, c_s)$ such that we have for all $h > 0$ and all $n \in \{0, \ldots, N\}$,*

$$\|u(t_n) - u_n\|_{H^r} \leq C\,T\,h^{s+1}\Big(\|f^{(s)}(0)\|_{H^{r+2}} + \int_0^{t_n} \|f^{(s+1)}(\tau)\|_{H^{r+2}}\,\mathrm{d}\tau\Big). \tag{2.12}$$

Proof. With the notation of the previous proof, using another Taylor series expansion of f in (2.10), we write

$$\delta_{n+1} = \delta_{n+1}^{(1)} + \delta_{n+1}^{(2)},$$

with

$$\begin{aligned}\delta_{n+1}^{(1)} = \Big(&\int_0^h e^{-(h-\tau)A}\int_0^\tau \frac{(\tau-\sigma)^{s-1}}{(s-1)!}\mathrm{d}\sigma\mathrm{d}\tau \\ &-\sum_{i=1}^{s}\int_0^h e^{-(h-\tau)A} l_i(\tau)\mathrm{d}\tau \int_0^{c_i h}\frac{(c_i h-\sigma)^{s-1}}{(s-1)!}\mathrm{d}\sigma\Big) f^{(s)}(t_n),\end{aligned}$$

and, after integration by parts,

$$\delta_{n+1}^{(2)} = \int_0^h e^{-(h-\tau)A} \int_0^\tau \frac{(\tau-\sigma)^s}{s!} f^{(s+1)}(t_n+\sigma)\mathrm{d}\sigma\mathrm{d}\tau$$
$$- \sum_{i=1}^s \int_0^h e^{-(h-\tau)A} l_i(\tau)\mathrm{d}\tau \int_0^{c_i h} \frac{(c_i h-\sigma)^s}{s!} f^{(s+1)}(t_n+\sigma)\mathrm{d}\sigma. \quad (2.13)$$

Accordingly, we set

$$e_n^{(1)} = \sum_{p=0}^{n-1} e^{-phA}\delta_{n-p}^{(1)} \qquad \text{and} \qquad e_n^{(2)} = \sum_{p=0}^{n-1} e^{-phA}\delta_{n-p}^{(2)}.$$

Recall that $\|e^{\iota h\Delta}\|_{H^r\to H^r} = 1$. On one hand, for some constant $C_1 > 0$ depending only on $(c_1,\ldots,c_s)$,we have $\|\delta_{n+1}^{(2)}\|_{H^r(\mathbb{T}^d)} \le C_1\, h^{s+1} \int_{t_n}^{t_{n+1}} \|f^{(s+1)}(\tau)\|_{H^r(\mathbb{T}^d)}\,\mathrm{d}\tau$. Therefore, we derive that

$$\|e_n^{(2)}\|_{H^r(\mathbb{T}^d)} \le C_1\, h^{s+1} \int_{t_0}^{t_n} \|f^{(s+1)}(\tau)\|_{H^r(\mathbb{T}^d)}\,\mathrm{d}\tau. \quad (2.14)$$

On the other hand, since

$$\delta_{n+1}^{(1)} = h^{s+1}\big(\varphi_{s+1}(-hA) - \frac{1}{s!}\sum_{i=1}^s c_i^s b_i(-hA)\big) f^{(s)}(t_n),$$

an Abel summation yields

$$e_n^{(1)} = h^{s+1}\psi_{s+1}(-hA)$$
$$\Big(\big(\sum_{p=0}^{n-1} e^{-phA}\big) f^{(s)}(0) + \sum_{p=0}^{n-2}\big(\sum_{k=0}^{p} e^{-khA}\big)\big(f^{(s)}(t_{n-p-2}) - f^{(s)}(t_{n-p-1})\big)\Big),$$

where $\psi_{s+1}(z) = \varphi_{s+1}(z) - \frac{1}{s!}\sum_{i=1}^s c_i^s b_i(z)$. Since the underlying Runge–Kutta method is of order $s+1$, Lemma 2.3 and the fact that $\varphi_{s+1}(0) = ((s+1)!)^{-1}$ ensure that $\psi_{s+1}(0) = 0$. Moreover, ψ_{s+1} is a holomorphic function on $\mathbb{C}$ and is bounded on $\iota\mathbb{R}$. We derive that there exists a holomorphic function $\tilde{\psi}_{s+1}$ that is bounded on $\iota\mathbb{R}$ such that $\forall z \in \mathbb{C}$, $\psi_{s+1}(z) = z\tilde{\psi}_{s+1}(z)$. Hence, there exists a positive constant C_2 depending only on $(c_1,\ldots,c_s)$ such that $\|\tilde{\psi}_{s+1}(-hA)\|_{H^r(\mathbb{T}^d)\to H^r(\mathbb{T}^d)} \le C_2$. We derive that

$$\|e_n^{(1)}\|_{H^r(\mathbb{T}^d)} \le C_2 h^{s+1}\Big(\big\| -hA\big(\sum_{p=0}^{n-1} e^{-phA}\big) f^{(s)}(0)\big\|_{H^r(\mathbb{T}^d)}$$
$$+ \sum_{p=0}^{n-2} \big\| -hA\big(\sum_{k=0}^{p} e^{-khA}\big) \int_{t_{n-p-2}}^{t_{n-p-1}} f^{(s+1)}(\tau)\mathrm{d}\tau\big\|_{H^r(\mathbb{T}^d)}\Big).$$

For all $k \in \mathbb{Z}^d$ and $p \in \{0,\ldots,N-1\}$,

$$\Big| -\iota h|k|_2^2 \sum_{\ell=0}^{p} e^{-\iota\ell h|k|_2^2}\Big| \le (p+1)h|k|_2^2 \le T|k|_2^2. \quad (2.15)$$

Therefore, for all $p \in \{0, \dots, N-1\}$ and $u \in H^{r+2}$,

$$\Big\| - hA \sum_{\ell=0}^{p} e^{-\ell hA} u \Big\|_{H^r} \le T \|u\|_{H^{r+2}} . \tag{2.16}$$

This allows us to bound the H^r-norm of $e_n^{(1)}$. Together with estimate (2.14), this ensures that inequality (2.12) holds true. ∎

Note that the order constant in the previous result depends on T. This is also the case when the exponential Runge–Kutta method (2.5) is applied to a linear parabolic problem (see [14], Theorem 2). In the case of linear Schrödinger problems (2.4), if the underlying Runge–Kutta method is of order $s+1$, it is possible to get an order $s+1$ constant that does not depend on T, with a restriction on the values of the time step. The latter has to be non-resonant in the following sense:

Lemma 2.5 *Assume the following non-resonance condition on the time step $h > 0$: there exists $\gamma > 0$ and $\nu > 1$ such that*

$$\forall\, N \in \mathbb{N}^*, \qquad \left| \frac{1 - e^{\iota h N}}{h} \right| \ge \frac{\gamma}{N^\nu}. \tag{2.17}$$

Then we have for all $n \in \{0, \dots, N\}$, for all $r \ge 0$ and all $u \in H^{r+2\nu+2}(\mathbb{T}^d)$,

$$\Big\| - hA \sum_{p=0}^{n-1} e^{-phA} u \Big\|_{H^r(\mathbb{T}^d)} \le \frac{2}{\gamma} \|u\|_{H^{r+2\nu+2}(\mathbb{T}^d)} . \tag{2.18}$$

Proof. With the help of (2.17), we get for $k \in \mathbb{Z}^d \setminus \{0\}$,

$$\Big| - \iota h |k|_2^2 \sum_{p=0}^{n-1} e^{-\iota p h |k|_2^2} \Big| \le \Big| \frac{2h|k|_2^2}{1 - e^{-\iota h |k|_2^2}} \Big| \le \frac{2}{\gamma} |k|_2^{2\nu+2}.$$

Therefore, estimate (2.18) holds true. ∎

Note that the set of time steps $h \in (0, h_0)$ that do not satisfy (2.17) has a Lebesgue measure in $o(h_0)$ as h_0 tends to 0. See for example [11], Chapter 10, Lemma 6.3.

In addition to the restriction on the values of the time step, a higher spatial regularity of the right-hand side f of (2.4) is assumed to prove the following:

Theorem 2.6 *Assume that $r \ge 0$, $\gamma > 0$ and $\nu > 1$ are given. Assume that the underlying Runge–Kutta method is of order $s+1$ and $f \in C^{s+1}([0,T], L^2(\mathbb{T}^d))$ is such that $f^{(s)} \in C^1([0,T], H^{r+2\nu+2})$. Then the exponential Runge–Kutta method of collocation type (2.5) applied to the linear problem (2.4) is of order $s+1$ for non-resonant time steps in the sense that there exists a positive constant C depending only on $(c_1, \dots, c_s)$ and γ such that if $h > 0$ satisfies (2.17), then we have for all $n \in \{0, \dots, N\}$,*

$$\|u(t_n) - u_n\|_{H^r} \le C\, h^{s+1} \Big(\|f^{(s)}(0)\|_{H^{r+2\nu+2}} + \int_0^{t_n} \|f^{(s+1)}(\tau)\|_{H^{r+2\nu+2}} \,\mathrm{d}\tau \Big). \tag{2.19}$$

Proof. With the help of Lemma 2.5, estimate (2.16) can be replaced with estimate (2.18) in the proof of Theorem 2.4 to get

$$\|e_n^{(1)}\|_{H^r} \le 2\frac{C_2}{\gamma} h^{s+1}\Big(\|f^{(s)}(0)\|_{H^{r+2\nu+2}} + \int_{t_0}^{t_{n-1}} \|f^{(s+1)}(\tau)\|_{H^{r+2\nu+2}}\,\mathrm{d}\tau\Big). \quad (2.20)$$

In addition to (2.14), we derive that (2.19) holds true. ■

The effect of resonant time steps on the global error over the finite time interval $[0, T]$ is illustrated by numerical experiments in Section 4. In particular, one can see the difference between time steps satisfying (2.17) for which estimate (2.19) is sharp and those that do not satisfy (2.17) for which estimate (2.12) is sharp.

