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ADIABATIC INTEGRATORS FOR HIGHLY OSCILLATORY SECOND-ORDER LINEAR DIFFERENTIAL EQUATIONS WITH TIME-VARYING EIGENDECOMPOSITION*

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Abstract.

Numerical integrators for second-order differential equations with time-dependent high frequencies are proposed and analysed. We derive two such methods, called the adiabatic midpoint rule and the adiabatic Magnus method. The integrators are based on a transformation of the problem to adiabatic variables and an expansion technique for the oscillatory integrals. They can be used with far larger step sizes than those required by traditional schemes, as is illustrated by numerical experiments. We prove second-order error bounds with step sizes significantly larger than the almost-period of the fastest oscillations.

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1 Introduction.

The integration of highly oscillatory differential equations has been a numerical challenge for a long time; see, e.g., the reviews in [6, 15]. To approximate the solution with sufficient accuracy, step sizes far smaller than the smallest approximate period of the oscillations must be taken with standard integrators. An early approach to taking larger time steps in oscillatory problems has been made by Gautschi [4], who presents trigonometric integrators for differential equations of the form $\ddot{x} + \omega^2 x = g(t, x)$ with a fixed frequency ω. His methods extend readily to $\ddot{x} + Ax = g(t, x)$ with a constant, symmetric, positive semi-definite matrix A of large norm. For this type of equations, García-Archilla, Sanz-Serna and Skeel [3] propose and analyse the mollified impulse method, and Hochbruck and Lubich [7] analyse Gautschi-type integrators. Grimm [5] extends this analysis to equations with a time-dependent matrix $A(t)$, which may be

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of large norm, but whose derivatives are supposed to be moderately bounded. Iserles [8] uses WKB analysis to study the performance of numerical methods for the scalar linear oscillator $\ddot{x} + a(t)x = 0$, where $\limsup_{t\to\infty} a(t) = +\infty$ and $|\mathrm{d}^k a(t)/\mathrm{d}t^k| = \mathrm{o}(a(t)^{1/k})$ for $k \geq 1$ and large t. As a suitable numerical method he presents a modified Magnus method. Methods of this type are further studied by Degani and Schiff [2].

In this paper, we consider the linear oscillatory system

$$\ddot{x}(t) + \frac{1}{\varepsilon^2} A(t)x(t) = 0, \quad 0 < \varepsilon \ll 1, \tag{1.1}$$

with a time-dependent, symmetric positive definite matrix $A(t)$ whose derivatives are bounded independently of ε. Equation (1.1) describes oscillations in a mechanical system that at the same time moves on a slower time scale. Some applications are folding the antenna of a satellite or the oscillations appearing in the steering and the front axle suspension of a car [16]. Apart from this direct practical interest, finding suitable numerical integrators for this equation is an important prerequisite for nonlinear problems, which will be treated in forthcoming work.

None of the known numerical methods yields an ε-independent accuracy with step sizes $h > \varepsilon$ when applied to (1.1). Here, we develop numerical integrators which give ε-uniform $\mathrm{O}(h^2)$ accuracy with large step sizes up to $h = \mathrm{O}(\sqrt{\varepsilon})$. They require only one evaluation and diagonalization of $A(t)$ per time step. The methods are invariant under rescaling $\varepsilon \to \sigma\varepsilon$ and $A(t) \to \sigma^2 A(t)$, since effectively they work only with the complete matrix $\frac{1}{\varepsilon^2} A(t)$. The approach taken here is closely related to that of [11–13] for the numerical integration of singularly perturbed Schrödinger equations.

In Section 2 we start with reformulating (1.1) as a first-order system, which is then transformed to *adiabatic* variables. The solution of the transformed differential equation is a smoother function $\eta(t)$, which is more accessible to numerical approximation. We also comment on the inhomogeneous version of (1.1). In Sections 3 and 4, we present two time-reversible integrators for (1.1) constructed via the transformed equation, named the adiabatic midpoint rule and the adiabatic Magnus method. Numerical examples are shown in Section 5, where the new schemes are compared with methods known from the literature. The error behaviour is illustrated both for well-separated frequencies and in the case of an avoided frequency crossing. Finally, Section 6 gives a detailed error analysis proving ε-uniform second-order accuracy of the proposed methods for $h < \sqrt{\varepsilon}$ in the case of separated frequencies. The error bounds depend on the smoothness of the eigendecomposition of $A(t)$, but not on bounds of derivatives of the highly oscillatory solution $x(t)$.

2 Transformation of the problem.

It is favourable to transform the problem instead of trying to solve Equation (1.1) directly. The reformulated equation is introduced in this section.

2.1 Assumptions.

Let the real, symmetric and positive definite matrix $A(t)$ be diagonalized as

$$A(t) = Q(t)\Omega(t)^2 Q(t)^{\mathrm{T}}, \qquad \Omega(t) = \operatorname{diag}(\omega_k(t)), \tag{2.1}$$

with an orthogonal matrix $Q(t)$ and a diagonal matrix $\Omega(t)$ containing the eigenfrequencies $\omega_k(t)$, that is, the square roots of the eigenvalues of $A(t)$. We assume that the eigendecomposition is sufficiently smooth: the functions $t \mapsto Q(t)$ and $t \mapsto \Omega(t)$ are supposed to be three times continuously differentiable, and each of the derivatives is bounded independently of ε.

We suppose, in addition, that the eigenfrequencies $\omega_k(t)$ remain separated and bounded away from 0: there is a $\delta > 0$ such that for any pair $\omega_k(t)$ and $\omega_l(t)$ with $k \neq l$, the lower bounds

$$|\omega_k(t) - \omega_l(t)| \geq \delta, \quad \omega_k(t) \geq \tfrac{1}{2}\delta \tag{2.2}$$

hold for all $t \in [t_0, t_{\mathrm{end}}]$.

2.2 Reformulation as a first-order system.

With

$$B(t) := A(t)^{1/2} = Q(t)\Omega(t)Q(t)^{\mathrm{T}} \quad \text{and} \quad \frac{1}{\varepsilon}B(t)y(t) = \dot{x}(t),$$

we obtain a system of first-order ordinary differential equations

$$\begin{pmatrix} \dot{x} \\ \dot{y} \end{pmatrix} = \frac{1}{\varepsilon}\begin{pmatrix} 0 & B(t) \\ -B(t) & 0 \end{pmatrix}\begin{pmatrix} x \\ y \end{pmatrix} + \begin{pmatrix} 0 & 0 \\ 0 & -B(t)^{-1}\dot{B}(t) \end{pmatrix}\begin{pmatrix} x \\ y \end{pmatrix}, \tag{2.3}$$

which will be the starting point for our approach. Compared with the equation treated in [11–13], a common feature is the presence of a skew-Hermitian time-dependent matrix multiplied by $1/\varepsilon$. A major difference is the appearance of the second term in (2.3) which changes the behaviour of solutions and poses additional difficulties for the numerical treatment.

From the eigendecomposition (2.1) we obtain the following one for the skew-symmetric matrix in (2.3):

$$H(t) := \begin{pmatrix} 0 & B(t) \\ -B(t) & 0 \end{pmatrix} = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \otimes B(t) = U(t)i\Lambda(t)U(t)^* \tag{2.4}$$

$$\text{with} \quad U(t) = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & i \\ i & 1 \end{pmatrix} \otimes Q(t), \quad \Lambda(t) = \begin{pmatrix} \Omega(t) & 0 \\ 0 & -\Omega(t) \end{pmatrix}.$$

Here i is the imaginary unit and U^* denotes the hermitian conjugate of the unitary matrix U.

2.3 Transformation to adiabatic variables.

Like in [11], we now pass to a smoother variable $\eta(t)$ which is called the adiabatic variable. Up to an oscillating phase, $\eta(t)$ is the coefficient vector of

$(x(t), y(t))^{\mathrm{T}}$ with respect to the eigenbasis of $H(t)$. It is defined as

$$\eta(t) = \exp\left(-\frac{i}{\varepsilon}\Phi(t)\right) U(t)^* \begin{pmatrix} x(t) \\ y(t) \end{pmatrix}, \tag{2.5}$$

where $\Phi(t)$ is the diagonal matrix that contains the integrals over the eigenvalues of $H(t)$:

$$\Phi(t) = \int_{t_0}^{t} \Lambda(s)\,\mathrm{d}s, \quad \Phi = \mathrm{diag}(\phi_j). \tag{2.6}$$

Differentiating (2.5) and substituting the result into (2.3) leads to an ordinary differential equation for η:

$$\begin{aligned} \dot\eta(t) \;=\; & \exp\left(-\frac{i}{\varepsilon}\Phi(t)\right) U(t)^* \begin{pmatrix} 0 & 0 \\ 0 & -B(t)^{-1}\dot B(t) \end{pmatrix} U(t) \exp\left(\frac{i}{\varepsilon}\Phi(t)\right)\eta(t) - \\ & - \exp\left(-\frac{i}{\varepsilon}\Phi(t)\right) U(t)^* \dot U(t) \exp\left(\frac{i}{\varepsilon}\Phi(t)\right)\eta(t). \end{aligned} \tag{2.7}$$

Equation (2.7) contains two ε-independent coupling matrices framed by rapidly oscillating diagonal matrices $\exp(\pm i\Phi(t)/\varepsilon)$.

One advantage of the transformed equation is that the right-hand side of (2.7) stays bounded independently of ε and the variable $\eta(t)$ is therefore smoother than the solution of (2.3). Another good reason for working with (2.7) rather than (2.3) is that, as $\varepsilon \to 0$, the solutions $\eta(t) = \eta_\varepsilon(t)$ converge strongly to solutions of a limit equation (see Section 2.5).

2.4 Notation.

We denote the coupling matrices in (2.7) by $V(t)$ and $W(t)$,

$$\begin{aligned} V &= U^* \begin{pmatrix} 0 & 0 \\ 0 & -B^{-1}\dot B \end{pmatrix} U = -\tfrac{1}{2} \begin{pmatrix} 1 & -i \\ i & 1 \end{pmatrix} \otimes \Omega^{-1}\big(\dot\Omega + [K,\ \Omega]\big), \\ W &= U^*\dot U = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \otimes K, \end{aligned}$$

with the skew-symmetric matrix $K = Q^{\mathrm{T}}\dot Q$ and the commutator $[K,\ \Omega] = K\Omega - \Omega K$. We let $V^D(t)$ be the diagonal part of $V(t)$,

$$V^D = -\tfrac{1}{2} \begin{pmatrix} \Omega^{-1}\dot\Omega & 0 \\ 0 & \Omega^{-1}\dot\Omega \end{pmatrix},$$

and $V^N(t) = V(t) - V^D(t)$ contains the off-diagonal entries. The real skew-symmetric matrix $W(t)$ has zero diagonal and will therefore be regrouped with $V^N(t)$ in the following.

