Arbitrary–order trigonometric Fourier collocation methods for multi-frequency oscillatory systems

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Abstract. We rigorously study a novel type of trigonometric Fourier collocation methods for solving multi-frequency oscillatory second-order ordinary differential equations (ODEs) $q''(t) + Mq(t) = f(q(t))$ with a principal frequency matrix $M \in \mathbb{R}^{d\times d}$. If M is symmetric and positive semi-definite and $f(q) = -\nabla U(q)$ for a smooth function $U(q)$, then this is a multi-frequency oscillatory Hamiltonian system with the Hamiltonian $H(q,p) = p^T p/2 + q^T Mq/2 + U(q)$, where $p = q'$. The solution of this system is a nonlinear multi-frequency oscillator. The new trigonometric Fourier collocation method takes advantage of the special structure brought by the linear term Mq and its construction incorporates the idea of collocation methods, the variation-of-constants formula and the local Fourier expansion of the system. The properties of the new methods are analysed. The analysis in the paper demonstrates an important feature, namely that the trigonometric Fourier collocation methods can be of an arbitrary order and when $M \to 0$, each trigonometric Fourier collocation method creates a particular Runge–Kutta–Nyström-type Fourier collocation method, which is symplectic under some conditions. This allows us to obtain arbitrary high order symplectic methods to deal with a special and important class of systems of second-order ODEs in an efficient way. The results of numerical experiments are quite promising and show that the trigonometric Fourier collocation methods are significantly more efficient in comparison with alternative approaches that have previously appeared in the literature.

Keywords: Second-order ordinary differential equations · Multi-frequency oscillatory systems · Trigonometric Fourier collocation methods · Multi-frequency oscillatory Hamiltonian systems · Quadratic invariant · Variation-of-constants formula · Symplectic methods

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1 Introduction

In this paper we are concerned with systems of multi-frequency oscillatory second-order differential equations of the form

$$q''(t) + Mq(t) = f(q(t)), \qquad q(0) = q_0, \quad q'(0) = q_0', \qquad t \in [0, t_{\text{end}}], \tag{1}$$

where M is a $d \times d$ positive semi-definite matrix implicitly containing the frequencies of the oscillatory problem and $f : \mathbb{R}^d \to \mathbb{R}^d$ is an analytic function. The solution of this system is a multi-frequency nonlinear oscillator because of the presence of the linear term Mq. (1) is a multi-frequency oscillatory system with multiple time scales and occurs in a wide variety of applications such as quantum physics, circuit simulations, flexible body dynamics, mechanics (see, e.g. [20, 10, 11, 21, 15, 56, 59]).

Once it is further assumed that M is symmetric and f is the negative gradient of a real-valued function $U(q)$, the system (1) is identical to the following initial value Hamiltonian system

$$\begin{aligned} \dot{q} &= \nabla_p H(q,p), \qquad & q(0) &= q_0, \\ \dot{p} &= -\nabla_q H(q,p), \qquad & p(0) &= p_0 \equiv q_0' \end{aligned} \tag{2}$$

with the Hamiltonian function

$$H(q,p) = \frac{1}{2} p^T p + \frac{1}{2} q^T M q + U(q). \tag{3}$$

This is an important system which has been investigated by many authors (see, e.g. [20, 10, 8, 11, 21]). In essence, numerous mechanical systems with a partitioned Hamiltonian function fit this pattern. Two fundamental properties of Hamiltonian systems are:

(a) the solutions preserve the Hamiltonian H, i.e., $H(q(t), p(t)) \equiv H(q_0, p_0)$ for any $t \geq 0$;

(b) the corresponding flow is symplectic, i.e., it preserves the differential 2-form $\sum_{i=1}^{d} dp_i \wedge dq_i$.