2.2.3 Concerning order $s + 2$

As in the case of exponential Runge–Kutta methods applied to linear parabolic problems studied in [14] (see Theorem 3), if its underlying Runge–Kutta method is of order $s + 2$ and one has sufficient spatial regularity in the right-hand side of (2.4), then the exponential Runge–Kutta method (2.5) applied to the linear problem (2.4) also has order $s + 2$. Before giving precise statements, let us recall the following: (see [14], Lemma 3)

Lemma 2.7 *If the underlying Runge–Kutta method is of order* $s + 2$*, then*

$$\sum_{i=1}^{s} c_i^{s+1} b_i(0) = \frac{1}{s+2}, \quad (2.21)$$

$$\sum_{i=1}^{s} c_i^{s} b_i'(0) = \frac{1}{(s+1)(s+2)}. \quad (2.22)$$

We are now able to prove the following:

Theorem 2.8 *Assume that* $r \ge 0$ *is given, the underlying Runge–Kutta method is of order* $s+2$ *and* $f \in C^{s+2}([0,T], L^2(\mathbb{T}^d))$ *is such that* $f^{(s)} \in C^2([0,T], H^{r+4})$*. Then the exponential Runge–Kutta method of collocation type* (2.5) *applied to the linear Schrödinger equation* (2.4) *is of order* $s + 2$ *in the sense that there exists a positive constant* C *depending only on* $(c_1, \dots, c_s)$ *such that for all* $h > 0$ *and all* $n \in \{0, \dots, N\}$*, we have*

$$\|u(t_n) - u_n\|_{H^r} \le C\,T\,h^{s+2}\Big(\|f^{(s)}(0)\|_{H^{r+4}} + \|f^{(s+1)}(0)\|_{H^{r+2}} + \int_0^{t_n} \|f^{(s+1)}(\tau)\|_{H^{r+4}}\,\mathrm{d}\tau + \int_0^{t_n} \|f^{(s+2)}(\tau)\|_{H^{r+2}}\,\mathrm{d}\tau\Big).$$

Proof. Let $\delta_{n+1}^{(2)}$ be defined by (2.13) and write $\delta_{n+1}^{(2)} = \delta_{n+1}^{(2,1)} + \delta_{n+1}^{(2,2)}$ with

$$\delta_{n+1}^{(2,1)} = h^{s+2}\Big(\varphi_{s+2}(-hA) - \frac{1}{(s+1)!}\sum_{i=1}^{s} c_i^{s+1} b_i(-hA)\Big) f^{(s+1)}(t_n),$$

and

$$\delta_{n+1}^{(2,2)} = \int_0^h e^{-(h-\tau)A} \int_0^\tau \frac{(\tau-\sigma)^{s+1}}{(s+1)!} f^{(s+2)}(t_n+\sigma)\mathrm{d}\sigma\mathrm{d}\tau$$
$$- \sum_{i=1}^s \int_0^h e^{-(h-\tau)A} l_i(\tau)\mathrm{d}\tau \int_0^{c_i h} \frac{(c_i h-\sigma)^{s+1}}{(s+1)!} f^{(s+2)}(t_n+\sigma)\mathrm{d}\sigma.$$

One deduces that there exists $C > 0$ depending only on $(c_1, \ldots, c_s)$ such that

$$\|\delta_{n+1}^{(2,2)}\|_{H^r} \leq C\, h^{s+2} \int_{t_n}^{t_{n+1}} \|f^{(s+2)}(\tau)\|_{H^r} \,\mathrm{d}\tau.$$

Therefore,

$$\begin{aligned} \|\sum_{p=0}^{n-1} e^{-phA} \delta_{n-p}^{(2,2)}\|_{H^r} &\leq C\, h^{s+2} \sum_{p=0}^{n-1} \int_{t_{n-p-1}}^{t_{n-p}} \|f^{(s+2)}(\tau)\|_{H^r} \,\mathrm{d}\tau \\ &\leq C\, h^{s+2} \int_{t_0}^{t_n} \|f^{(s+2)}(\tau)\|_{H^r} \,\mathrm{d}\tau. \end{aligned} \tag{2.23}$$

Since the underlying Runge–Kutta method is of order $s+2$, Lemma 2.7 ensures that $\sum_{i=1}^s c_i^{s+1} b_i(0) = \frac{1}{s+2}$ (see (2.21)). Moreover, $\varphi_{s+2}(0) = ((s+2)!)^{-1}$. Therefore, there exists a holomorphic function ζ_{s+2} on $\mathbb{C}$ such that

$$\forall z \in \mathbb{C}, \qquad \frac{1}{(s+1)!} \sum_{i=1}^s c_i^{s+1} b_i(z) - \varphi_{s+2}(z) = z\zeta_{s+2}(z).$$

Moreover, ζ_{s+2} is bounded on $\imath\mathbb{R}$. Hence, we have

$$\delta_{n+1}^{(2,1)} = -hAh^{s+2}\zeta_{s+2}(-hA) f^{(s+1)}(t_n),$$

and by an Abel summation,

$$\sum_{p=0}^{n-1} e^{-phA}\delta_{n-p}^{(2,1)} = h^{s+2}\zeta_{s+2}(-hA)\Big(-hA\big(\sum_{p=0}^{n-1} e^{-phA}\big) f^{(s+1)}(0)$$
$$+ \sum_{p=0}^{n-2} -hA\big(\sum_{k=0}^{p} e^{-khA}\big)\big(f^{(s+1)}(t_{n-p-2}) - f^{(s+1)}(t_{n-p-1})\big)\Big).$$

We derive with estimate (2.15) that there exists a positive constant C_1 depending only on $(c_1, \ldots, c_s)$ such that

$$\begin{aligned} &\|\sum_{p=0}^{n-1} e^{-phA}\delta_{n-p}^{(2,1)}\|_{H^r} \\ &\leq C_1\, T\, h^{s+2}\Big(\|f^{(s+1)}(0)\|_{H^{r+2}} + \int_{t_0}^{t_{n-1}} \|f^{(s+2)}(\tau)\|_{H^{r+2}}\,\mathrm{d}\tau\Big). \end{aligned} \tag{2.24}$$

To complete the proof, since the underlying Runge–Kutta method is of order $s+2$, we get by Lemmas 2.3 and 2.7 that $\sum_{i=1}^s c_i^s b_i(0) = \frac{1}{s+1}$ and $\sum_{i=1}^s c_i^s b_i'(0) = \frac{1}{(s+1)(s+2)}$ (see relation (2.22)). Therefore, there exists a holomorphic function κ_{s+2} on $\mathbb{C}$ such that $\varphi_{s+1}(z) - \frac{1}{s!}\sum_{i=1}^s c_i^s b_i(z) = z^2\kappa_{s+2}(z)$. Moreover, κ_{s+2} is bounded on $\imath\mathbb{R}$. As before, we get

$$\sum_{p=0}^{n-1} e^{-phA}\delta_{n-p}^{(1)} = -hh^{s+1}\kappa_{s+2}(-hA)\Big(-hA\big(\sum_{p=0}^{n-1} e^{-phA}\big)Af^{(s)}(0) + \sum_{p=0}^{n-2} -hA\big(\sum_{k=0}^{p} e^{-khA}\big)A\big(f^{(s)}(t_{n-p-2}) - f^{(s)}(t_{n-p-1})\big)\Big).$$

Therefore, using inequality (2.15), there exists a constant positive C_2 depending only on $(c_1,\dots,c_2)$ such that

$$\|\sum_{p=0}^{n-1} e^{-phA}\delta_{n-p}^{(1)}\|_{H^r} \leq C_2\, T\, h^{s+2}\Big(\|f^{(s)}(0)\|_{H^{r+4}} + \int_{t_0}^{t_{n-1}} \|f^{(s+1)}(\tau)\|_{H^{r+4}}\,\mathrm{d}\tau\Big). \qquad (2.25)$$

The conclusion follows by adding (2.23), (2.24) and (2.25) together. ■

In the previous theorem, the order constant depends on T. As in the previous section (see Theorem 2.6), if the underlying Runge–Kutta method is of order $s+2$, then the exponential Runge–Kutta method (2.5) applied to the linear Schrödinger problem (2.4) is of order $s+2$ with an order constant independent of T provided that the time step is non-resonant and the right-hand side f of (2.4) has higher spatial regularity. A precise statement is the following:

Theorem 2.9 *Assume that $r \geq 0$, $\gamma > 0$ and $\nu > 1$ are given as in Theorem 2.6. Assume that the underlying Runge–Kutta method is of order $s+2$ and that $f \in C^{s+2}([0,T], L^2(\mathbb{T}^d))$ is such that $f^{(s)} \in C^2([0,T], H^{r+2\nu+4}(\mathbb{T}^d))$. Then the exponential Runge–Kutta method of collocation type* (2.5) *applied to the linear Schrödinger equation* (2.4) *is of order $s+2$ for non-resonant time steps in the sense that there exists a positive constant C depending only on $(c_1,\dots,c_s)$ and γ such that if $h>0$ satisfies* (2.17)*, then we have for all $n \in \{0,\dots,N\}$,*

$$\|u(t_n) - u_n\|_{H^r} \leq C\, h^{s+2}\Big(\|f^{(s)}(0)\|_{H^{r+2\nu+4}} + \|f^{(s+1)}(0)\|_{H^{r+2\nu+2}} + \int_0^{t_n} \|f^{(s+1)}(\tau)\|_{H^{r+2\nu+4}}\,\mathrm{d}\tau + \int_0^{t_n} \|f^{(s+2)}(\tau)\|_{H^{r+2\nu+2}}\,\mathrm{d}\tau\Big).$$