We introduce $E(\Phi)$ as the matrix with entries $e_{kl}(\Phi)$ defined by

$$e_{kl}(\Phi) = \begin{cases} \exp\left(\dfrac{i}{\varepsilon}(\phi_l - \phi_k)\right) & \text{if } k \neq l, \\ 0 & \text{otherwise.} \end{cases} \tag{2.8}$$

Denoting the entrywise product of matrices by $\bullet$, Equation (2.7) can equivalently be written as

$$\dot\eta(t) = V^D(t)\eta(t) + \big(E(\Phi(t)) \bullet (V^N(t) - W(t))\big)\eta(t). \tag{2.9}$$

Next, $D(\Lambda)$ and $D^-(\Lambda)$ are defined as matrices with the entries

$$d_{kl}(\Lambda) = \lambda_l - \lambda_k, \qquad d^-_{kl}(\Lambda) = \begin{cases} (\lambda_l - \lambda_k)^{-1} & \text{if } k \neq l, \\ 0 & \text{otherwise.} \end{cases} \tag{2.10}$$

Note that $D^-(\Lambda)$ is not the inverse of $D(\Lambda)$, but the entrywise product yields $D(\Lambda) \bullet D^-(\Lambda) \bullet W = W$ for every matrix W with zero diagonal. The definitions of E, D, and D^- apply with any diagonal matrix Φ or Λ. For $\Phi(t)$ of (2.6), we note

$$\frac{\mathrm{d}}{\mathrm{d}t} E(\Phi(t)) = E(\Phi(t)) \bullet \frac{i}{\varepsilon} D(\Lambda(t)). \tag{2.11}$$

2.5 The adiabatic limit equation.

We show that the solutions $\eta(t) = \eta_\varepsilon(t)$ of (2.7) converge strongly to solutions $\eta_*(t)$ of the equation obtained by taking the weak limit for $\varepsilon \to 0$ in (2.9),

$$\dot\eta_* = V^D(t)\eta_*. \tag{2.12}$$

The diagonal matrix $V^D(t)$ is independent of ε and so the solution of (2.12) evolves on a time scale ~ 1 and shows no high-frequency oscillations at all. To estimate the difference $\eta(t) - \eta_*(t)$ we subtract (2.12) from (2.9) to obtain

$$\dot\eta - \dot\eta_* = V^D(\eta - \eta_*) + E(\Phi) \bullet \big(V^N - W\big)\eta.$$

We integrate this equation from 0 to t, insert $E(\Phi(t)) = \frac{\mathrm{d}}{\mathrm{d}t} E(\Phi(t)) \bullet \frac{\varepsilon}{i} D^-(\Lambda(t))$ and integrate by parts, obtaining

$$\begin{aligned} \eta(t) - \eta_*(t) \;=\; & \int_0^t V^D(s)(\eta(s) - \eta_*(s))\,\mathrm{d}s - \\ & - i\varepsilon\, E(\Phi(s)) \bullet D^-(\Lambda(s)) \bullet \big(V^N(s) - W(s)\big)\eta(s)\big|_0^t + \\ & + i\varepsilon \int_0^t E(\Phi(s)) \bullet \frac{\mathrm{d}}{\mathrm{d}s}\big(D^-(\Lambda(s)) \bullet \big(V^N(s) - W(s)\big)\big)\eta(s)\,\mathrm{d}s + \\ & + i\varepsilon \int_0^t E(\Phi(s)) \bullet D^-(\Lambda(s)) \bullet \big(V^N(s) - W(s)\big)\dot\eta(s)\,\mathrm{d}s \\ =\; & \int_0^t V^D(s)(\eta(s) - \eta_*(s))\,\mathrm{d}s + \mathrm{O}(\varepsilon), \end{aligned}$$

where we use $|\lambda_l(t) - \lambda_k(t)| \geq \delta$. For $\eta(0) = \eta_*(0)$ and for times $t = \mathrm{O}(1)$, we conclude with the Gronwall lemma

$$\eta(t) - \eta_*(t) = \mathrm{O}(\varepsilon). \tag{2.13}$$

Moreover, $\eta_*(t)$ is given explicitly as

$$\begin{aligned}\eta_*(t) &= \begin{pmatrix}1 & 0\\ 0 & 1\end{pmatrix} \otimes \exp\Big(-\tfrac{1}{2}\int_0^t \Omega(s)^{-1}\dot{\Omega}(s)\,\mathrm{d}s\Big)\eta(0)\\ &= \begin{pmatrix}1 & 0\\ 0 & 1\end{pmatrix} \otimes \Omega(t)^{-1/2}\Omega(0)^{1/2}\eta(0).\end{aligned}$$

2.6 Adiabatic invariants.

With the rescaling

$$\widehat{\eta}(t) = \begin{pmatrix}\Omega(t)^{1/2} & 0\\ 0 & \Omega(t)^{1/2}\end{pmatrix}\eta(t)$$

the above analysis shows, for times $t = \mathrm{O}(1)$,

$$\widehat{\eta}(t) = \widehat{\eta}(0) + \mathrm{O}(\varepsilon), \tag{2.14}$$

so that the components of $\widehat{\eta}$ are adiabatic invariants. This result is an analogue to the quantum-adiabatic theorem of Born and Fock [1].

The function $\widehat{\eta}$ satisfies the differential equation

$$\dot{\widehat{\eta}}(t) = \big(E(\Phi(t)) \bullet (\widehat{V}(t) - \widehat{W}(t))\big)\widehat{\eta}(t), \tag{2.15}$$

where the matrices

$$\begin{aligned}\widehat{V} &= -\tfrac{1}{2}\begin{pmatrix}1 & -i\\ i & 1\end{pmatrix} \otimes \Omega^{-1/2}[K,\ \Omega]\,\Omega^{-1/2},\\ \widehat{W} &= \begin{pmatrix}1 & 0\\ 0 & 1\end{pmatrix} \otimes \Omega^{1/2}K\Omega^{-1/2},\end{aligned}$$

again with $K = Q^{\mathrm{T}}\dot{Q}$, all have zero diagonal.

Numerical methods can be based on either of (2.9) or (2.15). We will describe the approach via (2.9). The corresponding method for (2.15) is obtained simply by replacing V and W with $\widehat{V}$ and $\widehat{W}$ and noting $\widehat{V}^D = 0$.

2.7 Inhomogeneous problems.

The approach extends to the inhomogeneous equation

$$\ddot{x}(t) + \frac{1}{\varepsilon^2}A(t)x(t) = \frac{1}{\varepsilon^2}f(t)$$

with a smooth function $f(t)$. With the transformation

$$z = x - A^{-1}f + \varepsilon^2 A^{-1}\frac{\mathrm{d}^2}{\mathrm{d}t^2}(A^{-1}f),$$

we obtain

$$\ddot{z} + \frac{1}{\varepsilon^2} A z = \varepsilon^2 \frac{\mathrm{d}^2}{\mathrm{d}t^2}\left(A^{-1} \frac{\mathrm{d}^2}{\mathrm{d}t^2}(A^{-1} f)\right),$$

where dropping the ε^2 term leads to an error of $\mathrm{O}(\varepsilon^4)$ in the solution. The right-hand term can therefore be omitted in the approximation if an accuracy $\mathrm{O}(h^2)$ with step sizes $h > \varepsilon$ is desired. The truncated differential equation for $z(t)$ is again of the form (1.1).

Alternatively, the inhomogeneity can be directly accommodated in the adiabatic midpoint rule of the next section, using the inhomogeneous extension of (2.7) which contains the additional term

$$\exp\left(-\frac{i}{\varepsilon}\Phi(t)\right) U(t)^* \begin{pmatrix} 0 \\ \frac{1}{\varepsilon} B(t)^{-1} f(t) \end{pmatrix}.$$

Here, however, the remaining factor $1/\varepsilon$ may lead to reduced accuracy.

3 The adiabatic midpoint rule.

We derive a symmetric method with an $\mathrm{O}(h^3)$ local error. The construction is similar to that of "Method I" for singularly perturbed Schrödinger equations presented in [13].

3.1 Derivation of the method.

Let h be the step size and fix a time $t_n = t_0 + nh$. We start with integrating the transformed equation (2.9) from t_{n-1} to t_{n+1} and from t_n to $t_n + \theta h$, getting

$$\begin{aligned} \eta(t_{n+1}) &= \eta(t_{n-1}) + h \int_{-1}^{1} \big(E(\Phi(t_n+\theta h)) \bullet \big(V^N - W\big)(t_n+\theta h) + \\ &\quad + V^D(t_n+\theta h)\big)\eta(t_n+\theta h)\,\mathrm{d}\theta, \qquad (3.1) \\ \eta(t_n+\theta h) &= \eta(t_n) + h \int_{0}^{\theta} \big(E(\Phi(t_n+\sigma h)) \bullet \big(V^N - W\big)(t_n+\sigma h) + \\ &\quad + V^D(t_n+\sigma h)\big)\eta(t_n+\sigma h)\,\mathrm{d}\sigma, \qquad (3.2) \end{aligned}$$

respectively. Now, we substitute the expression $\eta(t_n+\theta h)$ in (3.1) with the right-hand side of (3.2) and replace the intermediate values $V(t_n+\theta h)$ and $W(t_n+\theta h)$ by the Taylor expansions

$$\begin{aligned} V(t_n+\theta h) &= V(t_n) + \theta h \dot{V}(t_n) + \mathrm{O}(\theta^2 h^2), \\ W(t_n+\theta h) &= W(t_n) + \theta h \dot{W}(t_n) + \mathrm{O}(\theta^2 h^2). \end{aligned} \qquad (3.3)$$

