

Proof. One has to impose $d_{1,1} = 0$ and $d_{p,j} = 0$ in eq. (5.7). Then, coefficients $\omega_{i,j}$ vanish, because all the successive commutators $[K(h), \dots, [K(h), \tilde{K}(h)] \dots]$ appearing in the BCH formula applied to $e^{K(h)} e^{\tilde{K}(h)}$ contain only pure imaginary terms up to order $\mathcal{O}(h^{2p+1})$. \square

In consequence, if the problem (5.1) is defined in a Lie group \mathcal{G} , then the scheme S_h of order p is conjugate to a method that preserves the Lie group structure up to order $2p+1$. This is so up to order $2p+2$ if Ψ_h is symmetric-conjugate and the order p is even, due to the particular structure of K_h in that case [5]. On the other hand, if Ψ_h is symmetric-conjugate and its order p is odd, then the resulting AC method is time-symmetric and of order $p+1$.

5.2 New alternating-conjugate methods

The analysis of the previous subsection shows that, in addition to concatenating a given method Ψ_h of order p (say palindromic or symmetric-conjugate) with the same scheme with complex conjugate coefficients, one can also get an alternating-conjugate method of order $p \geq 2$ by considering Ψ_h as in Proposition 5.1, namely by requiring the following order conditions:

$$\begin{aligned} \Re(k_{1,1}) &= \frac{1}{2}, & \Re(k_{p,j}) &= 0; & j &= 1, \dots, c(p) \\ k_{\ell,j} &= 0, & \ell &= 2, \dots, p-1; & j &= 1, \dots, c(\ell). \end{aligned} \quad (5.12)$$

The simplest AC method of order $p = 2$ corresponds of course to the composition $S_h = \Phi_{\alpha h} \Phi_{\bar{\alpha} h}$ with

$$\Phi_{\alpha h} = e^{K(h)} \quad \text{and} \quad K(h) = \alpha h M + \alpha^2 h^2 Y_2 + \alpha^3 h^3 Y_3 + \dots$$

By imposing $\Re(\alpha) = \frac{1}{2}$, $\Re(\alpha^2) = 0$ we get $\alpha = \frac{1}{2}(1 \pm i)$, i.e., we recover method (5.2).

Analogously, for an AC method of order 3 within this family one has to take $\Psi_h = \Phi_{\alpha_1 h} \Phi_{\alpha_2 h} \Phi_{\alpha_3 h}$ to satisfy the 5 required conditions (5.12). Although there are solutions with $\alpha_3 \in \mathbb{R}$, it is more efficient to consider Φ_h in the composition (5.4) as a 2nd-order time-symmetric method, namely

$$\Psi_h = \Psi_{\alpha_1 h}^{[2]} \Psi_{\alpha_2 h}^{[2]} \dots \Psi_{\alpha_r h}^{[2]}. \quad (5.13)$$

Now the number of order conditions (5.12) to achieve a method of order 3, 4, 5, 6 is, respectively, 2, 4, 7 and 11. This is the strategy we follow next to construct higher order schemes with the minimum number of basic methods (or *stages*). We denote, for brevity, the whole AC method by its sequence of coefficients:

$$S_h = (\alpha_1, \alpha_2, \dots, \alpha_r, \bar{\alpha}_1, \bar{\alpha}_2, \dots, \bar{\alpha}_r).$$

Order 3. The two order conditions, $\Re(k_{1,1}) = \frac{1}{2}$, $\Re(k_{3,1}) = 0$ can be satisfied with just one basic scheme, $\Psi_{\alpha_1 h}^{[2]}$, if

$$\alpha_1 = \frac{1}{2} \pm i \frac{1}{2\sqrt{3}}.$$

In this way we recover the scheme (2.5), which is both symmetric-conjugate and AC. Notice that if $\Psi_h^{[2]}$ is taken as the Strang splitting (2.3) for two operators, then the number of exponentials is 5 instead of 12 with a composition of the Lie–Trotter scheme.