Proof. With the help of Lemma 2.5, estimate (2.24) can be replaced by the following estimate

$$\|\sum_{p=0}^{n-1} e^{-phA}\delta_{n-p}^{(2,1)}\|_{H^r} \leq \frac{C_1}{\gamma} h^{s+2}\Big(\|f^{(s+1)}(0)\|_{H^{r+2\nu+2}} + \int_{t_0}^{t_{n-1}} \|f^{(s+2)}(\tau)\|_{H^{r+2\nu+2}}\,\mathrm{d}\tau\Big), \qquad (2.26)$$

where $C_1 > 0$ depends only on $(c_1, \dots, c_n)$. The same lemma yields the existence of a positive constant C_2 depending only on $(c_1, \dots, c_s)$ such that

$$\begin{aligned}
&\| \sum_{p=0}^{n-1} e^{-phA} \delta_{n-p}^{(1)} \|_{H^r} \\
&\leq \frac{C_2}{\gamma} h^{s+2} \Big(\|f^{(s)}(0)\|_{H^{r+2\nu+4}} + \int_{t_0}^{t_{n-1}} \|f^{(s+1)}(\tau)\|_{H^{r+2\nu+4}} \, \mathrm{d}\tau \Big). \quad (2.27)
\end{aligned}$$

This estimate replaces inequality (2.25). As in the proof of the previous theorem, the conclusion follows by adding (2.23), (2.26) and (2.27) together. ■

3 Semi-linear problems

3.1 Notation

We consider the following semi-linear Cauchy problem

$$\begin{array}{rclr}
\partial_t u(t,x) + A\, u(t,x) & = & g(t, u(t,x)) & (t,x) \in [0,T] \times \mathbb{T}^d \\
u(0,x) & = & u_0(x) & x \in \mathbb{T}^d
\end{array} \quad (3.1)$$

where $T > 0$, $A = -\iota\Delta$, $r \geq 0$, $u_0 \in H^r(\mathbb{T}^d)$ and g are given. In the following and in many applications, for all $t \in [0,T]$, $g(t)$ comes from a non-linear function from $\mathbb{C}$ to $\mathbb{C}$. For example, for the so-called cubic non-linear Schrödinger equation, $g(t,u) = g(t)(u) = i|u|^2 u$. In order to solve numerically the problem (3.1), we consider the following numerical methods, also called *exponential Runge–Kutta methods of collocation type*. We also refer to [14] for a derivation of such methods for semi-linear problems based on the variation-of-constants formula. We assume that $s \in \mathbb{N}^*$, $c_1, \dots, c_s \in [0,1]$, $h > 0$ are given and set $N = \lfloor T/h \rfloor$. We also assume that if $(i,j) \in \{1, \dots, s\}^2$ are such that $i \neq j$, then $c_i \neq c_j$. We denote for all $n \in \{0, \dots, N\}$, $t_n = nh$. For such n, if $u_n \in H^r(\mathbb{T}^d)$ is a given approximation of the exact solution $u(t_n)$ of the problem (3.1), then we construct an approximation u_{n+1} of $u(t_{n+1})$ by first solving the non-linear system consisting of the s following equations

$$u_{n,i} = e^{-c_i hA} u_n + h \sum_{j=1}^{s} a_{i,j}(-hA) g(t_n + c_j h, u_{n,j}), \qquad i \in \{1, \dots, s\}. \quad (3.2)$$

The s unknown quantities are $u_{n,1}, \dots, u_{n,s} \in H^r(\mathbb{T}^d)$ and the s^2 coefficients $(a_{i,j}(-hA))_{(i,j) \in \{1,\dots,s\}^2}$ are defined by

$$a_{i,j}(-hA) = \frac{1}{h} \int_0^{c_i h} e^{-(c_i h - \tau)A} l_j(\tau) \mathrm{d}\tau.$$

We recall that the $(l_j)_{j \in \{1,\dots,s\}}$ are the Lagrange polynomials defined in (2.7). Then, we define

$$u_{n+1} = e^{-hA} u_n + h \sum_{i=1}^{s} b_i(-hA) g(t_n + c_i h, u_{n,i}). \quad (3.3)$$

Recall that the coefficients $(b_i)_{i\in\{1,\dots,s\}}$ are defined in (2.6). Note that for all $(i,j) \in \{1,\dots,s\}^2$, $a_{i,j}(-hA) \in \mathrm{span}(\varphi_0(c_ihA),\dots,\varphi_{s-1}(c_ihA))$ and the coefficients in each linear combination depend only on the choice of the points $(c_1,\dots,c_s)$. Hence, each coefficient $a_{i,j}(z)$ is bounded on $\iota\mathbb{R}$ by a constant depending only on the choice of $(c_1,\dots,c_s)$. In the following, $\mathcal{C}$ denotes a bound of the functions $(b_i(z))_{i\in\{1,\dots,s\}}$ and $(a_{i,j}(z))_{(i,j)\in\{1,\dots,s\}^2}$ on $\iota\mathbb{R}$ depending only on the choice of $(c_1,\dots,c_s)$.

In the case $A = 0$, the non-linear Cauchy problem (3.1) reduces to the collection of non-linear ODEs for $x \in \mathbb{T}^d$

$$\frac{\mathrm{d}u}{\mathrm{d}t}(t,x) = g(t,u(t,x)), \qquad\qquad t \in [0,T],$$

with initial values $u(0,x) = u_0(x)$. Moreover, the exponential Runge–Kutta method of collocation type (3.2)-(3.3) reduces to a classical Runge–Kutta method whose coefficients are $(a_{i,j}(0))_{(i,j)\in\{1,\dots,s\}^2}$ and $(b_i(0))_{i\in\{1,\dots,s\}}$, since in that case for all $(i,j) \in \{1,\dots,s\}^2$,

$$a_{i,j}(-hA) = a_{i,j}(0)\mathrm{Id} \qquad \text{and} \qquad b_i(-hA) = b_i(0)\mathrm{Id}.$$

This method is called the *underlying Runge–Kutta method*.

For $t \in [0,T]$, we denote $f(t) = g(t,u(t))$, the right-hand side of (3.1), where u denotes the exact solution of the problem.

The space $H^r(\mathbb{T}^d)^s$ is a Hilbert space when endowed with the norm

$$\left\|(u_1,\dots,u_s)\right\|_{r,s} = \Big(\sum_{i=1}^{s} \left\|u_i\right\|^2_{H^r(\mathbb{T}^d)}\Big)^{1/2}. \tag{3.4}$$

For $R \geq 0$, we denote by $B(0,R)$ the set of $\boldsymbol{u} \in H^r(\mathbb{T}^d)^s$ such that $\left\|\boldsymbol{u}\right\|_{r,s} \leq R$.

3.2 Existence and uniqueness of the numerical solution

This section is devoted to the proof of existence and uniqueness of the numerical solution $(u_0,\dots,u_N)$ provided by the exponential Runge–Kutta method (3.2)-(3.3) of the semi-linear problem (3.1) for h sufficiently small and with some suitable assumptions on the exact solution and the right-hand side of (3.1). We will also give a first bound for the numerical error.

Our assumptions on the exact solution u of (3.1) and the non-linearity g are the following:

Hypothesis 3.1 *The function g satisfies:*

$$\forall t \in [0,T], \qquad g(t,0) = 0.$$

Hypothesis 3.2 *The non-linearity g in the right-hand side of* (3.1) *is Lipschitz-continuous in the sense that there exists $L > 0$ and $\rho > 0$ such that for all $t \in [0,T]$ and for all $u, v \in H^r(\mathbb{T}^d)$ satisfying $\|u\|_{H^r(\mathbb{T}^d)} \leq \rho$ and $\|v\|_{H^r(\mathbb{T}^d)} \leq \rho$, we have*

$$\|g(t,u) - g(t,v)\|_{H^r(\mathbb{T}^d)} \leq L\|u - v\|_{H^r(\mathbb{T}^d)} . \tag{3.5}$$

Hypothesis 3.3 *Equation* (3.1) *admits an exact solution $u : [0,T] \to H^r(\mathbb{T}^d)$ that is sufficiently smooth. In particular, there exists $R > 0$ such that for all $t \in [0,T]$, $\|u(t)\|_{H^r(\mathbb{T}^d)} \leq R$.*

Hypothesis 3.4 *The mapping $f : [0,T] \to H^r(\mathbb{T}^d)$ is sufficiently smooth.*

In applications, Hypothesis 3.4 will often be a consequence of Hypothesis 3.3 and of the regularity of the function g.

Note that these assumptions are fulfilled in many cases of interest, for example in the case of the cubic non-linear Schrödinger equation, at least when $r > d/2$ and $r - d/2 \notin \mathbb{N}$. This can be seen, for example, by adapting classical results of non-linear analysis (see for example [1], Chapter II, Proposition 2.2). Precise statements of the adaptations can be found in [6].

Under these assumptions, if ρ is sufficiently big (see (3.7)) and h is sufficiently small (see (3.6)), then for all $n \in \{0, \ldots, N\}$ the non-linear system (3.2) has a unique solution $(u_{n,1}, \ldots, u_{n,s}) \in H^r(\mathbb{T})^s$ such that $\|(u_{n,1}, \ldots, u_{n,s})\|_{r,s} \leq 3R\sqrt{s}$. Moreover, the approximation u_{n+1} defined by (3.3) is such that $\|u_{n+1}\|_{H^s(\mathbb{T}^d)} \leq 2R$. To prove these assertions, we start with the following lemma:

Lemma 3.5 *Assume that $h_0 > 0$ is such that*

$$h_0 \leq (3\mathcal{C}Ls^2)^{-1}, \tag{3.6}$$

and

$$\rho \geq 3R\sqrt{s}. \tag{3.7}$$

Then for all $h \in (0, h_0)$, $t \in [0, T-h]$ and $y \in H^r(\mathbb{T}^d)$ such that $\|y\|_{H^r(\mathbb{T}^d)} \leq 2R$, the non-linear system

$$\begin{array}{rcl} v_1 &=& e^{-c_1 hA} y + h \sum_{j=1}^{s} a_{1,j}(-hA) g(t + c_j h, v_j) \\ \vdots & & \vdots \\ v_s &=& e^{-c_s hA} y + h \sum_{j=1}^{s} a_{s,j}(-hA) g(t + c_j h, v_j), \end{array}$$

admits a unique solution $\boldsymbol{v} = (v_1, \ldots, v_s) \in B(0, 3R\sqrt{s})$.