Substituting $\eta(t_n+\sigma h) = \eta(t_n) + \mathrm{O}(\sigma h)$ in (3.2) then leads to

$$\eta(t_{n+1}) = \eta(t_{n-1}) + h\mathcal{A}(t_n)\eta(t_n) + h^2\mathcal{B}(t_n)\eta(t_n) + h^2\mathcal{C}(t_n)\eta(t_n) + \mathrm{O}(h^3)$$

with the matrices

$$\mathcal{A}(t) = \int_{-1}^{1} E(\Phi(t+\theta h))\,\mathrm{d}\theta \bullet \big(V^N(t) - W(t)\big) + 2V^D(t), \tag{3.4}$$

$$\mathcal{B}(t) = \int_{-1}^{1} \theta E(\Phi(t+\theta h))\,\mathrm{d}\theta \bullet \big(\dot{V}^N(t) - \dot{W}(t)\big), \tag{3.5}$$

$$\begin{aligned}\mathcal{C}(t) = {} & \int_{-1}^{1} \big(E(\Phi(t+\theta h)) \bullet \big(V^N(t) - W(t)\big)\big) \times \\ & \times \int_{0}^{\theta} E(\Phi(t+\sigma h)) \bullet \big(V^N(t) - W(t)\big)\,\mathrm{d}\sigma\,\mathrm{d}\theta + \\ & + \int_{-1}^{1} \theta E(\Phi(t+\theta h))\,\mathrm{d}\theta \bullet \big(V^N(t) - W(t)\big) V^D(t) + \\ & + V^D(t) \int_{-1}^{1} \int_{0}^{\theta} E(\Phi(t+\sigma h))\,\mathrm{d}\sigma\,\mathrm{d}\theta \bullet \big(V^N(t) - W(t)\big).\end{aligned} \tag{3.6}$$

These are the basic equations for the construction of the numerical method. We need sufficiently accurate approximations to $\mathcal{A}(t_n)$, $\mathcal{B}(t_n)$, and $\mathcal{C}(t_n)$. First, $V(t_n)$ and $W(t_n)$ are replaced by V_n and W_n given by

$$\begin{aligned} V_n &= -\tfrac{1}{2} \begin{pmatrix} 1 & -i \\ i & 1 \end{pmatrix} \otimes \Omega(t_n)^{-1} (\dot{\Omega}_n + [K_n,\ \Omega(t_n)]), \\ W_n &= \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \otimes K_n, \end{aligned} \tag{3.7}$$

with the symmetric difference quotients

$$\dot{\Omega}_n = \frac{1}{2h}\big(\Omega(t_{n+1}) - \Omega(t_{n-1})\big), \qquad K_n = \frac{1}{2h} Q(t_n)^{\mathrm{T}} \big(Q(t_{n+1}) - Q(t_{n-1})\big).$$

We denote by V_n^D the diagonal part of V_n, and by $V_n^N = V_n - V_n^D$ the off-diagonal part. The diagonals of K_n and hence also W_n are set to zero, since $K(t)$ and $W(t)$ have zero diagonal. The corresponding derivatives are approximated by

$$\dot{V}_n = \frac{1}{h}(V_{n+1/2} - V_{n-1/2}), \qquad \dot{W}_n = \frac{1}{h}(W_{n+1/2} - W_{n-1/2}), \tag{3.8}$$

where

$$\begin{aligned} V_{n+1/2} &= -\tfrac{1}{2} \begin{pmatrix} 1 & -i \\ i & 1 \end{pmatrix} \otimes \Omega_{n+1/2}^{-1} \big(\dot{\Omega}_{n+1/2} + [K_{n+1/2},\ \Omega_{n+1/2}]\big), \\ W_{n+1/2} &= \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \otimes K_{n+1/2}, \end{aligned} \tag{3.9}$$

with

$$\begin{aligned} \Omega_{n+1/2} &= \tfrac{1}{2}\big(\Omega(t_{n+1}) + \Omega(t_n)\big), \qquad \dot{\Omega}_{n+1/2} = \frac{1}{h}\big(\Omega(t_{n+1}) - \Omega(t_n)\big), \\ K_{n+1/2} &= \frac{1}{2h}\big(Q(t_{n+1}) + Q(t_n)\big)^{\mathrm{T}} \big(Q(t_{n+1}) - Q(t_n)\big). \end{aligned}$$

Next, we make a quadratic phase approximation in $E(\Phi)$ appearing in $\mathcal{A}(t_n)$, $\mathcal{B}(t_n)$, and $\mathcal{C}(t_n)$:

$$\Phi(t_n+\theta h) \approx \Phi(t_n) + \theta h \Lambda(t_n) + \tfrac{1}{2}\theta^2 h^2 \dot{\Lambda}(t_n). \tag{3.10}$$

Here, the derivative $\dot{\Lambda}(t_n)$ is approximated by the symmetric difference quotient

$$\dot{\Lambda}_n = \frac{1}{2h}\big(\Lambda(t_{n+1}) - \Lambda(t_{n-1})\big) = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \otimes \dot{\Omega}_n \tag{3.11}$$

and the integral $\Phi(t_n) = \int_{t_0}^{t_n} \Lambda(s)\,\mathrm{d}s$ is approximated by Φ_n defined recursively by the Simpson rule,

$$\Phi_{n+1} = \Phi_{n-1} + \frac{h}{3}\big(\Lambda(t_{n+1}) + 4\Lambda(t_n) + \Lambda(t_{n-1})\big). \tag{3.12}$$

With these approximations we replace the oscillatory matrix-valued function $E(\Phi(t_n+\theta h))$ by

$$\begin{aligned} E_n(\theta) &= E(\Phi_n + \theta h \Lambda(t_n) + \tfrac{1}{2}\theta^2 h^2 \dot{\Lambda}_n) \\ &= E(\Phi_n) \bullet E(\theta h \Lambda(t_n)) \bullet E(\tfrac{1}{2}\theta^2 h^2 \dot{\Lambda}_n), \end{aligned} \tag{3.13}$$

and so we arrive at the following scheme:

$$\eta_{n+1} = \eta_{n-1} + h\widetilde{\mathcal{A}}_n \eta_n + h^2 \widetilde{\mathcal{B}}_n \eta_n + h^2 \widetilde{\mathcal{C}}_n \eta_n, \tag{3.14}$$

where, with the matrices with zero diagonal abbreviated as

$$Z_n = V_n^N - W_n, \qquad \dot{Z}_n = \dot{V}_n^N - \dot{W}_n, \tag{3.15}$$

we have the following approximations to the matrices $\mathcal{A}(t_n)$, $\mathcal{B}(t_n)$, $\mathcal{C}(t_n)$ of (3.4)–(3.6):

$$\widetilde{\mathcal{A}}_n = \int_{-1}^{1} E_n(\theta)\,\mathrm{d}\theta \bullet Z_n + 2V_n^D, \tag{3.16}$$

$$\widetilde{\mathcal{B}}_n = \int_{-1}^{1} \theta E_n(\theta)\,\mathrm{d}\theta \bullet \dot{Z}_n, \tag{3.17}$$

$$\begin{aligned} \widetilde{\mathcal{C}}_n = {} & \int_{-1}^{1} \big(E_n(\theta) \bullet Z_n\big)\left(\int_0^{\theta} E_n(\sigma)\,\mathrm{d}\sigma \bullet Z_n\right)\mathrm{d}\theta + \\ & + \left(\int_{-1}^{1} \theta E_n(\theta)\,\mathrm{d}\theta \bullet Z_n\right) V_n^D + V_n^D \left(\int_{-1}^{1}\int_0^{\theta} E_n(\sigma)\,\mathrm{d}\sigma\,\mathrm{d}\theta \bullet Z_n\right). \end{aligned} \tag{3.18}$$

3.2 Computing the oscillatory integrals.

An expansion technique similar to that of [13] is now used to compute the oscillatory integrals in (3.16)–(3.18). We start with the integral in $\widetilde{\mathcal{B}}_n$. Integration

by parts yields*

$$
\begin{aligned}
(3.19)\qquad &\int_{-1}^{1} \theta E(\theta h \Lambda(t_n)) \bullet E(\tfrac{1}{2}\theta^2 h^2 \dot{\Lambda}_n)\,\mathrm{d}\theta \\
&= E(\theta h \Lambda(t_n) + \tfrac{1}{2}\theta^2 h^2 \dot{\Lambda}_n) \bullet \\
&\quad \bullet \left(\theta \frac{\varepsilon}{ih} D^-(\Lambda(t_n)) - \left(\frac{\varepsilon}{ih} D^-(\Lambda(t_n)) \right)^{\bullet 2} \right) \Big|_{\theta=-1}^{1} - \\
&\quad - \int_{-1}^{1} E(\theta h \Lambda(t_n) + \tfrac{1}{2}\theta^2 h^2 \dot{\Lambda}_n) \bullet \\
&\quad \bullet \left(\theta \frac{\varepsilon}{ih} D^-(\Lambda(t_n)) - \left(\frac{\varepsilon}{ih} D^-(\Lambda(t_n)) \right)^{\bullet 2} \right) \bullet \\
&\quad \bullet \theta \frac{ih^2}{\varepsilon} D(\dot{\Lambda}_n)\,\mathrm{d}\theta,
\end{aligned}
$$

with the matrices $D(\Lambda)$ and $D^-(\Lambda)$ defined by (2.10). The last integral is of magnitude $\mathrm{O}(h)$ and hence

$$
(3.20)\qquad \int_{-1}^{1} \theta E(\theta h \Lambda(t_n) + \tfrac{1}{2}\theta^2 h^2 \dot{\Lambda}_n)\,\mathrm{d}\theta = \mathcal{I}_1 + \mathrm{O}(h) \quad \text{with}
$$

$$
\begin{aligned}
(3.21)\qquad \mathcal{I}_1 &= \mathcal{J} \bullet \mathcal{E}_1 - \mathcal{J} \bullet \mathcal{J} \bullet \mathcal{E}_0, \\
(3.22)\qquad \mathcal{E}_1 &= \theta E(\theta h \Lambda(t_n) + \tfrac{1}{2}\theta^2 h^2 \dot{\Lambda}_n)\big|_{\theta=-1}^{1}, \\
(3.23)\qquad \mathcal{E}_0 &= E(\theta h \Lambda(t_n) + \tfrac{1}{2}\theta^2 h^2 \dot{\Lambda}_n)\big|_{\theta=-1}^{1}, \\
(3.24)\qquad \mathcal{J} &= \frac{\varepsilon}{ih} D^-(\Lambda(t_n)).
\end{aligned}
$$

Next, we look at the integral in $\widetilde{\mathcal{A}}_n$. Again we integrate by parts and use (3.20):

$$
\begin{aligned}
(3.25)\qquad &\int_{-1}^{1} E(\theta h \Lambda(t_n) + \tfrac{1}{2}\theta^2 h^2 \dot{\Lambda}_n)\,\mathrm{d}\theta = \mathcal{I}_0 + \mathrm{O}(h^2) \\
&\qquad \text{with } \mathcal{I}_0 = \mathcal{J} \bullet \mathcal{E}_0 - \mathcal{J} \bullet \mathcal{I}_1 \bullet \frac{ih^2}{\varepsilon} D(\dot{\Lambda}_n).
\end{aligned}
$$