An important feature of ordinary differential equations (ODEs) is first integrals. Much work deals with the conservation of invariants (first integrals) by numerical methods, e.g. [23, 33, 32, 21, 6, 22, 38, 12]. We consider the quadratic invariant $Q = q^T Dp$ of (1). The quadratic form Q is a first integral of (1) if and only if $p^T Dp + q^T D(f(q) - Mq) = 0$ for all $p, q \in \mathbb{R}^d$. This implies that D is a skew-symmetric matrix and that $q^T D(f(q) - Mq) = 0$ for any $q \in \mathbb{R}^d$. It has been pointed out in [23, 21] that symplecticity is a quadratic first integral acting on the vector fields of a differential equation and every numerical method that preserves quadratic first integrals is a symplectic method for the corresponding Hamiltonian system.

For the Hamiltonian differential equations

$$y' = J^{-1} \nabla H(y) \tag{4}$$

with a skew-symmetric constant matrix J and the Hamiltonian $H(y)$, various numerical methods including symplectic methods and energy-preserving methods have been proposed and we refer the reader to [45, 48, 42, 43, 50, 40, 29, 38, 30, 22, 19, 5, 9, 7, 2, 1, 3, 35] for some related work. These methods are applicable to (2) since (2) can be rewritten in the form (4). However, it is noted that the system (1) or (2) is oscillatory due to the special structure brought by the linear term Mq. In the last few decades, the theory of numerical methods for oscillatory differential equations has reached a certain maturity. Many efficient codes, mainly based on Runge–Kutta–Nyström (RKN) methods and exponentially/trigonometrically-fitted methods, have become available. Among these various methods, exponential/trigonometric integrators are a very powerful approach and we refer to [27] for a survey work on exponential integrators. Other work related to exponential/trigonometric integrators can be found in [25, 20, 26, 21, 50, 28, 57] for instance. Much has been done to use the special structure brought by the term Mq to solve (1) effectively and we refer the reader to [17, 25, 20, 13, 16, 50, 15, 60, 58, 55, 36, 52, 57, 53, 56, 51, 59] for example.

The motivation for developing exponential/trigonometric algorithms for the oscillatory system (1) with the linear part Mq originates in a variety of research fields such as astronomy, quantum physics, molecular dynamics, mechanics, theoretical physics, semi-discrete wave equations approximated by the method of lines, and others from both applied and pure mathematics. It is apparent that the exponential/trigonometric methods taking advantage of the special structure brought by the term Mq not only produce an improved qualitative behaviour, but also allow for a more accurate long-term integration than with general-purpose methods. Inspired by this point, this paper is devoted to deriving and analysing a novel kind of trigonometric method (trigonometric Fourier collocation method) for (1).

When $M \to 0$, (1) reduces to a special and important class of systems of second-order ODEs expressed in the traditional form

$$q''(t) = f(q(t)), \qquad q(0) = q_0, \quad q'(0) = q'_0, \qquad t \in [0, t_{\text{end}}]. \tag{5}$$

Its corresponding Hamiltonian system and quadratic invariant can be described by the above statements for (1) with $M \to 0$. Therefore, we are hopeful of obtaining efficient methods for (5) based on the methods designed for (1) when $M \to 0$.

The main aim of this paper is to design a novel trigonometric Fourier collocation method of arbitrary order for solving multi-frequency oscillatory systems (1) and to obtain arbitrary order symplectic methods for system (5) based on the new trigonometric Fourier collocation method. This *trigonometric Fourier collocation (TFC)* method is a kind of collocation method: collocation methods for ODEs (see, e.g. [54, 23, 31, 21, 19]) have a long history. An interesting feature of collocation methods is that we not only get a discrete set of approximations, but also a continuous approximation to the solution. The TFC methods not only share this feature of collocation methods, but also incorporate the special structure originating in the term Mq. Moreover, they are derived by truncating the

local Fourier expansion of the system and thus it is very simple to get arbitrarily high order methods for solving (1). In addition, the TFC methods are applicable to the system (1) with no regard to symmetry of M. Besides, when $M \to 0$, our TFC method also sets out a special and efficient arbitrary order symplectic RKN approach to solving the special and important class of second-order ODEs (5). The fact stated above renders the TFC methods a very powerful and efficient approach in applications.

With this premise, this paper is organized as follows. Section 2 presents the local Fourier expansion of (1). The TFC methods are formulated in Section 3 and are analysed in Section 4. Section 5 is devoted to reporting several numerical experiments to demonstrate the efficiency of our novel approximation. Some conclusions are included in Section 6.