Proof. For $h \in (0, h_0)$, $t \in [0, T-h]$, $y \in H^r(\mathbb{T}^d)$ such that $\|y\|_{H^r(\mathbb{T}^d)} \le 2R$, we define the function

$$f_{h,t,y} : \left(\begin{array}{ccc} H^r(\mathbb{T}^d)^s & \longrightarrow & H^r(\mathbb{T}^d)^s \\ (v_i)_{1 \le i \le s} & \longmapsto & \left(e^{-c_i hA} y + h \sum_{j=1}^s a_{i,j}(-hA) g(t + c_j h, v_j) \right)_{1 \le i \le s} \end{array} \right).$$

Hypothesis 3.2 and inequality (3.7) ensure that for all $(v_1, \dots, v_s) \in B(0, 3R\sqrt{s})$, we have

$$\|f_{t,h,y}(v_1, \dots, v_s) - (e^{-c_1 hA} y, \dots, e^{-c_s hA} y)\|_{r,s} \le \mathcal{C} h s^{3/2} L(3R\sqrt{s}).$$

Since $\|(e^{-c_1 hA} y, \dots, e^{-c_s hA} y)\|_{r,s} \le 2R\sqrt{s}$, the triangle inequality and (3.6) imply that

$$\|f_{t,h,y}(v_1, \dots, v_s)\|_{r,s} \le 3R\sqrt{s}.$$

Therefore, $f_{t,h,y}(B(0, 3R\sqrt{s})) \subset B(0, 3R\sqrt{s})$.
On the other hand, for $\boldsymbol{v} = (v_1, \dots, v_s) \in B(0, 3R\sqrt{s})$ and $\boldsymbol{w} = (w_1, \dots, w_s) \in B(0, 3R\sqrt{s})$, by Hypothesis 3.2 we have

$$\|f_{t,h,y}(\boldsymbol{v}) - f_{t,h,y}(\boldsymbol{w})\|_{r,s} \le \mathcal{C} L h s \|\boldsymbol{v} - \boldsymbol{w}\|_{r,s}.$$

Hence, using (3.6), one derives that

$$\|f_{t,h,y}(\boldsymbol{v}) - f_{t,h,y}(\boldsymbol{w})\|_{r,s} \le \frac{h}{h_0} \|\boldsymbol{v} - \boldsymbol{w}\|_{r,s}.$$

Since $h h_0^{-1} < 1$, equation $\boldsymbol{x} = f_{t,h,y}(\boldsymbol{x})$ has exactly one solution in $B(0, 3R\sqrt{s})$ by the classical Picard fixed-point theorem. ■

We are now able to prove that if h_0 satisfies another smallness condition, then, for all $h \in (0, h_0)$, the exponential Runge–Kutta method of collocation type (3.2)-(3.3) provides a unique numerical solution with for all $n \in \{0, \dots, N\}$, $\|(u_{n,1}, \dots, u_{n,s})\|_{r,s} \in B(0, 3R\sqrt{s})$ and $\|u_n\|_{H^r(\mathbb{T}^d)} \le 2R$. Moreover, such an s-stage method is of order s when applied to the semi-linear Schrödinger problem (3.1).

Theorem 3.6 *Assume Hypotheses 3.1, 3.2, 3.3 and 3.4 are satisfied with* (3.7). *Set* $\kappa_s = (s+1)\left(\frac{1}{s!} + \frac{\mathcal{C}s}{(s-1)!}\right)$. *Assume that* $h_0 > 0$ *satisfies* (3.6), *and*

$$h_0^s \le R\left(\kappa_s e^{2\mathcal{C}sTL} \int_0^T \|f^{(s)}(\tau)\|_{H^r(\mathbb{T}^d)} \mathrm{d}\tau\right)^{-1}. \tag{3.8}$$

Then, for all $h \in (0, h_0)$, *the exponential Runge–Kutta method* (3.2)-(3.3) *provides a unique numerical solution such that for all* $n \in \{0, \dots, N\}$, $\|u_n\|_{H^s(\mathbb{T}^d)} \le 2R$ *and* $\|(u_{n,1}, \dots, u_{n,s})\|_{r,s} \le 3R\sqrt{s}$. *Moreover, for all* $n \in \{0, \dots, N\}$,

$$\|u_n - u(t_n)\|_{H^r(\mathbb{T}^d)} \le \kappa_s e^{2\mathcal{C}sLT} h^s \int_0^{t_n} \|f^{(s)}(\tau)\|_{H^r(\mathbb{T}^d)} \mathrm{d}\tau. \tag{3.9}$$

We recall that for all $n \in \{0, \dots, N\}$, $0 \le t_n \le T$.

Proof. Let $h \in (0, h_0)$. We prove the result by induction. Assume $n \in \{0, \dots, N-1\}$ is such that $\|u_n\|_{H^r(\mathbb{T}^d)} \le 2R$. Lemma 3.5 ensures that the non-linear system (3.2) has a unique solution $(u_{n,1}, \dots, u_{n,s}) \in B(0, 3R\sqrt{s})$. Moreover, Hypotheses 3.3 and 3.4 ensure that, for the exact solution, we have

$$u(t_{n+1}) = e^{-hA}u(t_n) + h\sum_{i=1}^{s} b_i(-hA)f(t_n + c_i h) + \delta_{n+1}, \tag{3.10}$$

with

$$\begin{aligned}\delta_{n+1} = &\int_0^h e^{-(h-\tau)A}\int_0^\tau \frac{(\tau-\sigma)^{s-1}}{(s-1)!}f^{(s)}(t_n+\sigma)\mathrm{d}\sigma\mathrm{d}\tau \\ &-h\sum_{i=1}^{s} b_i(-hA)\int_0^{c_i h}\frac{(c_i h-\tau)^{s-1}}{(s-1)!}f^{(s)}(t_n+\tau)\mathrm{d}\tau,\end{aligned}$$

using the quadrature rule properties. Similarly, for all $i \in \{1, \dots, s\}$, we have

$$u(t_n + c_i h) = e^{-c_i hA}u(t_n) + h\sum_{j=1}^{s} a_{i,j}(-hA)f(t_n + c_j h) + \Delta_{n,i}, \tag{3.11}$$

where

$$\begin{aligned}\Delta_{n,i} = &\int_0^{c_i h} e^{-(c_i h-\tau)A}\int_0^\tau \frac{(\tau-\sigma)^{s-1}}{(s-1)!}f^{(s)}(t_n+\sigma)\mathrm{d}\sigma\mathrm{d}\tau \\ &-h\sum_{j=1}^{s} a_{i,j}(-hA)\int_0^{c_j h}\frac{(c_j h-\tau)^{s-1}}{(s-1)!}f^{(s)}(t_n+\tau)\mathrm{d}\tau.\end{aligned} \tag{3.12}$$

Hence, if we denote $e_n = u_n - u(t_n)$ and $e_{n,i} = u_{n,i} - u(t_n + c_i h)$, then we have

$$e_{n,i} = e^{-c_i hA}e_n + h\sum_{j=1}^{s} a_{i,j}(-hA)\big(g(t_n + c_j h, u_{n,j}) - f(t_n + c_j h)\big) - \Delta_{n,i}. \tag{3.13}$$

For all $i \in \{1, \dots, s\}$, we have $\|e^{-c_i hA}\|_{H^r \to H^r} = 1$ and hence

$$\|e_{n,i}\|_{H^r(\mathbb{T}^d)} \le \|e_n\|_{H^r(\mathbb{T}^d)} + h\mathcal{C}L\Big(\sum_{j=1}^{s}\|e_{n,j}\|_{H^r(\mathbb{T}^d)}\Big) + \|\Delta_{n,i}\|_{H^r(\mathbb{T}^d)}. \tag{3.14}$$

Summing these s inequalities and using (3.6), we get

$$\sum_{j=1}^{s}\|e_{n,j}\|_{H^r(\mathbb{T}^d)} \le 2s\|e_n\|_{H^r(\mathbb{T}^d)} + 2\sum_{i=1}^{s}\|\Delta_{n,i}\|_{H^r(\mathbb{T}^d)}. \tag{3.15}$$

On the other hand, subtracting (3.10) from (3.3) yields

$$e_{n+1} = e^{-hA}e_n + h\sum_{i=1}^{s} b_i(-hA)\Big(g(t_n + c_i h, u_{n,i}) - f(t_n + c_i h)\Big) - \delta_{n+1}. \tag{3.16}$$

Hence,

$$\|e_{n+1}\|_{H^r(\mathbb{T}^d)} \leq \|e_n\|_{H^r(\mathbb{T}^d)} + h\mathcal{C}L\sum_{i=1}^{s}\|e_{n,i}\|_{H^r(\mathbb{T}^d)} + \|\delta_{n+1}\|_{H^r(\mathbb{T}^d)}. \tag{3.17}$$