The term $\widetilde{\mathcal{C}}_n$ is more complicated. It consists of three terms, contains double integrals and both matrix multiplication and entrywise multiplication. For the inner integral in the first term we obtain by partial integration as above

$$
(3.26)\qquad \int_0^{\theta} E_n(\sigma)\,\mathrm{d}\sigma = \mathcal{J} \bullet (E_n(\theta) - E_n(0)) + \mathrm{O}(h),
$$

* $X^{\bullet 2}$ denotes the entrywise power, i.e. $X^{\bullet 2} = X \bullet X$.

and hence the first term of $\widetilde{\mathcal{C}}_n$ becomes

$$\begin{aligned}\int_{-1}^{1} \big(E(\Phi_n + \theta h\Lambda(t_n) + \tfrac{1}{2}\theta^2 h^2 \dot\Lambda_n) \bullet Z_n\big) \times \\ \times \big(E(\Phi_n + \theta h\Lambda(t_n) + \tfrac{1}{2}\theta^2 h^2 \dot\Lambda_n) \bullet \mathcal{J} \bullet Z_n\big)\,\mathrm{d}\theta - \\ - \int_{-1}^{1} \big(E(\Phi_n) \bullet E(\theta h\Lambda(t_n) + \tfrac{1}{2}\theta^2 h^2 \dot\Lambda_n) \bullet Z_n\big) \times \\ \times \big(E(\Phi_n) \bullet \mathcal{J} \bullet Z_n\big)\,\mathrm{d}\theta + \mathrm{O}(h).\end{aligned}$$

We note that

$$(E(\Phi) \bullet M_1)(E(\Phi) \bullet M_2) = (E(\Phi) + I) \bullet (M_1 M_2)$$

holds by definition of $E(\Phi)$ for all diagonal matrices Φ and all matrices M_1, M_2 with zero diagonal; I denotes the identity matrix. Applying this equality and integrating gives

$$\begin{aligned}\big(E(\Phi_n) \bullet \mathcal{J} \bullet \mathcal{E}_0 + 2I\big) \bullet \big(Z_n(\mathcal{J} \bullet Z_n)\big) - \\ - \big(E(\Phi_n) + I\big) \bullet \big((\mathcal{J} \bullet \mathcal{E}_0 \bullet Z_n)(\mathcal{J} \bullet Z_n)\big)\end{aligned}$$

as an approximation to the first term of $\widetilde{\mathcal{C}}_n$ with an error of $\mathrm{O}(h)$.

The second term of $\widetilde{\mathcal{C}}_n$ is similar to $\widetilde{\mathcal{B}}_n$ and can be integrated in the same way, yielding

$$\bigg(\int_{-1}^{1} \theta E_n(\theta)\,\mathrm{d}\theta \bullet Z_n\bigg) V_n^D = \big(E(\Phi_n) \bullet \mathcal{I}_1 \bullet Z_n\big) V_n^D + \mathrm{O}(h).$$

The third term again contains a double integral. With (3.26) and (3.25) it gives

$$\begin{aligned}V_n^D \bigg(\int_{-1}^{1}\int_{0}^{\theta} E_n(\sigma)\,\mathrm{d}\sigma\,\mathrm{d}\theta \bullet Z_n\bigg) \\ = V_n^D\big(E(\Phi_n) \bullet \mathcal{J} \bullet \mathcal{J} \bullet \mathcal{E}_0 \bullet Z_n\big) - 2V_n^D\big(E(\Phi_n) \bullet \mathcal{J} \bullet Z_n\big) + \mathrm{O}(h).\end{aligned}$$

Altogether, we obtain an $\mathrm{O}(h)$-approximation $\mathcal{C}_n$ to $\widetilde{\mathcal{C}}_n$ as

$$\begin{aligned}\mathcal{C}_n \;=\; & \big(E(\Phi_n) \bullet \mathcal{J} \bullet \mathcal{E}_0 + 2I\big) \bullet \big(Z_n(\mathcal{J} \bullet Z_n)\big) - \\ & - \big(E(\Phi_n) + I\big) \bullet \big((\mathcal{J} \bullet \mathcal{E}_0 \bullet Z_n)(\mathcal{J} \bullet Z_n)\big) + \\ & + \big(E(\Phi_n) \bullet \mathcal{I}_1 \bullet Z_n\big) V_n^D + \\ & + V_n^D\big(E(\Phi_n) \bullet \mathcal{J} \bullet \mathcal{J} \bullet \mathcal{E}_0 \bullet Z_n\big) - 2V_n^D\big(E(\Phi_n) \bullet \mathcal{J} \bullet Z_n\big),\end{aligned} \tag{3.27}$$

and now we can implement the method in the following way.

3.3 The algorithm of the adiabatic midpoint rule.

Let η_n, η_{n-1}, $Q(t_n)$, $Q(t_{n-1})$, $\Omega(t_n)$, $\Omega(t_{n-1})$, Φ_n, Φ_{n-1}, $V_{n-1/2}$, $W_{n-1/2}$ be given from previous steps. Then, proceed as follows for step $n+1$:

1. Evaluate $A(t_{n+1})$, diagonalize
$$A(t_{n+1}) = Q(t_{n+1})\Omega(t_{n+1})^2 Q(t_{n+1})^{\mathrm{T}}$$
and determine $U(t_{n+1})$ and $\Lambda(t_{n+1})$ from (2.4).
2. Compute V_n, W_n, $V_{n+1/2}$, $W_{n+1/2}$, $\dot{V}_n$, $\dot{W}_n$, and $\dot{\Lambda}_n$ with (3.7)–(3.11), and Z_n, $\dot{Z}_n$ with (3.15).
3. Compute $\mathcal{J}, \mathcal{E}_0, \mathcal{E}_1, \mathcal{I}_0, \mathcal{I}_1$ with (3.21)–(3.25).
4. Compute $\mathcal{A}_n = E(\Phi_n) \bullet \mathcal{I}_0 \bullet Z_n + 2V_n^D$.
5. Compute $\mathcal{B}_n = E(\Phi_n) \bullet \mathcal{I}_1 \bullet \dot{Z}_n$.
6. Compute $\mathcal{C}_n$ with (3.27).
7. Update $\eta_{n+1} = \eta_{n-1} + h\mathcal{A}_n\eta_n + h^2\mathcal{B}_n\eta_n + h^2\mathcal{C}_n\eta_n$.
8. Compute Φ_{n+1} with (3.12).
9. Transform back from η to (x, y) and $\dot{x}$:
$$\begin{pmatrix} x_{n+1} \\ y_{n+1} \end{pmatrix} = U(t_{n+1}) \exp\left(\frac{i}{\varepsilon}\Phi_{n+1}\right)\eta_{n+1},$$
$$\dot{x}_{n+1} = \frac{1}{\varepsilon}\, Q(t_{n+1})\Omega(t_{n+1})Q(t_{n+1})^{\mathrm{T}} y_{n+1}.$$

Note that the method, though complicated to formulate, requires just one evaluation and diagonalization of $A(t)$ per time step. Care should be taken that the ordering of the eigenvalues in $\Omega(t)$ stays the same for all time steps and that the diagonalization of $A(t)$ does not produce artificial sign changes of the eigenvectors.

As starting step, we use
$$\eta_1 = \eta_0 + h\mathcal{A}_0\eta_0 + h^2\mathcal{B}_0\eta_0 + h^2\mathcal{C}_0\eta_0$$
with integration from 0 to 1 instead of -1 to 1. For the computation of W_0, V_0, $\dot{W}_0$, $\dot{V}_0$, Φ_1, and Λ_0 with the above formulas, we need two additional evaluations of A at $t_{1/2} = t_0 + h/2$ and $t_{-1/2} = t_0 - h/2$.

4 The adiabatic Magnus method.

4.1 A symmetric Magnus method.

Magnus [14] represents the solution of a linear differential equation
$$\dot{\eta}(t) = L(t)\eta(t)$$
with a time-dependent matrix $L(t)$ as
$$\eta(t) = \exp(M(t))\eta(t_0),$$
where $M(t)$ is given by the Magnus series

$$\begin{aligned} M(t) \;=\; & \int_{t_0}^{t} L(\tau)\,\mathrm{d}\tau - \frac{1}{2}\int_{t_0}^{t}\left[\int_{t_0}^{\tau} L(\sigma)\,\mathrm{d}\sigma,\; L(\tau)\right]\mathrm{d}\tau + \\ & + \frac{1}{4}\int_{t_0}^{t}\left[\int_{t_0}^{\tau}\left[\int_{t_0}^{\sigma} L(\mu)\,\mathrm{d}\mu,\; L(\sigma)\right]\mathrm{d}\sigma,\; L(\tau)\right]\mathrm{d}\tau + \\ & + \frac{1}{12}\int_{t_0}^{t}\left[\int_{t_0}^{\tau} L(\sigma)\,\mathrm{d}\sigma,\; \left[\int_{t_0}^{\tau} L(\mu)\,\mathrm{d}\mu,\; L(\tau)\right]\right]\mathrm{d}\tau + \cdots . \end{aligned}$$

The brackets $[\cdot,\cdot]$ denote the commutator $[X,\ Y] = XY - YX$. For a numerical treatment, the series is truncated and the integrals are replaced by quadrature approximations; see, e.g., [10].

We want the method to be time-symmetric, so we take the mean of one step forward in time and the inverse of one step backward in time. We put

$$\begin{aligned} M_n^{\pm} \;&=\; h\int_{-1}^{1} L(t_n+\theta h)\,\mathrm{d}\theta \mp \frac{h^2}{2}\int_{-1}^{1}\left[\int_{-1}^{\theta} L(t_n \pm \sigma h)\,\mathrm{d}\sigma,\; L(t_n \pm \theta h)\right]\mathrm{d}\theta, \\ M_n \;&=\; (M_n^{+} + M_n^{-})/2, \end{aligned}$$

and set

$$\eta_{n+1} = \exp(M_n)\eta_{n-1}.$$

In our case of the differential equation (2.9) with

$$L(t) = V^D(t) + E(\Phi(t)) \bullet (V^N(t) - W(t)),$$

the calculation of the integrals is the crucial point because the matrix function $L(t)$ is highly oscillatory. In a similar situation, Iserles [9] proposes to use Filon quadrature. However, since here only one evaluation of $L(t)$ per time step is desired, we apply the techniques presented in the previous section. Again, $\Phi(t_n + \theta h)$, $V(t_n + \theta h)$, and $W(t_n + \theta h)$ are replaced by the corresponding Taylor expansions. These substitutions lead to terms which are identical or very similar to (3.16), (3.17), and (3.18), and the techniques developed to compute the integrals of the previous section can again be applied. We omit the details of the construction and just state the algorithm.