2 Local Fourier expansion of (1)

Before considering the Fourier expansion, we commence by recalling matrix-valued functions which have been first defined in [60]:

$$\phi_i(M) := \sum_{l=0}^{\infty} \frac{(-1)^l M^l}{(2l+i)!}, \qquad i = 0, 1. \tag{6}$$

These functions reduce to the ϕ-functions used in Gautschi-type trigonometric or exponential integrators in [25, 20, 21] when M is a symmetric and positive semi-definite matrix. We note an important fact, namely that the convergent Taylor expansion in (6) depends directly on M and is applicable not only to symmetric matrices but also to nonsymmetric ones. By this definition and the formulation of our methods presented in next section, it can be observed that our methods are applicable to the system (1) with no regard to symmetry of M. This is the reason why we use the definition (6) in this paper.

Concerning the variation-of-constants formula for (1) given in [58], we have the following result on the exact solution of the system (1) and its derivative:

$$\begin{aligned} q(h) &= \phi_0(V)q_0 + h\phi_1(V)p_0 + h^2 \int_0^1 (1-z)\phi_1\big((1-z)^2V\big) f(q(hz))dz, \\ p(h) &= -hM\phi_1(V)q_0 + \phi_0(V)p_0 + h \int_0^1 \phi_0\big((1-z)^2V\big) f(q(hz))dz \end{aligned} \tag{7}$$

for $h > 0$, where $V = h^2M$.

In what follows we consider the multi-frequency oscillatory system (1) restricted to the interval $[0, h]$:

$$q''(t) + Mq(t) = f(q(t)), \qquad q(0) = q_0, \quad q'(0) = q_0', \qquad t \in [0, h]. \tag{8}$$

Choose an orthogonal polynomial basis $\{\widehat{P}_j\}_{j=0}^{\infty}$ on the interval $[0, 1]$: e.g., the shifted Legendre polynomials over the interval $[0, 1]$, scaled in order to be orthonormal. Consequently,

$$\int_0^1 \widehat{P}_i(x)\widehat{P}_j(x)dx = \delta_{ij}, \qquad \deg\big(\widehat{P}_j\big) = j, \qquad i, j \geq 0,$$

where δ_{ij} is the Kronecker symbol. We rewrite the right-hand side of (8) as

$$f(q(\xi h)) = \sum_{j=0}^{\infty} \widehat{P}_j(\xi)\gamma_j(q), \quad \xi \in [0,1]; \qquad \gamma_j(q) := \int_0^1 \widehat{P}_j(\tau) f(q(\tau h))d\tau. \quad (9)$$

(To simplify the notation, we use $\gamma_j(q)$ to denote the coefficients involved in the Fourier expansion, replacing the more complete notation $\gamma_j(h, f(q))$.)

Combining (7) and (9), we immediately have the following result.

Theorem 21 *The solution of* (8) *and its derivative satisfy*

$$\begin{aligned} q(h) &= \phi_0(V)q_0 + h\phi_1(V)p_0 + h^2 \sum_{j=0}^{\infty} I_{1,j}\gamma_j(q), \\ p(h) &= -hM\phi_1(V)q_0 + \phi_0(V)p_0 + h\sum_{j=0}^{\infty} I_{2,j}\gamma_j(q), \end{aligned} \quad (10)$$

where

$$I_{1,j} := \int_0^1 \widehat{P}_j(z)(1-z)\phi_1\big((1-z)^2V\big)dz, \quad I_{2,j} := \int_0^1 \widehat{P}_j(z)\phi_0\big((1-z)^2V\big)dz. \quad (11)$$

The main point in designing practical schemes to solve (1) is based on truncating the series (9) after $r \geq 2$ terms and this replaces the initial value problem (1) by the approximate problem

$$\begin{aligned} \tilde{q}'(\xi h) &= \tilde{p}(\xi h), & \tilde{q}(0) &= q_0, \\ \tilde{p}'(\xi h) &= -M\tilde{q}(\xi h) + \sum_{j=0}^{r-1} \widehat{P}_j(\xi)\gamma_j(\tilde{q}), & \tilde{p}(0) &= p_0. \end{aligned}$$