Using (3.15), we thus get

$$\begin{aligned}
&\|e_{n+1}\|_{H^r(\mathbb{T}^d)}\\
&\leq \|e_n\|_{H^r(\mathbb{T}^d)} + 2h\mathcal{C}L\Big(s\|e_n\|_{H^r(\mathbb{T}^d)} + \sum_{j=1}^{s}\|\Delta_{n,j}\|_{H^r(\mathbb{T}^d)}\Big) + \|\delta_{n+1}\|_{H^r(\mathbb{T}^d)}\\
&\leq (1+2h\mathcal{C}sL)\|e_n\|_{H^r(\mathbb{T}^d)} + \sum_{j=1}^{s}\|\Delta_{n,j}\|_{H^r(\mathbb{T}^d)} + \|\delta_{n+1}\|_{H^r(\mathbb{T}^d)}\\
&\leq \sum_{p=0}^{n}(1+2h\mathcal{C}sL)^p\Big(\sum_{j=1}^{s}\|\Delta_{n-p,j}\|_{H^r(\mathbb{T}^d)} + \|\delta_{n+1-p}\|_{H^r(\mathbb{T}^d)}\Big)\\
&\leq e^{2Nh\mathcal{C}sL}\sum_{p=0}^{n}\Big(\sum_{j=1}^{s}\|\Delta_{n-p,j}\|_{H^r(\mathbb{T}^d)} + \|\delta_{n+1-p}\|_{H^r(\mathbb{T}^d)}\Big),
\end{aligned}$$

using also (3.6). Using relation (2.10) (which still holds for non-linear problems) and relation (3.12), we get that for all $j \in \{1,\dots,s\}$ and all $p \in \{0,\dots,n\}$,

$$\|\Delta_{n-p,j}\|_{H^r(\mathbb{T}^d)}, \|\delta_{n+1-p}\|_{H^r(\mathbb{T}^d)} \leq \Big(\frac{1}{s!} + \frac{\mathcal{C}s}{(s-1)!}\Big)h^s\int_{t_{n-p}}^{t_{n-p+1}}\|f^{(s)}(\tau)\|_{H^r(\mathbb{T}^d)}\,\mathrm{d}\tau. \tag{3.18}$$

We derive

$$\|e_{n+1}\|_{H^r(\mathbb{T}^d)} \leq e^{2Nh\mathcal{C}sL}(s+1)\Big(\frac{1}{s!} + \frac{\mathcal{C}s}{(s-1)!}\Big)h^s\int_{t_0}^{t_{n+1}}\|f^{(s)}(\tau)\|_{H^r(\mathbb{T}^d)}\,\mathrm{d}\tau.$$

In view of (3.8), we derive that $\|e_{n+1}\|_{H^r(\mathbb{T}^d)} \leq R$. Hence, by triangle inequality, we get $\|u_{n+1}\|_{H^r(\mathbb{T}^d)} \leq \|u(t_{n+1})\|_{H^r(\mathbb{T}^d)} + \|e_{n+1}\|_{H^r(\mathbb{T}^d)} \leq R+R$ and estimate (3.9) holds true. ■

3.3 A sufficient condition for order $s+1$

As in the linear case (see Theorem 2.4 and Theorem 2.6), the exponential Runge–Kutta method of collocation type (3.2)-(3.3) applied to the non-linear Schrödinger equation (3.1) is of order $s+1$ provided that the underlying Runge–Kutta method is of order $s+1$. A precise result is stated in Theorem 3.8. Note that this result is very similar to the one obtained in [14] in the case of semi-linear parabolic problems (see [14], Theorem 5). Let us start with a discrete Gronwall Lemma:

Lemma 3.7 *Let X be a subset[2] of $\mathbb{R}^+$. Assume that $T > 0$ and $a \geq 0$ are given. There exists a positive constant C such that for all non-negative functions*

[2]Namely, X will be $(0, h_0)$ or the set of $h \in (0, h_0)$ satisfying (2.17).

b defined on X and all sequences $(\varepsilon_n)_{n\in\mathbb{N}}$ of non-negative real numbers satisfying for all $h \in X$ and $n \in \mathbb{N}$ with $0 \leq nh \leq T$, $\varepsilon_n \leq ah\sum_{k=0}^{n-1}\varepsilon_k + b(h)$, we have

$$\varepsilon_n \leq Cb(h).$$

Theorem 3.8 *Under the hypotheses of Theorem 3.6, if $f^{(s)} \in C^1([0,T], H^{r+2})$ and the underlying Runge-Kutta method is of order $s+1$, then there exists a positive constant $C > 0$ depending only on $(c_1, \ldots, c_s)$, L, and T such that for all $h \in (0, h_0)$, we have for all $n \in \{0, \ldots, N\}$,*

$$\|u_n - u(t_n)\|_{H^r} \leq C\, h^{s+1} \left(\|f^{(s)}(0)\|_{H^{r+2}} \right.$$
$$\left. + \int_0^T \|f^{(s+1)}(\tau)\|_{H^{r+2}}\, \mathrm{d}\tau + \int_0^T \|f^{(s)}(\tau)\|_{H^r}\, \mathrm{d}\tau \right).$$

Proof. By induction, relation (3.16) becomes

$$e_n = h\left(\sum_{k=0}^{n-1} e^{-khA} d_{n-k-1}\right) - \sum_{k=0}^{n-1} e^{-khA}\delta_{n-k},$$

where $d_k = \sum_{i=1}^s b_i(-hA)(g(t_k + c_i h, u_{k,i}) - f(t_k + c_i h))$. As in the proof of Theorem 2.4, there exists a constant $C_1 > 0$ depending only on $(c_1, \ldots, c_s)$ such that

$$\|\sum_{k=0}^{n-1} e^{-khA}\delta_{n-k}\|_{H^r} \leq C_1 h^{s+1}\Big(\|f^{(s)}(0)\|_{H^{r+2}} + \int_0^{t_{n-1}} \|f^{(s+1)}(\tau)\|_{H^{r+2}}\, \mathrm{d}\tau\Big). \tag{3.19}$$

On the other hand, with Hypothesis 3.2, we have

$$\|\sum_{k=0}^{n-1} e^{-khA} d_{n-k-1}\|_{H^r} \leq \mathcal{C}L \sum_{k=0}^{n-1}\sum_{i=1}^{s} \|e_{k,i}\|_{H^r}.$$

Then, using (3.15), we deduce

$$\|\sum_{k=0}^{n-1} e^{-khA} d_{n-k-1}\|_{H^r} \leq 2s\mathcal{C}L \sum_{k=0}^{n-1} \|e_k\|_{H^r} + 2\mathcal{C}L \sum_{k=0}^{n-1}\sum_{i=1}^{s} \|\Delta_{k,i}\|_{H^r}.$$

Estimate (3.18) provides the existence of a constant $C_2 > 0$ depending only on $(c_1, \ldots, c_s)$ and s such that

$$\sum_{k=0}^{n-1}\sum_{i=1}^{s} \|\Delta_{k,i}\|_{H^r} \leq C_2 h^s \int_0^{t_n} \|f^{(s)}(\tau)\|_{H^r}\, \mathrm{d}\tau.$$

Hence,

$$\|e_n\|_{H^r} \leq 2sh\mathcal{C}L \sum_{k=0}^{n-1} \|e_k\|_{H^r} + h^{s+1}\left(2\mathcal{C}LC_2 \int_0^T \|f^{(s)}(\tau)\|_{H^r}\, \mathrm{d}\tau\right.$$
$$\left. + C_1\Big(\|f^{(s)}(0)\|_{H^{r+2}} + \int_0^T \|f^{(s+1)}(\tau)\|_{H^{r+2}}\, \mathrm{d}\tau\Big)\right).$$

We conclude with the help of Lemma 3.7 with $\varepsilon_n = \|e_n\|_{H^r}$, $a = 2s\mathcal{C}L$ and b equal the term multiplied by h^{s+1} in the previous estimate. ■

Remark 3.9 *Note that in this non-linear case, the order constant C appearing in Theorem 3.8 depends a priori exponentially on T. This contrasts the linear case (see Theorem 2.4 and Theorem 2.6).*

Remark 3.10 *We could write a counterpart of Theorem 3.8 for non-resonant time steps with suitable assumptions on f essentially by modifying inequality* (3.19)*. However, we would still get an order constant depending on T (see Theorem 2.6 for the corresponding result for linear problems) and the fact is that we did not manage to observe resonances for non-linear problems (see section 4 for numerical experiments).*

3.4 Achieving order $s + 2$

In order to give sufficient algebraic conditions on the coefficients of the underlying Runge–Kutta method for the s-stage exponential Runge–Kutta method of collocation type (3.2)-(3.3) to be of order $s+2$, we reinforce our hypothesis on the smoothness of the non-linearity g. The function g is assumed to be smooth in the sense of functions from $\mathbb{R}^2$ to $\mathbb{R}^2$. For convenience, we denote, for example, for $v \in \mathbb{C} = \mathbb{R}^2$, $\frac{\partial g}{\partial u}(t, v)$ the $\mathbb{R}$-linear mapping from $\mathbb{C} = \mathbb{R}^2$ to $\mathbb{C} = \mathbb{R}^2$ corresponding to the first derivative of $g(t, u)$ as a function of $u \in \mathbb{R}^2$. For $v \in H^r(\mathbb{T}^d)$, we also denote by $\frac{\partial g}{\partial u}(t, v)$ the induced mapping between functions on $\mathbb{T}^d$ defined for a function w on $\mathbb{T}^d$ by

$$\forall x \in \mathbb{T}^d, \qquad \frac{\partial g}{\partial u}(t, v)(w)(x) = \frac{\partial g}{\partial u}(t, v(x))(w(x)).$$

Our additional hypotheses on the non-linearity g are the following:

Hypothesis 3.11 *Assume that there exists positive constants L_1 and $\tilde{L}_1$ such that*

$$\forall t \in [0, T], \quad \forall v \in H^r(\mathbb{T}^d), \qquad \|\frac{\partial g}{\partial u}(t, u(t))v\|_{H^r(\mathbb{T}^d)} \leq L_1 \|v\|_{H^r(\mathbb{T}^d)},$$

and

$$\forall t \in [0, T], \quad \forall v \in H^{r+2}(\mathbb{T}^d), \qquad \|\frac{\partial g}{\partial u}(t, u(t))v\|_{H^{r+2}(\mathbb{T}^d)} \leq \tilde{L}_1 \|v\|_{H^{r+2}(\mathbb{T}^d)}.$$