4.2 The algorithm of the adiabatic Magnus method.

1. to 5. Proceed as for the adiabatic midpoint rule.
6. Compute

$$\begin{aligned} \mathcal{C}_n \;=\; & \tfrac{1}{2}(E(\Phi_n)\bullet\mathcal{J}\bullet\mathcal{E}_0 + 2I)\bullet[Z_n,\ \mathcal{J}\bullet Z_n] + \\ & + \tfrac{1}{4}[E(\Phi_n)\bullet\mathcal{J}\bullet\mathcal{E}_1\bullet Z_n,\ E(\Phi_n)\bullet\mathcal{J}\bullet\mathcal{E}_0\bullet Z_n] + \\ & + \tfrac{1}{2}[E(\Phi_n)\bullet\mathcal{I}_1\bullet Z_n, V_n^D]. \end{aligned}$$

7. Compute M_n and η_{n+1}:

$$\begin{aligned} M_n \;&=\; h\mathcal{A}_n + h^2\mathcal{B}_n + h^2\mathcal{C}_n, \\ \eta_{n+1} \;&=\; \exp(M_n)\eta_{n-1}. \end{aligned}$$

8. to 9. Proceed as for the adiabatic midpoint rule.
A starting step can be obtained as for the adiabatic midpoint rule or by modifying the Magnus step.

5 Numerical experiments.

In this section, we illustrate the performance of the adiabatic integrators. We use a simple model problem which shows the characteristic features that appear also in higher-dimensional situations. With a parameter δ, let

$$A(t) = \begin{pmatrix} (t+3)^2+\delta^2 & 3\delta(t+2) \\ 3\delta(t+2) & (2t+3)^2+\delta^2 \end{pmatrix} = \begin{pmatrix} t+3 & \delta \\ \delta & 2t+3 \end{pmatrix}^2.$$

The diagonalization $A(t) = Q(t)\Omega(t)^2 Q(t)^{\mathrm{T}}$ is given by

$$\begin{aligned} \Omega(t) &= \begin{pmatrix} \frac{3}{2}t+3+\frac{1}{2}\sqrt{t^2+4\delta^2} & 0 \\ 0 & \frac{3}{2}t+3-\frac{1}{2}\sqrt{t^2+4\delta^2} \end{pmatrix}, \\ Q(t) &= \begin{pmatrix} \cos\xi(t) & -\sin\xi(t) \\ \sin\xi(t) & \cos\xi(t) \end{pmatrix} \quad \text{with } \xi(t) = \tfrac{\pi}{4} + \tfrac{1}{2}\arctan\bigl(\tfrac{t}{2\delta}\bigr). \end{aligned}$$

The parameter $\delta > 0$ has a strong influence on the behaviour of the eigenfrequencies of $A(t)$ and on the solution of (2.9). To show this influence, we will consider the following examples where in all cases, the solutions are computed on the interval $[-1,\ 1]$ with $\varepsilon = 0.01$:

- For $\delta = 1$, the eigenfrequencies of $A(t)$ stay well separated at all times t and the norm of the coupling matrix W stays rather small, as can be seen in Figure 5.1, left-hand side.
- For $\delta = 0.1$, the eigenfrequencies of $A(t)$ show a so-called avoided crossing (Figure 5.1, in the middle), i.e. the eigenvalues approach each other until $t \approx 0$, where they almost intersect and then separate again. The minimal distance between eigenvalues is 2δ. This behaviour is accompanied by a sudden increase of coupling between the corresponding components, as can be seen in Figure 5.1 (lower row) where the norm of $W(t)$ is plotted. There is no significant variation in the norm of the other coupling matrix $V(t)$.
- For $\delta = 0.01$, both effects – the approach of the eigenfrequencies and the growth of the coupling – increase (Figure 5.1, right-hand side). It is not visible in the figure that the two frequencies do not intersect.

The two methods presented above are compared with other numerical schemes:

- Gautschi's method [4] applied to Equation (1.1),
$$x_{n+1} - 2\cos\left(\frac{h}{\varepsilon}B(t_n)\right)x_n + x_{n-1} = 0;$$
- the Magnus method of order 2 applied to (2.3),
$$\begin{pmatrix} x_{n+1} \\ y_{n+1} \end{pmatrix} = \exp\left(\int_{t_n}^{t_{n+1}} L(t)\,\mathrm{d}t\right)\begin{pmatrix} x_n \\ y_n \end{pmatrix},$$
where now $L(t)$ is the combined matrix on the right-hand side of (2.3);

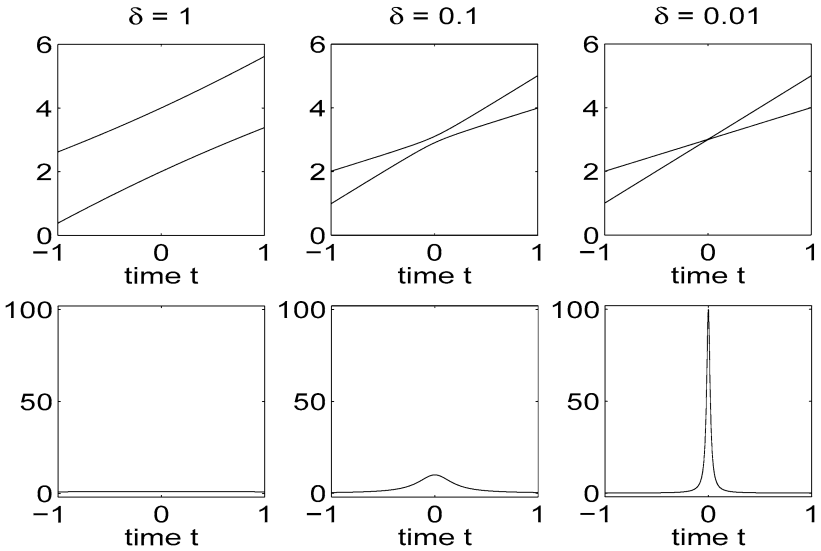

Figure 5.1: Upper row: Eigenfrequencies $\omega_k(t)$ for $\delta = 1$ (left-hand side), $\delta = 0.1$ (in the middle), and $\delta = 0.01$ (right-hand side). Lower row: $\|W(t)\|$ for the same values of δ.

- the modified Magnus method of classical order 4 as presented by Iserles [8].

In the Magnus methods, the occurring integrals are approximated by Gaussian quadrature of order 4. Since these methods require more than one function evaluation per time step, we do not only display the error versus the step size, but also the error versus the number of function evaluations.

5.1 Well-separated frequencies.

For $\delta = 1$, the frequencies stay well separated at all times t. In Figure 5.2, we illustrate the improvement obtained from transforming the original differential equation (1.1) to Equation (2.7). On the left-hand side, the first solution component of (1.1) is displayed and on the right-hand side that of (2.7). As predicted by (2.13), the oscillations of η are of magnitude $\mathrm{O}(\varepsilon)$ around a smooth solution of the adiabatic limit equation (2.12).

The average error in η is plotted in logarithmic scale versus the step size in Figure 5.3 and versus the number of required function evaluations in Figure 5.4. For small step sizes $h < \varepsilon$, the Modified Magnus method shows order 4, the other methods order 2 as expected. For the more interesting range $h > \varepsilon$, the accuracy of most schemes is subject to resonances for certain values of h. The Gautschi method is obviously the least accurate one, but in fact it is still by far more accurate than standard integrators like, e.g., the trapezoidal rule (not displayed). The adiabatic integrators show comparable accuracy to the Magnus schemes for $\varepsilon = 0.01$, but they are considerably more accurate for smaller values of ε. The differences are even more pronounced in the numbers of matrix evaluations.

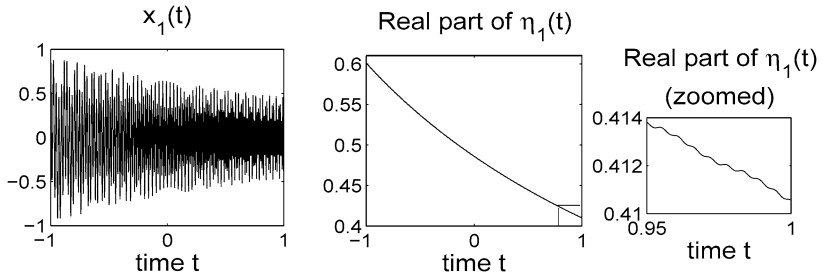

Figure 5.2: Left-hand side: First entry of the solution of the original equation (1.1) ($\varepsilon = 0.01$, $\delta = 1$). Centre: First entry of the solution of the transformed equation (2.7). Right-hand side: Magnification of the region marked by the small box.

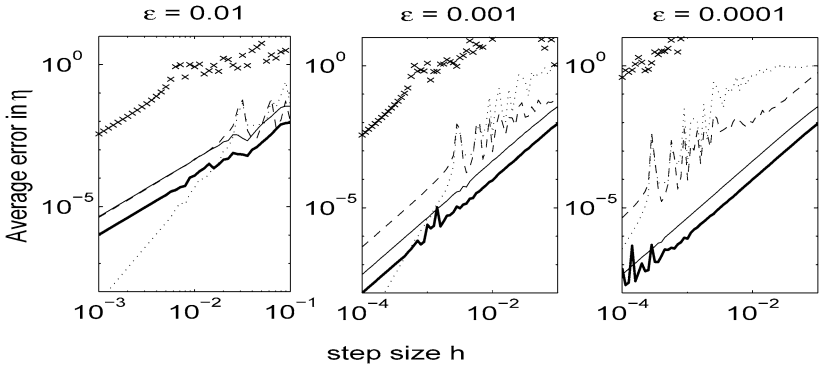

Figure 5.3: Error versus step size of the adiabatic midpoint rule (solid line) and the adiabatic Magnus method (bold solid line) compared with other schemes: the modified Magnus method of order 4 (dotted line), the standard Magnus method (dashed line) and the Gautschi method (crosses); $\delta = 1$.