Hypothesis 3.12 *Assume that there exists a positive constant L_2 such that for all $t \in [0, T]$ and $u, v, w \in H^r(\mathbb{T}^d)$ satisfying* $\max\{\|u\|_{H^r}, \|v\|_{H^r}, \|w\|_{H^r}\} \leq 2R$, *one has*

$$\|g(t, v) - g(t, w) - \frac{\partial g}{\partial u}(t, u)(v - w)\|_{H^r} \leq L_2 \Big(\|u - v\|_{H^r} + \|u - w\|_{H^r}\Big) \|v - w\|_{H^r}.$$

Hypothesis 3.13 *Assume that there exists positive constants L_3 and $\tilde{L}_3$ such that for all $t \in [0,T]$ and $v, w \in H^{r+2}(\mathbb{T}^d)$, one has*

$$\|\frac{\partial^2 g}{\partial u^2}(t,u(t))(v,w)\|_{H^r} \leq L_3 \|v\|_{H^r} \|w\|_{H^r},$$

$$\|\frac{\partial^2 g}{\partial t \partial u}(t,u(t))v\|_{H^r} \leq L_3 \|v\|_{H^r},$$

$$\|\frac{\partial^2 g}{\partial u^2}(t,u(t))(v,w)\|_{H^{r+2}} \leq \tilde{L}_3 \|v\|_{H^{r+2}} \|w\|_{H^{r+2}},$$

and

$$\|\frac{\partial^2 g}{\partial t \partial u}(t,u(t))v\|_{H^{r+2}} \leq \tilde{L}_3 \|v\|_{H^{r+2}}.$$

Such hypotheses on g are coupled with (and may imply) the following one on the exact solution u of problem (3.1) that reinforces Hypothesis 3.3:

Hypothesis 3.14 *Equation* (3.1) *has an exact solution $u : [0,T] \to H^{r+2}(\mathbb{T}^d)$ that is sufficiently smooth. In particular, $u_0 \in H^{r+2}(\mathbb{T}^d)$.*

Notice that Hypotheses (3.11), (3.12) and (3.13) are satisfied in many cases of interest, for example for the cubic Schrödinger equation when $r > d/2$ with $r - d/2 \notin \mathbb{N}$ provided that u is sufficiently smooth (see [6] for details).

Under these hypotheses, we prove that the exponential Runge–Kutta method (3.2)-(3.3) applied to the semi-linear Schrödinger equation (3.1) is of order $s+2$ provided that the underlying Runge–Kutta method is of order $s+2$.

Theorem 3.15 *Assume that $r \geq 0$ is given. Assume that the underlying Runge–Kutta method is of order $s+2$, and that the hypotheses of Theorem 3.6, Hypothesis 3.11, Hypothesis 3.12, Hypothesis 3.13 and Hypothesis 3.14 are fulfilled. If $f \in C^{s+2}([0,T], H^{r+4})$, then there exists a positive constant $C > 0$ such that for all $h \in (0, h_0)$ and all $n \in \{0, \ldots, N\}$, one has*

$$\|u(t_n) - u_n\|_{H^r} \leq C h^{s+2}.$$

Remark 3.16 Of course, the constant C appearing in Theorem 3.15 also involves the final time $T > 0$ and integrals of norms of the time-derivatives of f over $[0,T]$.

Proof. Let us set for $n \in \{0, \ldots, N\}$

$$J_n = \frac{\partial g}{\partial u}(t_n, u(t_n)),$$

and

$$\tilde{d}_{n,i} = g(t_n + c_i h, u_{n,i}) - g(t_n + c_i h, u(t_n + c_i h)) - J_n e_{n,i}.$$

As before, subtracting (3.10) from (3.3) yields

$$e_{n+1} = e^{-hA} e_n - \delta_{n+1} + h \sum_{i=1}^{s} b_i(-hA) J_n e_{n,i} + h \sum_{i=1}^{s} b_i(-hA) \tilde{d}_{n,i}.$$

By induction, we derive that for all $n \in \{0, \dots, N-1\}$,

$$
\begin{aligned}
e_{n+1} = &-\sum_{p=0}^{n} e^{-phA}\delta_{n+1-p} && (3.20)\\
&+ \quad h\sum_{i=1}^{s} b_i(-hA)\sum_{p=0}^{n} e^{-phA}J_{n-p}\big(e_{n-p,i}+\Delta_{n-p,i}\big) && (3.21)\\
&- \quad h\sum_{i=1}^{s} b_i(-hA)\sum_{p=0}^{n} e^{-phA}J_{n-p}\Delta_{n-p,i} && (3.22)\\
&+ \quad h\sum_{i=1}^{s} b_i(-hA)\sum_{p=0}^{n} e^{-phA}\tilde{d}_{n-p,i}. && (3.23)
\end{aligned}
$$

Since the underlying Runge–Kutta method is of order $s+2$, one deduces, as in the proof of Theorem 2.8 that there exists a positive constant C_1 such that for all h and n,

$$
\begin{aligned}
\|\sum_{p=0}^{n} e^{-phA}\delta_{n+1-p}\|_{H^r} \leq C_1\, h^{s+2}\Big(&\|f^{(s)}(0)\|_{H^{r+4}} + \|f^{(s+1)}(0)\|_{H^{r+2}}\\
&+\int_0^T \|f^{(s+1)}(\tau)\|_{H^{r+4}}\,\mathrm{d}\tau + \int_0^T \|f^{(s+2)}(\tau)\|_{H^{r+2}}\Big). \qquad (3.24)
\end{aligned}
$$

To bound the error term (3.21), one uses (3.13) and then (3.15) to derive that

$$
\begin{aligned}
\|e_{n-p,i}+\Delta_{n-p,i}\|_{H^r} &\leq \|e_{n-p}\|_{H^r} + \mathcal{C}hL\sum_{j=1}^{s}\|e_{n-p,j}\|_{H^r}\\
&\leq (1+2\mathcal{C}h_0Ls)\|e_{n-p}\|_{H^r} + 2\mathcal{C}Lh\sum_{j=1}^{s}\|\Delta_{n-p,j}\|_{H^r}.
\end{aligned}
$$

Using Hypothesis 3.11 and estimate (3.18), we derive that[3]

$$
\begin{aligned}
&\Big\|h\sum_{i=1}^{s} b_i(-hA)\sum_{p=0}^{n} e^{-phA}J_{n-p,i}\big(e_{n-p,i}+\Delta_{n-p,i}\big)\Big\|_{H^r}\\
&\leq \mathcal{C}hs\left(\sum_{p=0}^{n} L_1\Big((1+2\mathcal{C}h_0Ls)\|e_{n-p}\|_{H^r} + 2\mathcal{C}Lh\sum_{j=1}^{s}\|\Delta_{n-p,j}\|_{H^r}\Big)\right)\\
&\leq \mathcal{C}hsL_1(1+2\mathcal{C}h_0Ls)\sum_{p=0}^{n}\|e_p\|_{H^r} + 2\mathcal{C}^2LL_1\kappa_s h^{s+2}\int_0^T \|f^{(s)}(\tau)\|_{H^r}\,\mathrm{d}\tau.
\end{aligned}
$$

Hence, there exists positive constants C_2 and C_3 such that for all h and n, the H^r-norm of the term (3.21) is bounded by $C_2 h\sum_{p=0}^{n}\|e_p\|_{H^r} + C_3h^{s+2}$.

[3]See the definition of κ_s in Theorem 3.6.

In order to bound the H^r-norm of the error term (3.22), we set

$$\psi_{i,s+1}(z) = \varphi_{s+1}(c_i z) c_i^{s+1} - \frac{1}{s\,!} \sum_{j=1}^{s} a_{i,j}(z) c_j^s,$$

and write

$$\Delta_{n-p,i} = h^{s+1} \psi_{i,s+1}(-hA) f^{(s)}(t_{n-p}) + \widetilde{\Delta}_{n-p,i},$$

to get

$$h \sum_{i=1}^{s} b_i(-hA) \sum_{p=0}^{n} e^{-phA} J_{n-p} \Delta_{n-p,i} =$$

$$- h \sum_{i=1}^{s} b_i(0) \sum_{p=0}^{n} e^{-phA} J_{n-p} h^{s+1} \psi_{i,s+1}(0) f^{(s)}(t_{n-p}) \tag{3.25}$$

$$- h \sum_{i=1}^{s} b_i(-hA) \sum_{p=0}^{n} e^{-phA} J_{n-p} h^{s+1} \big(\psi_{i,s+1}(-hA) - \psi_{i,s+1}(0)\big) f^{(s)}(t_{n-p}) \tag{3.26}$$

$$- h \sum_{i=1}^{s} \big(b_i(-hA) - b_i(0)\big) \sum_{p=0}^{n} e^{-phA} J_{n-p} h^{s+1} \psi_{i,s+1}(0) f^{(s)}(t_{n-p}) \tag{3.27}$$

$$+ h \sum_{i=1}^{s} b_i(-hA) \sum_{p=0}^{n} e^{-phA} J_{n-p} \widetilde{\Delta}_{n-p,i}. \tag{3.28}$$

Since the underlying Runge–Kutta method is of order at least $s+2$, we derive that

$$\sum_{i=1}^{s} b_i(0) \psi_{i,s+1}(0) = 0,$$

and therefore the term (3.25) reads

$$h^{s+2} \sum_{p=0}^{n} e^{-phA} J_{n-p} \Big(\sum_{i=1}^{s} b_i(0) \psi_{i,s+1}(0) \Big) f^{(s)}(t_{n-p}) = 0.$$

On the other hand, there exists s holomorphic functions $(\Psi_{i,s+1})_{i \in \{1,\dots,s\}}$ such that

$$\forall i \in \{1, \dots, s\}, \quad \forall z \in \mathbb{C}, \qquad \psi_{i,s+1}(z) - \psi_{i,s+1}(0) = z \Psi_{i,s+1}(z).$$

Note that the functions $(\Psi_{i,s+1})_{i \in \{1,\dots,s\}}$ are bounded on $\imath\mathbb{R}$. Let $M > 0$ be a bound for these functions. For all $i \in \{i, \dots, s\}$, an Abel summation yields

$$\sum_{p=0}^{n} e^{-phA} J_{n-p} \Psi_{i,s+1}(-hA) \big(-hA \big) f^{(s)}(t_{n-p}) =$$

$$\Big(\sum_{p=0}^{n} e^{-phA} \Big) J_0 \Psi_{i,s+1}(-hA) \big(-hA \big) f^{(s)}(0)$$

$$+ \sum_{p=0}^{n-1} \Big(\sum_{q=0}^{p} e^{-qhA} \Big) \int_{t_{n-p-1}}^{t_{n-p}} \frac{\mathrm{d}}{\mathrm{d}t} \Big[\frac{\partial g}{\partial u}(t, u(t)) \Psi_{i,s+1}(-hA) \big(-hA \big) f^{(s)}(t) \Big] \mathrm{d}t.$$

On one hand,

$$\Big\|\Big(\sum_{p=0}^{n} e^{-phA}\Big) J_0 \Psi_{i,s+1}(-hA)\big(-hA\big) f^{(s)}(0)\Big\|_{H^r} \leq TL_1 M \|f^{(s)}(0)\|_{H^{r+2}}.$$

On the other hand, since after differentiating and using Hypothesis 3.11 and 3.13, one has

$$\begin{aligned}&\Big\|\frac{\mathrm{d}}{\mathrm{d}t}\Big[\frac{\partial g}{\partial u}(t,u(t))\Psi_{i,s+1}(-hA)\big(-hA\big)f^{(s)}(t)\Big]\Big\|_{H^r}\\ &\leq \ hL_3 M\|f^{(s)}(t)\|_{H^{r+2}} + hL_3 M\widetilde{R}\|f^{(s)}(t)\|_{H^{r+2}} + hL_1 M\|f^{(s+1)}(t)\|_{H^{r+2}},\end{aligned}$$

where $\widetilde{R}$ denotes the maximum of $\|u'(t)\|_{H^r}$ on $[0,T]$ (see Hypothesis 3.3), we deduce that there exists a positive constant C_4 such that for all h and n, the term (3.26) has an H^r-norm bounded by $C_4 h^{s+2}$.
The same kind of calculations yields, denoting $(\theta_i)_{i\in\{1,\dots,s\}}$ the holomorphic functions such that

$$\forall i \in \{1,\dots,n\}, \quad \forall z\in\mathbb{C}, \qquad b_i(z)-b_i(0) = z\theta_i(z) = \theta_i(z)z,$$

$$\begin{aligned}&\sum_{i=1}^{s}\big(b_i(-hA)-b_i(0)\big)\sum_{p=0}^{n} e^{-phA} J_{n-p}\psi_{i,s+1}(0) f^{(s)}(t_{n-p}) =\\ &\quad \psi_{i,s+1}(0)\Big(\sum_{p=0}^{n} e^{-phA}\Big)\theta_i(-hA)\big(-hA\big)J_0 f^{(s)}(0)\\ &+\ \psi_{i,s+1}(0)\sum_{p=0}^{n-1}\Big(\sum_{q=0}^{p} e^{-qhA}\Big)\theta_i(-hA)\big(-hA\big)\int_{t_{n-p-1}}^{t_{n-p}}\frac{\mathrm{d}}{\mathrm{d}t}\Big[\frac{\partial g}{\partial u}(t,u(t))f^{(s)}(t)\Big]\mathrm{d}t.\end{aligned}$$

If we also denote by M a positive constant bounding the functions $(\theta_i)_{i\in\{1,\dots,s\}}$, then

$$\begin{aligned}&\Big\|e^{-qhA}\theta_i(-hA)\big(-hA\big)\int_{t_{n-p-1}}^{t_{n-p}}\frac{\mathrm{d}}{\mathrm{d}t}\Big[\frac{\partial g}{\partial u}(t,u(t))f^{(s)}(t)\Big]\mathrm{d}t\Big\|_{H^r}\\ &\leq \ Mh\int_{t_{n-p-1}}^{t_{n-p}}\Big\|A\frac{\mathrm{d}}{\mathrm{d}t}\Big[\frac{\partial g}{\partial u}(t,u(t))f^{(s)}(t)\Big]\Big\|_{H^r}\mathrm{d}t\\ &\leq \ Mh\int_{t_{n-p-1}}^{t_{n-p}}\Big\|\frac{\mathrm{d}}{\mathrm{d}t}\Big[\frac{\partial g}{\partial u}(t,u(t))f^{(s)}(t)\Big]\Big\|_{H^{r+2}}\mathrm{d}t.\end{aligned}$$

Hypotheses 3.11 and 3.13 ensure that

$$\begin{aligned}&\|\frac{\mathrm{d}}{\mathrm{d}t}\Big[\frac{\partial g}{\partial u}(t,u(t))f^{(s)}(t)\Big]\|_{H^{r+2}}\,\mathrm{d}t\\ &\leq \ \tilde{L}_3(1+\widetilde{R})\int_{t_{n-p-1}}^{t_{n-p}}\|f^{(s)}(t)\|_{H^{r+2}}\,\mathrm{d}t + \tilde{L}_1\int_{t_{n-p-1}}^{t_{n-p}}\|f^{(s+1)}(t)\|_{H^{r+2}}\,\mathrm{d}t,\end{aligned}$$

if $\widetilde{R}$ stands for a bound of $\|u'(t)\|_{H^{r+2}}$ on $[0,T]$(see Hypothesis 3.14). Hence, the H^r-norm of term (3.27) is bounded by $C_5 h^{s+2}$ for some positive constant C_5.

One can easily check by using Hypothesis 3.11 that there exists a positive constant C_6 such that for all h and n, the H^r-norm of term (3.28) is bounded by $C_6 h^{s+2}$. Hence, term (3.22) is bounded for all h and n by $(C_4+C_5+C_6)h^{s+2}$. Eventually, one can estimate term (3.23) by writing, for $i \in \{1,\ldots,s\}$, $h \in (0,h_0)$, $n \in \{0,\ldots,N-1\}$, and $p \in \{0,\ldots,n\}$, using Hypothesis 3.12

$$\|\tilde{d}_{n-p,i}\|_{H^r} \leq L_2\Big(\|u(t_{n-p})-u_{n-p,i}\|_{H^r}+\|u(t_{n-p})-u(t_{n-p}+c_ih)\|_{H^r}\Big)\|e_{n-p,i}\|_{H^r}.$$

Therefore, we get that

$$\begin{aligned}
&\Big\|h\sum_{i=1}^{s} b_i(-hA)\sum_{p=0}^{n} e^{-phA}\tilde{d}_{n-p,i}\Big\|_{H^r} \\
&\quad\leq\ \mathcal{C}L_2 h\sum_{p=0}^{n}\sum_{i=1}^{s}\Big(\|e_{n-p,i}\|_{H^r}^2+\widetilde{R}h\|e_{n-p,i}\|_{H^r}\Big).
\end{aligned}$$

Note that we have using (3.15) and (3.18)

$$\begin{aligned}
\sum_{i=1}^{s}\|e_{n-p,i}\|_{H^r}^2 &\leq \Big(\sum_{i=1}^{s}\|e_{n-p,i}\|_{H^r}\Big)^2 \\
&\leq (s+1)\Big(4s^2\|e_{n-p}\|_{H^r}^2+4\sum_{i=1}^{s}\|\Delta_{n-p,i}\|_{H^r}^2\Big) \\
&\leq (s+1)\Big(4s^2\|e_{n-p}\|_{H^r}^2+4s\kappa_s^2h^{2s+1}\int_{t_{n-p}}^{t_{n-p+1}}\|f^{(s)}(\tau)\|_{H^r}^2\,\mathrm{d}\tau\Big) \\
&\leq (s+1)\Big(4s^2R\|e_{n-p}\|_{H^r}+4s\kappa_s^2h^{2s+1}\int_{t_{n-p}}^{t_{n-p+1}}\|f^{(s)}(\tau)\|_{H^r}^2\,\mathrm{d}\tau\Big).
\end{aligned}$$

We derive that there exists a positive constant C_7 such that for all h and n, the H^r-norm of term (3.23) is bounded by

$$C_7 h\sum_{p=0}^{n}\|e_p\|_{H^r}+C_7h^{s+2}.$$

The conclusion follows using Lemma 3.7. ∎

4 Numerical experiments

We provide two kinds of numerical experiments to illustrate our results. Both of them have been performed with $s=2$ collocation points.

- The first method we choose is defined by $c_1=\frac{1}{2}$ and $c_2=1$. This method does not satisfy relation (2.11). Hence, its underlying Runge–Kutta method exactly is of order 2.
- The other method we choose is defined by $c_1=\frac{1}{3}$ and $c_2=1$. This method satisfies relation (2.11) but not relation (2.21). Hence, its underlying Runge–Kutta method exactly is of order 3.

4.1 Linear problems

Firstly, we consider a linear problem (2.4) with dimension $d = 1$. The functions u_0 and f are chosen in such a way that the exact solution of the problem is $u(t,x) = e^{\iota\left(\frac{t}{2}\right)^2 \sin(x)}$. We set the final time $T = 2\pi$. We apply Methods 1 and 2 to this problem for different time steps $h > 0$ such that T/h is an integer. We plot in logarithmic scales the L^2-norm of the final error $e_{\frac{T}{h}}$ as a function of h on Figure 1. Calculations are carried out with Fast Fourier Transforms with 2^8 modes.

One can see that, in both cases, the error plot lies between two different straight lines with same slope. The upper line is reached when $T/h = 2\pi/h$ is close to the square of an integer, that is to say when the time step is resonant (for example, when $T/h = 2\pi/10^{-1.2019} \sim 100 = 10^2$, relation (2.17) does not hold). In this case, inequality (2.12) of Theorem 2.4 holds and seems to be sharp. On the other hand, for non-resonant time steps, estimate (2.19) of Theorem 2.6 holds and seems to be sharp. Of course, estimate (2.12) also holds, but it does not seem to be sharp anymore.