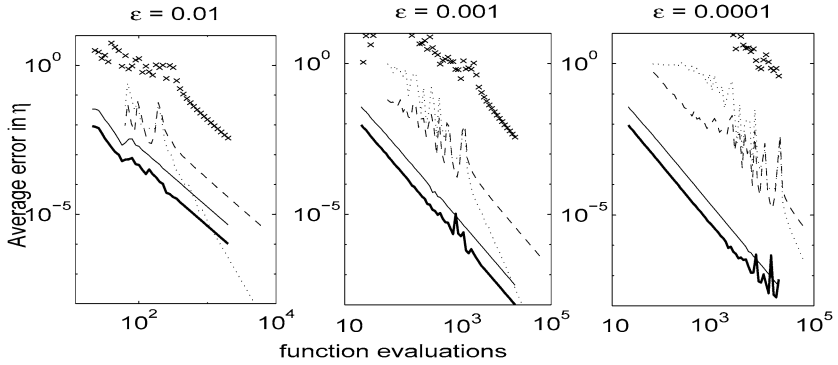

Figure 5.4: Error versus the number of function evaluations for the same methods and data as before.

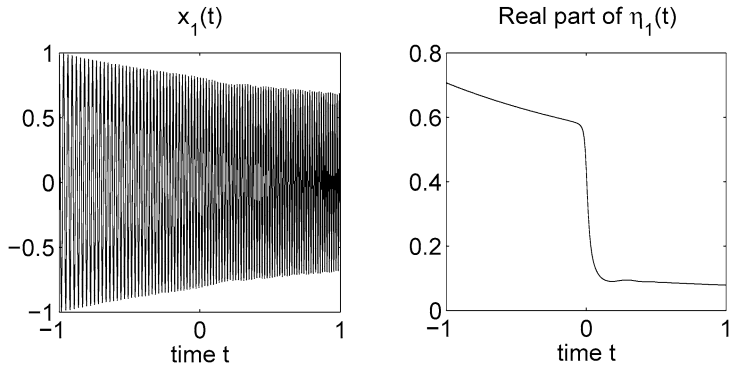

Figure 5.5: Left-hand side: First entry of the solution of the original equation (1.1). Right-hand side: First entry of the solution of the transformed equation (2.7); $\varepsilon = 0.01$, $\delta = 0.01$.

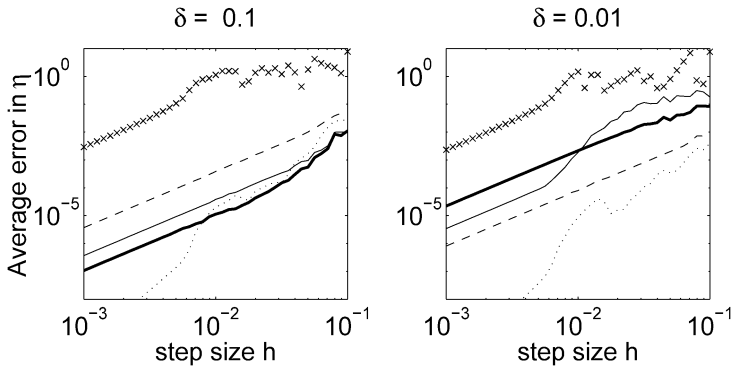

Figure 5.6: Error versus step size for the same methods as before, $\varepsilon = 0.01$.

5.2 Almost-crossing of frequencies.

Figure 5.5 shows what happens if δ is reduced to ε and the eigenfrequencies of $A(t)$ pass through an avoided crossing. At $t \approx 0$, where these eigenvalues have their minimal distance, the entries of $\eta(t)$ leave their range of $O(\varepsilon)$ around a smooth function and jump to new levels, since (2.13) ceases to be valid. Before the avoided crossing, the situation is similar to the case considered before and our methods apply with very small errors. The main part of the error comes from the avoided crossing.

As is shown in Figure 5.1, $W(t)$ changes rapidly during the avoided crossing, but the methods approximate this matrix only piecewise linearly. The finite difference approximations in (3.7)–(3.9) lose accuracy now that $W(t)$ changes abruptly. In addition, some of the entries $1/(\lambda_l - \lambda_k)$ of the matrix $D^-(\Lambda)$ become large during the close encounter of the eigenvalues.

Figure 5.6 compares the errors of the adiabatic midpoint rule and the adiabatic Magnus method with those of the other numerical schemes described above. On the left-hand side, δ is chosen as $\sqrt{\varepsilon}$ and on the right-hand side, $\delta = \varepsilon = 0.01$. Most of the graphs are much smoother than in the first examples, because now

it is not the small scale oscillations that sum up to the main error, but the non-adiabatic transitions on the larger scale. For $\delta = \sqrt{\varepsilon}$ and for $h > \varepsilon$, the range of step sizes we are interested in, the new methods show comparable results to the modified Magnus method, whereas the standard Magnus method seems to have more difficulties in this example. Again, the Gautschi method shows the lowest accuracy.

For $\delta = \varepsilon$ (right-hand side of Figure 5.6) or smaller values of δ, the jump of η gets steeper and the Magnus methods benefit from their fourth-order integral approximation. The adiabatic integrators lose accuracy in the narrow transition zone. It can be expected that the behaviour is improved by an adaptive step size selection, possibly using only a linear phase approximation for $\Phi(t)$, as in [11].

6 Error analysis.

In this section, we give a rigorous proof of the observed second-order accuracy for the adiabatic midpoint and Magnus methods for large step sizes up to $h < \sqrt{\varepsilon}$.

6.1 Error of the adiabatic midpoint rule.

General assumptions for the whole section are:

1. $A(t)$ is a real, symmetric and positive definite matrix with the diagonalization $A(t) = Q(t)\Omega(t)^2 Q(t)^{\mathrm{T}}$ for every $t \in [t_0,\ t_{\mathrm{end}}]$.
2. The eigenfrequencies $\omega_k(t)$ remain separated and bounded away from 0: there is a $\delta > 0$ such that for any pair $\omega_k(t)$ and $\omega_l(t)$ with $k \neq l$, the lower bounds
$$|\omega_k(t) - \omega_l(t)| \geq \delta, \quad \omega_k(t) \geq \tfrac{1}{2}\delta$$
hold for all $t \in [t_0, t_{\mathrm{end}}]$.
3. The functions $t \mapsto Q(t)$ and $t \mapsto \Omega(t)$ are three times continuously differentiable with derivatives bounded independently of ε.
4. The initial values satisfy $\|x(0)\| \leq C_0$ and $\|\dot{x}(0)\| \leq C_0/\varepsilon$ with a constant C_0 independent of ε.
5. The time step h satisfies $h < \sqrt{\varepsilon}$.

The time step restriction is much weaker than the condition $h \ll \varepsilon$ required for standard integrators.

THEOREM 6.1. *Let η_n and x_n, $\dot{x}_n$ denote the approximations given by the adiabatic midpoint rule and assume that conditions* 1–5 *hold. Then, the errors at $t_n = t_0 + nh \in [t_0,\ t_{\mathrm{end}}]$ are bounded by*

$$\|\eta_n - \eta(t_n)\| \leq C_1 h^2,$$
$$\|x_n - x(t_n)\| + \varepsilon\|\dot{x}_n - \dot{x}(t_n)\| \leq C_2 h^2,$$

where the constants C_1 and C_2 depend only on δ of Assumption 2*, on the bounds of the derivatives in Assumption* 3*, on the bounds of the initial values, and on the length of the time interval. In particular, C_1 and C_2 are independent of ε, h, and n with $t_n \in [t_0,\ t_{\mathrm{end}}]$.*

PROOF. For convenience, we give the proof only for $h > \varepsilon$. The less interesting case $h < \varepsilon$ can be treated by similar arguments. In some aspects, the error analysis is similar to the error analysis of [12] and we refer to that paper for some details we omit here. As in [12], the main part of the proof is to show that the local error is of size $\mathrm{O}(h^3)$,

$$\left\|\eta(t_{n+1}) - \big(\eta(t_{n-1}) + h\mathcal{A}_n\eta(t_n) + h^2\mathcal{B}_n\eta(t_n) + h^2\mathcal{C}_n\eta(t_n)\big)\right\| \le Ch^3 \tag{6.1}$$

with a constant C independent of ε. The statement of Theorem 6.1 then follows from a discrete version of Gronwall's lemma and the estimate for x and y is a consequence of the transformation (2.5) and the accuracy of the Simpson rule. To prove (6.1), we use the following notations.

- Define $\widehat{\mathcal{A}}_n$, $\widehat{\mathcal{B}}_n$, and $\widehat{\mathcal{C}}_n$ as in (3.4), (3.5), and (3.7), respectively, but with $W(t_n)$ replaced by W_n, $V(t_n)$ replaced by V_n and the same replacements made for $\dot{W}(t_n)$ and $\dot{V}(t_n)$.
- Define $\check{\mathcal{A}}_n$, $\check{\mathcal{B}}_n$, and $\check{\mathcal{C}}_n$ as in (3.16), (3.17), and (3.18), respectively, but with Φ_n replaced by $\Phi(t_n)$ and $\dot{\Lambda}_n$ replaced by $\dot{\Lambda}(t_n)$.

With this definitions, the local error can be split into four parts

$$\begin{aligned}
&\eta(t_{n+1}) - \big(\eta(t_{n-1}) + h\mathcal{A}_n\eta(t_n) + h^2\mathcal{B}_n\eta(t_n) + h^2\mathcal{C}_n\eta(t_n)\big)\\
&\quad= \eta(t_{n+1}) - \big(\eta(t_{n-1}) + h\widehat{\mathcal{A}}_n\eta(t_n) + h^2\widehat{\mathcal{B}}_n\eta(t_n) + h^2\widehat{\mathcal{C}}_n\eta(t_n)\big) + && (6.2)\\
&\qquad+ \big(h\widehat{\mathcal{A}}_n + h^2\widehat{\mathcal{B}}_n + h^2\widehat{\mathcal{C}}_n\big)\eta(t_n) - \big(h\check{\mathcal{A}}_n + h^2\check{\mathcal{B}}_n + h^2\check{\mathcal{C}}_n\big)\eta(t_n) + && (6.3)\\
&\qquad+ \big(h\check{\mathcal{A}}_n + h^2\check{\mathcal{B}}_n + h^2\check{\mathcal{C}}_n\big)\eta(t_n) - \big(h\widetilde{\mathcal{A}}_n + h^2\widetilde{\mathcal{B}}_n + h^2\widetilde{\mathcal{C}}_n\big)\eta(t_n) + && (6.4)\\
&\qquad+ \big(h\widetilde{\mathcal{A}}_n + h^2\widetilde{\mathcal{B}}_n + h^2\widetilde{\mathcal{C}}_n\big)\eta(t_n) - \big(h\mathcal{A}_n + h^2\mathcal{B}_n + h^2\mathcal{C}_n\big)\eta(t_n) && (6.5)
\end{aligned}$$

with the following interpretation: (6.2) is the error resulting from replacing the intermediate values of W and V via (3.3), (3.7), and (3.8) and from freezing $\eta(t_n + \sigma h) \approx \eta(t_n)$. Replacing $\Phi(t_n + \theta h)$ by the Taylor expansion is the origin of difference (6.3). The approximation of $\Phi(t_n)$ by the Simpson rule (3.12) causes (6.4), whereas (6.5) is introduced by solving the integrals approximately, as it is done in Section 3.2.