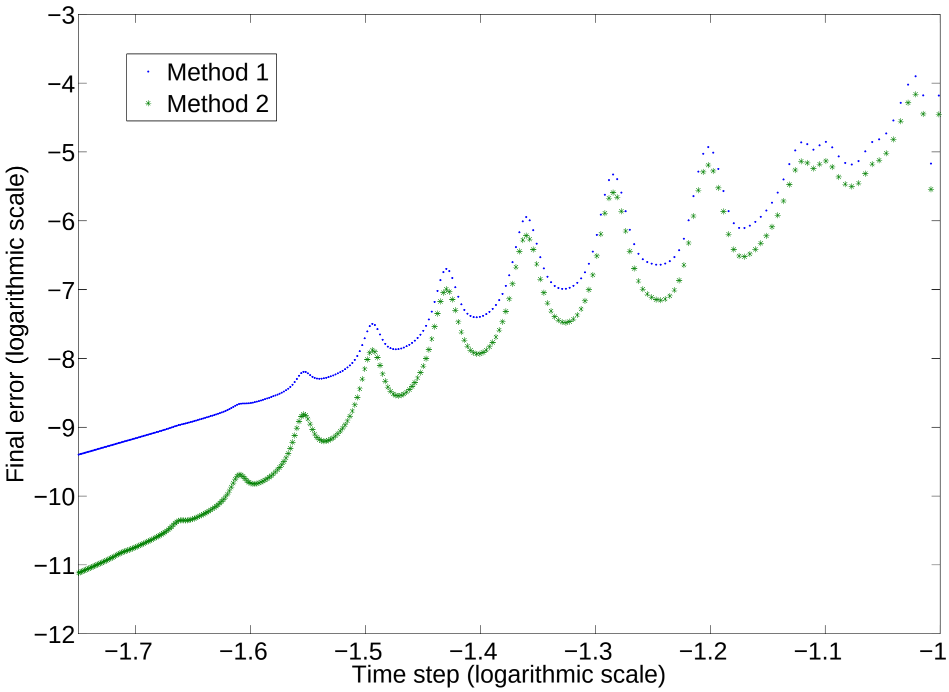

Figure 1: Final error as a function of the time step for a linear Schrödinger problem. Method 1 (upper dotted line) and 2 (lower starred line). Logarithmic scales.

4.2 Semi-linear problems

Secondly, we consider a semi-linear problem (3.1) with dimension $d = 1$. The non-linearity is $g(u) = i|u|^2 u$ and the initial datum is $u_0(x) = \frac{1+e^{2ix}}{2+\sin(x)}$. We set the final time $T = 2\pi$. We apply Methods 1 and 2 to this problem for different time steps $h > 0$ such that T/h is an integer. We plot in logarithmic scales the L^2-norm of the final error $e_{\frac{T}{h}}$ as a function of h on Figure 2. Calculations are carried out with Fast Fourier Transforms with 2^8 modes.

One can see that no resonance occurs for time steps between 10^{-3} and 10^{-1}, even when T/h is the square of an integer, and that both methods have a numerical order consistent with Theorems 3.6 and 3.8: the upper straight line has a numerical slope close to 2, while the lower straight line has a numerical slope close to 3.

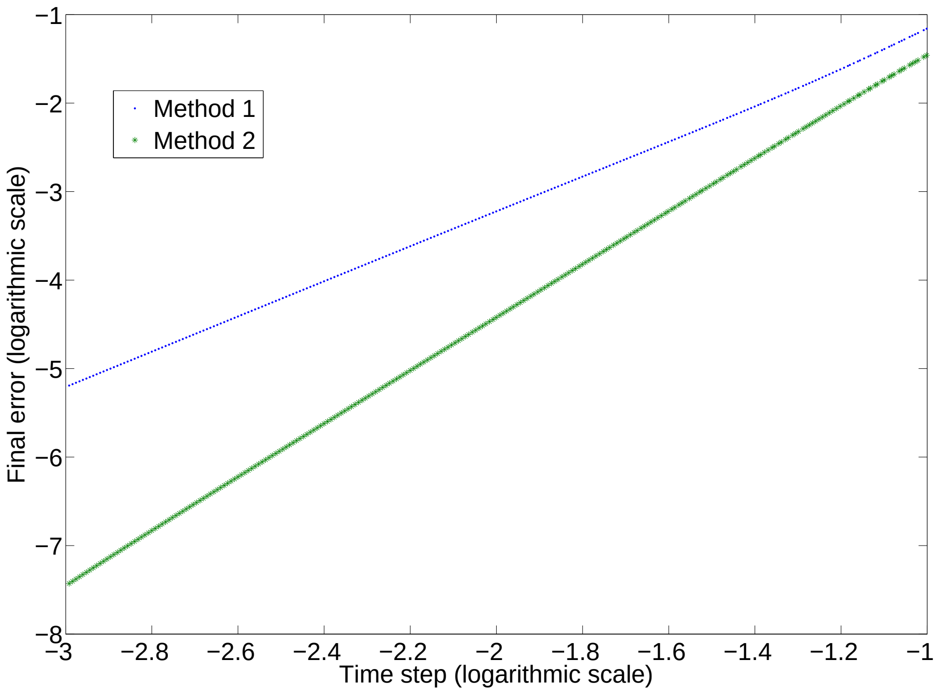

Figure 2: Final error as a function of the time step for the cubic Schrödinger equation. Method 1 (upper dotted line, numerical slope 1.9932) and Method 2 (lower starred line, numerical slope 2.9874). Logarithmic scales.

5 Conclusion

This paper provides a numerical analysis of exponential Runge–Kutta methods of collocation type applied to the linear and semi-linear Schrödinger equations on a d-dimensional torus. These methods have been studied in [14] when applied to *parabolic* problems.

This paper shows how the results of [14] extend to the case of the Schrödinger equation and provides sufficient conditions to achieve orders s, $s+1$ and $s+2$ using an s-stage method (see Theorems 2.1, 2.4, 2.6, 2.8 and 2.9 for linear Schrödinger problems and Theorems 3.6, 3.8 and 3.15 for non-linear Schrödinger problems). Essentially, when solving Schrödinger problems, the methods behave as they do when solving parabolic problems : under some suitable assumptions (on the right-hand side or on the non-linearity), an s-stage method is of order s and can achieve orders $s+1$ and $s+2$. However, the proofs of the results presented in this paper require some hypotheses (for example on the regularity of the exact solution of the problem, like Hypotheses 3.3 and 3.14) that seem more restrictive in the Schrödinger context than the corresponding ones in the parabolic context. Moreover, this paper points out a major difference between parabolic problems and Schrödinger problems solved by such exponential Runge–Kutta methods: it shows and explains the effect of resonant and non-resonant time steps over finite time intervals when solving linear Schrödinger problems (see Theorems 2.6 and 2.9).

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References

[1] A. Alinhac, P. Gérard, *Opérateurs pseudo-différentiels et théorie de Nash-Moser*, InterÉditions/Éditions du CNRS

[2] H. Berland, A.L. Islas, C.M. Schober, *Conservation of phase space properties using exponential integrators on the cubic Schrödinger equation*, Journal of Computational Physics, 255(1):284-299 (2007)

[3] H. Berland, B. Skaflestad, *Solving the nonlinear Schrödinger equation using exponential integrators*, Proceedings SIMS 2005 46th Conference on Simulation and Modeling. Trondheim, Norway

[4] D. Cohen, E. Hairer, C. Lubich, *Long-time analysis of nonlinearly perturbed wave equations via modulated Fourier expansions*, to appear in Arch. Ration. Mech. Anal

[5] D. Cohen, E. Hairer, C. Lubich, *Conservation of energy, momentum and actions in numerical discretizations of nonlinear wave equations*, April 2007, preprint

[6] G. Dujardin, *Étude de schémas de discrétisation en temps de l'équation de Schrödinger*, PhD thesis, 2008.

[7] G. Dujardin, E. Faou, *Normal form and long time analysis of splitting schemes for the linear Schrödinger equation with small potential*, Numerische Mathematik 106, Number 2 (2007) 223-262

[8] B. Garcìa-Archilla, J. Sanz-Serna, R. Skeel, *Long-time-step methods for oscillatory differential equations*, SIAM J. Sci. Comput., 30(3):930-963, 1998

[9] V. Grimm, M. Hochbruck, *Error analysis of exponential integrators for oscillatory second-order differential equations*, J. Phys. A; Math. Gen., 39:5495-5507, 2006

[10] E. Hairer, C. Lubich, Spectral semi-discretisations of weakly nonlinear wave equations over long times, August 2007. To appear in J. FoCM

[11] E. Hairer, C. Lubich, G. Wanner, *Geometric Numerical Integration. Structure-preserving Algorithms for Ordinary Differential Equations*, Second Edition, Springer, Berlin, 2006

[12] M. Hochbruck, C. Lubich, *A Gautschi-type method for oscillatory second-order differential equations*, Numer. Math., 83:403-426, 1999

[13] M. Hochbruck, A. Ostermann, *Explicit exponential Runge–Kutta methods for semilinear parabolic problems*, SIAM J. Numer. Anal. 43, No. 3, 1069-1090, 2005

[14] M. Hochbruck, A. Ostermann, *Exponential Runge–Kutta methods for parabolic problems*, Appl. Numer. Math. 53, Issues 2-4, 323-339, 2005

[15] B. Minchev, W.M. Wright, *A review of exponential integrators for semilinear problems*, Tech. rep. 2/05. Department of Mathematical Sciences, Norwegian University of Science and Technology, Trondheim, Norway

[16] J.M. Sanz-Serna, *Modified impulse methods for highly oscillatory differential equations*, SIAM J. Numer. Anal., 46(2):1040-1059, 2008