For simplicity, we denote with C indistinguished constants and instead of

$$\sup_t \|W(t)\|, \quad \sup_t \|V(t)\|, \quad \sup_t \|\ddot{\Lambda}(t)\|, \quad \sup_t \left\|\frac{\partial^3}{\partial t^3}U(t)\right\|, \quad \dots$$

where the suprema are taken over all $t \in [t_0,\ t_{\mathrm{end}}]$, we use the short forms

$$\|W\|, \quad \|V\|, \quad \|\ddot{\Lambda}\|, \quad \left\|\frac{\partial^3}{\partial t^3}U\right\|, \quad \text{etc.}$$

One difference to the terms occuring in [12] is the presence of a second coupling matrix V in all $\mathcal{A}(t_n)$, $\mathcal{B}(t_n)$, and $\mathcal{C}(t_n)$. By splitting this matrix in a diagonal part V^D and a part with zero diagonal V^N, we can treat the difference $V^N - W$ with the techniques from [12] and only add the term containing V^D. Other

additional terms occur in $\mathcal{C}(t_n)$, which here contains two terms with double integrals and one term similar to $\mathcal{B}(t_n)$.

6.1.1 Estimating (6.2).

One can easily conclude the following estimates for (3.7) and (3.8)

$$\begin{aligned} \|W(t_n) - W_n\| &\le Ch^2 \|\partial^3 U\|, \qquad \|V(t_n) - V_n\| \le Ch^2 \|\partial^3 B\|, \\ \|\dot{W}(t_n) - \dot{W}_n\| &\le Ch \|\partial^3 U\|, \qquad \|\dot{V}(t_n) - \dot{V}_n\| \le Ch \|\partial^3 B\|, \end{aligned}$$

and derive

$$\begin{aligned} \|W(t_n + \theta h) - W_n - \theta h \dot{W}_n\| &\le Ch^2(\|\partial^3 U\| + \|\ddot{W}\|), \quad \text{analogously} \\ \|V(t_n + \theta h) - V_n - \theta h \dot{V}_n\| &\le Ch^2(\|\partial^3 B\| + \|\ddot{W}\|), \quad \text{and} \\ \|W(t_n + \theta h) - W_n\| &\le Ch\|\dot{W}\| + \mathrm{O}(h^2), \\ \|V(t_n + \theta h) - V_n\| &\le Ch\|\dot{V}\| + \mathrm{O}(h^2). \end{aligned}$$

Using $|\sigma| \le 1$ we get the estimate $\|\eta(t_n + \sigma h) - \eta(t_n)\| \le Ch \|V - W\|$ from

$$\begin{aligned} \eta(t_n + \sigma h) - \eta(t_n) \;=\; h \int_0^\sigma \big(E(\Phi(t_n + \xi h)) \bullet \big(V^N - W\big)(t_n + \xi h)\big)\eta(t_n + \xi h) + \\ + V^D(t_n + \xi h)\eta(t_n + \xi h)\,\mathrm{d}\xi. \end{aligned}$$

With these inequalities, we can compute the following bound for (6.2)

$$Ch^3(\|\partial^3 B\| + \|\partial^3 U\| + \|\ddot{V} - \ddot{W}\| + \|\dot{V} - \dot{W}\|\,\|V - W\| + \|V - W\|^3 + \|V - W\|^2\|V\|).$$

6.1.2 Estimating (6.3).

We denote with $\theta^3 h^3 R(t, \theta h)$ the remainder of the Taylor expansion (3.10), i.e.

$$\Phi(t + \theta h) = \Phi(t) + \theta h \Lambda(t) + \tfrac{1}{2}\theta^2 h^2 \dot{\Lambda}(t) + \theta^3 h^3 R(t, \theta h), \text{ and } \|R(t, \theta h)\| \le C\|\ddot{\Lambda}\|.$$

Moreover, we define a matrix-valued and with respect to t continuously differentiable function by

$$F(t, x) = D(R(t, x)) \bullet \int_0^1 E(\xi x^3 R(t, x))\,\mathrm{d}\xi = \frac{\varepsilon}{ix^3}\big(E(x^3 R(t, x)) - E(0)\big)$$

for $x \neq 0$, and by the corresponding limit for $x = 0$. $F(t, x)$ is bounded by

$$\|F(t, x)\| = C\|R(t, x)\| \le C\|\ddot{\Lambda}\|. \tag{6.6}$$

We start with a part of (6.3), using this definition and get

$$\begin{aligned}
&(h\widehat{\mathcal{A}}_n + h^2\widehat{\mathcal{B}}_n) - (h\check{\mathcal{A}}_n + h^2\check{\mathcal{B}}_n) \\
&\quad = hE(\Phi(t_n)) \bullet \int_{-1}^{1} E\big(\theta h\Lambda(t_n) + \tfrac{1}{2}\theta^2 h^2 \dot{\Lambda}(t_n)\big) \bullet \\
&\qquad \bullet \frac{i\theta^3 h^3}{\varepsilon} F(t_n, \theta h)\,\mathrm{d}\theta \bullet \big(V_n^N - W_n\big) + \\
&\qquad + \mathrm{O}(h^4).
\end{aligned}$$

Now, we examine the integral more closely, which is exactly the same as in [12]. Omitting further details, integration by parts yields

$$\begin{aligned}
&\int_{-1}^{1} E\big(\theta h\Lambda(t_n) + \tfrac{1}{2}\theta^2 h^2 \dot{\Lambda}(t_n)\big) \bullet \frac{i\theta^3 h^3}{\varepsilon} F(t_n, \theta h)\,\mathrm{d}\theta \\
&\quad = \int_{-1}^{\theta} E(\sigma h\Lambda(t_n))\,\mathrm{d}\sigma \bullet E\big(\tfrac{1}{2}\theta^2 h^2 \dot{\Lambda}(t_n)\big) \bullet \frac{i\theta^3 h^3}{\varepsilon} F(t_n, \theta h)\Big|_{\theta=-1}^{1} - \\
&\qquad - \int_{-1}^{1}\int_{-1}^{\theta} E(\sigma h\Lambda(t_n))\,\mathrm{d}\sigma \bullet \frac{\mathrm{d}}{\mathrm{d}\theta}\left(E\big(\tfrac{1}{2}\theta^2 h^2 \dot{\Lambda}(t_n)\big) \bullet \frac{i\theta^3 h^3}{\varepsilon} F(t_n, \theta h)\right) \mathrm{d}\theta.
\end{aligned}$$

With

$$\int_{-1}^{\theta} E(\sigma h\Lambda(t_n))\,\mathrm{d}\sigma = \frac{\varepsilon}{ih} D^-(\Lambda(t_n)) \bullet \big(E(\theta h\Lambda(t_n)) - E(-h\Lambda(t_n))\big)$$

and

$$\begin{aligned}
&\frac{\mathrm{d}}{\mathrm{d}\theta}\left(E\big(\tfrac{1}{2}\theta^2 h^2 \dot{\Lambda}(t_n)\big) \bullet \frac{i\theta^3 h^3}{\varepsilon} F(t_n, \theta h)\right) \\
&\quad = \frac{i\theta h^2}{\varepsilon} D(\dot{\Lambda}(t_n)) \bullet E\big(\tfrac{1}{2}\theta^2 h^2 \dot{\Lambda}(t_n)\big) \bullet \frac{i\theta^3 h^3}{\varepsilon} F(t_n, \theta h) + \\
&\qquad + E\big(\tfrac{1}{2}\theta^2 h^2 \dot{\Lambda}(t_n)\big) \bullet \frac{ih^3}{\varepsilon} \frac{\mathrm{d}}{\mathrm{d}\theta}\big(\theta^3 F(t_n, \theta h)\big),
\end{aligned}$$

this enables the estimate

$$\|(h\widehat{\mathcal{A}}_n + h^2\widehat{\mathcal{B}}_n)\eta(t_n) - (h\check{\mathcal{A}}_n + h^2\check{\mathcal{B}}_n)\eta(t_n)\| \le C\frac{h^3}{\delta}\|\ddot{\Lambda}\|\,\|V - W\| + \mathrm{O}(h^4).$$

Besides the above conclusions, we have used that, by assumption, $\frac{h^2}{\varepsilon} \le 1$ and that

$$\begin{aligned}
&\|D(\dot{\Lambda}(t_n))\| \le C, \qquad \|F(t_n, \theta h)\| \le C\|\ddot{\Lambda}\|, \qquad \|D^-(\Lambda(t_n))\| \le \frac{C}{\delta}, \\
&\left\| \frac{\mathrm{d}}{\mathrm{d}\theta}\big(\theta^3 F(t_n, \theta h)\big)\right\| \le C\|F(t_n, \theta h)\| + \mathrm{O}(h).
\end{aligned}$$

The difference between the first terms of $\widehat{\mathcal{C}}_n - \check{\mathcal{C}}_n$ is the same occuring in [12] and can be rewritten as

$$\begin{aligned}
&\int_{-1}^{1} \Big(E\big(\Phi(t_n) + \theta h \Lambda(t_n) + \tfrac{1}{2}\theta^2 h^2 \dot{\Lambda}(t_n)\big) \bullet \frac{i\theta^3 h^3}{\varepsilon} F(t_n, \theta h) \bullet \big(V_n^N - W_n\big) \Big) \times \\
&\quad \times \Big(\int_0^{\theta} E\big(\Phi(t_n + \sigma h)\big) \bullet \big(V_n^N - W_n\big)\, \mathrm{d}\sigma \Big)\, \mathrm{d}\theta + \\
&\quad + \int_{-1}^{1} \big(E\big(\Phi(t_n) + \theta h \Lambda(t_n) + \tfrac{1}{2}\theta^2 h^2 \dot{\Lambda}(t_n)\big) \bullet \big(V_n^N - W_n\big) \big) \times \\
&\quad \times \Big(\int_0^{\theta} E\big(\Phi(t_n) + \sigma h \Lambda(t_n) + \tfrac{1}{2}\sigma^2 h^2 \dot{\Lambda}(t_n)\big) \bullet \frac{i\sigma^3 h^3}{\varepsilon} F(t_n, \sigma h) \bullet \\
&\quad \bullet \big(V_n^N - W_n\big)\, \mathrm{d}\sigma \Big)\, \mathrm{d}\theta.
\end{aligned}$$

With the inequalities mentioned above and the assumption $\frac{h^2}{\varepsilon} \leq 1$, we can estimate the norm of this difference by $Ch\,\|\ddot{\Lambda}\|\,\|V - W\|^2 + \mathrm{O}(h^2)$ and turn to the difference of the second terms, which can be treated like the difference $\widehat{\mathcal{B}}_n - \check{\mathcal{B}}_n$. It holds that

$$\begin{aligned}
&\Big\| \Big(\int_{-1}^{1} \theta E(\Phi(t_n + \theta h))\, \mathrm{d}\theta - \int_{-1}^{1} \theta E\big(\Phi(t_n) + \theta h \Lambda(t_n) + \tfrac{1}{2}\theta^2 h^2 \dot{\Lambda}(t_n)\big)\, \mathrm{d}\theta \Big) \bullet \\
&\quad \bullet \big(V_n^N - W_n\big)\, V_n^D \Big\| \leq Ch\|\ddot{\Lambda}\|\,\|V - W\|\,\|V\| + \mathrm{O}(h^2);
\end{aligned}$$

and the same estimate is valid for the difference of the third terms of $\widehat{\mathcal{C}}_n - \check{\mathcal{C}}_n$, because of their similarity to the first terms.

Altogether, (6.3) is bounded by

$$Ch^3 \|\ddot{\Lambda}\|\,\|V - W\| \Big(\frac{1}{\delta} + \|V - W\| + \|V\| \Big).$$

6.1.3 Estimating (6.4).

The errors of the Simpson rule (3.12) and the difference quotient (3.11) are

$$\begin{aligned}
\|\Phi(t_n) - \Phi_n\| &\leq Ch^4\, \|\partial^3 \Lambda\|, \\
\|\dot{\Lambda}(t_n) - \dot{\Lambda}_n\| &\leq Ch^2\, \|\partial^3 \Lambda\|.
\end{aligned}$$

By using the assumption $\frac{ih^2}{\varepsilon} \leq 1$, we conclude directly

$$\|\check{\mathcal{A}}_n - \widetilde{\mathcal{A}}_n\| \leq Ch^2\, \|\partial^3 \Lambda\|\,\|V - W\|.$$

Since $\|\check{\mathcal{B}}_n - \widetilde{\mathcal{B}}_n\|$ and $\|\check{\mathcal{C}}_n - \widetilde{\mathcal{C}}_n\|$ only produce errors of higher order, we get the bound $Ch^3\,\|\partial^3 \Lambda\|\,\|V - W\|$ for (6.4).

6.1.4 Estimating (6.5).

We have

$$\widetilde{\mathcal{B}}_n - \mathcal{B}_n = E(\Phi_n) \bullet \left(\int_{-1}^{1} \theta E\big(\theta h \Lambda(t_n) + \tfrac{1}{2}\theta^2 h^2 \dot{\Lambda}_n\big)\, \mathrm{d}\theta - \mathcal{I}_1 \right) \bullet \big(\dot{V}_n^N - \dot{W}_n\big).$$

The error made in (3.19) can easily (see [12]) be transformed to

$$\begin{aligned} &\int_{-1}^{1} \theta E\big(\theta h \Lambda(t_n) + \tfrac{1}{2}\theta^2 h^2 \dot{\Lambda}_n\big)\, \mathrm{d}\theta - \mathcal{I}_1 \\ &\quad = -hD^-(\Lambda(t_n)) \bullet D(\dot{\Lambda}_n) \bullet \\ &\qquad \bullet \int_{-1}^{1} \left(\theta E(\theta h \Lambda(t_n)) + E(-h\Lambda(t_n)) - \right. \\ &\qquad \left. - \int_{-1}^{\theta} E(\sigma h \Lambda(t_n))\, \mathrm{d}\sigma \right) \bullet \theta E\big(\tfrac{1}{2}\theta^2 h^2 \dot{\Lambda}_n\big)\, \mathrm{d}\theta, \end{aligned}$$

from which we conclude

$$\left\| \int_{-1}^{1} \theta E\big(\theta h \Lambda(t_n) + \tfrac{1}{2}\theta^2 h^2 \dot{\Lambda}_n\big)\, \mathrm{d}\theta - \mathcal{I}_1 \right\| \leq C\frac{h}{\delta}. \tag{6.7}$$

Next, we examine

$$\begin{aligned} \widetilde{\mathcal{A}}_n - \mathcal{A}_n \;=\; & E(\Phi_n) \bullet \left(\int_{-1}^{1} E\big(\theta h \Lambda(t_n) + \tfrac{1}{2}\theta^2 h^2 \dot{\Lambda}_n\big)\, \mathrm{d}\theta - \right. \\ & \left. - \left(\frac{\varepsilon}{ih} D^-(\Lambda(t_n)) \bullet \mathcal{E}_0 - hD^-(\Lambda(t_n)) \bullet D(\dot{\Lambda}_n) \bullet \mathcal{I}_1 \right) \right) \bullet \\ & \bullet \big(V_n^N - W_n\big). \end{aligned}$$

From Equation (3.25), it follows that

$$\left\| \int_{-1}^{1} E\big(\theta h \Lambda(t_n) + \tfrac{1}{2}\theta^2 h^2 \dot{\Lambda}_n\big)\, \mathrm{d}\theta - \frac{\varepsilon}{ih} D^-(\Lambda(t_n)) \bullet \mathcal{E}_0 \right\| \leq C\frac{h}{\delta}$$

and with (6.7)

$$\|\widetilde{\mathcal{A}}_n - \mathcal{A}_n\| \leq C\left(\frac{h}{\delta}\right)^2 \|V - W\|,$$

since the remainder term is similar to (3.19).

Together with (6.7), we get the estimate

$$\|(h\widetilde{\mathcal{A}}_n + h^2\widetilde{\mathcal{B}}_n)\eta(t_n) - (h\mathcal{A}_n + h^2\mathcal{B}_n)\eta(t_n)\| \leq Ch^3\left(\frac{\|V - W\|}{\delta^2} + \frac{\|\dot{V} - \dot{W}\|}{\delta} \right).$$

Analogously, it can be shown that

$$\|h^2\widetilde{\mathcal{C}}_n\eta(t_n) - h^2\mathcal{C}_n\eta(t_n)\| \leq C\frac{h^3}{\delta^2}\|V - W\|\big(\|V - W\|\,(1 + \delta) + 2\|V\|\delta + \|V\|\big).$$

This is the final estimate to complete the proof of statement (6.1).

The error of the starting step is also bounded by $O(h^2)$ as can be seen by similar arguments. □

6.2 Error of the adiabatic Magnus method.

THEOREM 6.2. *Under the assumptions of Theorem* 6.1*, the errors of the adiabatic Magnus method introduced in Section* 4 *are bounded by*

$$\begin{aligned} \|\eta_n - \eta(t_n)\| &\leq C_1 h^2, \\ \|x_n - x(t_n)\| + \varepsilon \|\dot{x}_n - \dot{x}(t_n)\| &\leq C_2 h^2, \end{aligned}$$

with constants C_1 and C_2 depending on the same terms as in Theorem 6.1.

PROOF. Truncating the Magnus series after the first commutator is known to cause a local error of $O(h^5)$ if the product of the step size and the highest frequency is small, but this estimate is not uniform in ε. Nevertheless, the truncation error is still $O(h^3)$ uniformly in ε even with $h > \varepsilon$, since all truncated terms of the Magnus expansion contain at least three integrals and since the integrand is uniformly bounded with respect to ε. The other errors (induced by the use of Taylor expansions, difference quotients and approximate evaluations of the integrals) can be estimated as it was done in the proof of Theorem 6.1. □

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REFERENCES

1. M. Born and V. Fock, *Beweis des Adiabatensatzes*, Z. Phys., 51 (1928), pp. 165–180.
2. I. Degani and J. Schiff, *Right correction Magnus series approach for integration of linear ordinary differential equations with highly oscillatory solution*, Report MCS03-04, Weizmann Institute of Science, Israel, 2003.
3. B. García-Archilla, J. M. Sanz-Serna, and R. D. Skeel, *Long-time-step methods for oscillatory differential equations*, SIAM J. Sci. Comput., 20 (1998), pp. 930–963.
4. W. Gautschi, *Numerical integration of ordinary differential equations based on trigonometric polynomials*, Numer. Math., 3 (1961), pp. 381–397.
5. V. Grimm, *Exponentielle Integratoren als Lange–Zeitschritt–Verfahren für oszillatorische Differentialgleichungen zweiter Ordnung*, Doctoral Thesis, Mathematisches Institut, Universität Düsseldorf, 2002.
6. E. Hairer, C. Lubich, and G. Wanner, *Geometric Numerical Integration*, Springer-Verlag, Berlin, 2002, Ch. XIII.
7. M. Hochbruck and C. Lubich, *A Gautschi-type method for oscillatory second-order differential equations*, Numer. Math., 83 (1999), pp. 403–426.
8. A. Iserles, *On the global error of discretization methods for highly oscillatory ordinary differential equations*, BIT, 42 (2002), pp. 561–599.
9. A. Iserles, *On the numerical quadrature of highly oscillating integrals I: Fourier transforms*, Technical Report, NA2003/05, DAMTP University of Cambridge, 2003.
10. A. Iserles, H. Z. Munthe-Kaas, S. P. Nørsett, and A. Zanna, *Lie-group methods*, Acta Numerica, (2000), pp. 215–365.

11. T. Jahnke and C. Lubich, *Numerical integrators for quantum dynamics close to the adiabatic limit*, Numer. Math., 94 (2003), pp. 289–314.
12. T. Jahnke, *Numerische Verfahren für fast adiabatische Quantendynamik*, Doctoral Thesis, Mathematisches Institut, Universität Tübingen, 2003.
13. T. Jahnke, *Long-time-step integrators for almost-adiabatic quantum dynamics*, SIAM J. Sci. Comp., 25 (2004), pp. 2145–2164.
14. W. Magnus, *On the exponential solution of differential equations for a linear operator*, Comm. Pure Appl. Math., VII (1954), pp. 649–673.
15. L. R. Petzold, L. O. Jay, and J. Yen, *Numerical solution of highly oscillatory ordinary differential equations*, Acta Numerica, 7 (1997), pp. 437–483.
16. V. Stejskal and M. Valášek, *Kinematics and Dynamics of Machinery*, Marcel Dekker Inc., New York, 1996, Ch. IX.