The implicit solution of the new problem is

$$\begin{aligned} \tilde{q}(h) &= \phi_0(V)q_0 + h\phi_1(V)p_0 + h^2 \sum_{j=0}^{r-1} I_{1,j}\gamma_j(\tilde{q}), \\ \tilde{p}(h) &= -hM\phi_1(V)q_0 + \phi_0(V)p_0 + h\sum_{j=0}^{r-1} I_{2,j}\gamma_j(\tilde{q}). \end{aligned} \quad (12)$$

3 Formulation of the TFC methods

It is clear that the scheme (12) itself falls well short of being a practical method unless the integrals $I_{1,j},\ I_{2,j},\ \gamma_j(\tilde{q})$ in (12) can be approximated.

3.1 The computation of $I_{1,j}$, $I_{2,j}$

According to the definition of shifted Legendre polynomials on the interval $[0,1]$,

$$\widehat{P}_j(x) = (-1)^j \sqrt{2j+1} \sum_{k=0}^{j} \binom{j}{k} \binom{j+k}{k} (-x)^k, \qquad j = 0, 1, \ldots, \qquad x \in [0,1], \tag{13}$$

we arrive at

$$\begin{aligned} I_{1,j} =& \int_0^1 \widehat{P}_j(z)(1-z)\phi_1\big((1-z)^2 V\big) dz \\ =& \sqrt{2j+1} \sum_{l=0}^{\infty} (-1)^j \sum_{k=0}^{j} \binom{j}{k} \binom{j+k}{k} \int_0^1 (-z)^k (1-z)^{2l+1} dz \frac{(-1)^l V^l}{(2l+1)!} \\ =& \sqrt{2j+1} \sum_{l=0}^{\infty} \sum_{k=0}^{j} (-1)^{j+k} \binom{j}{k} \binom{j+k}{k} \frac{k!(2l+1)!}{(2l+k+2)!} \frac{(-1)^l V^l}{(2l+1)!} \\ =& \sqrt{2j+1} \sum_{l=0}^{\infty} \sum_{k=0}^{j} \frac{(-1)^{j+k+l}(j+k)!}{k!(j-k)!(2l+k+2)!} V^l, \qquad j = 0, 1, \ldots. \end{aligned}$$

Recall that a *generalized hypergeometric function* (see [41, 47]) is

$${}_mF_n \left[\begin{matrix} \alpha_1, \alpha_2, \ldots, \alpha_m; \\ \beta_1, \beta_2, \ldots, \beta_n; \end{matrix} x \right] = \sum_{l=0}^{\infty} \frac{\prod_{i=1}^{m} (\alpha_i)_l}{\prod_{i=1}^{n} (\beta_i)_l} \frac{x^l}{l!}, \tag{14}$$

where the *Pochhammer symbol* $(z)_l$ is defined as $(z)_0 = 1$ and $(z)_l = z(z+1)\cdots(z+l-1)$, $l \in \mathbb{N}$. The parameters α_i and β_i are arbitrary complex numbers, except that β_i can be neither zero nor a negative integer. $I_{1,j}$ can be formulated as

$$\begin{aligned} I_{1,j} =& \sqrt{2j+1} \sum_{l=0}^{\infty} \frac{(-1)^{j+l}}{(2l+2)!} {}_2F_1 \left[\begin{matrix} -j, j+1; \\ 2l+3; \end{matrix} 1 \right] V^l \\ =& \sqrt{2j+1} \sum_{l=[j/2]}^{\infty} \frac{(-1)^{j+l}(2l+1)!}{(2l+2+j)!(2l+1-j)!} V^l, \end{aligned}$$

where we have used the standard formula to sum up ${}_2F_1$ functions with unit argument (see [41]).

For $n \geq 0$, $(2l+n)! = n!2^{2l}(\frac{n+1}{2})_l(\frac{n+2}{2})_l$ and from this, it follows that

$$\begin{aligned}
I_{1,2j} =&\sqrt{4j+1}\sum_{l=j}^{\infty}\frac{(-1)^{2j+l}(2l+1)!}{(2l+2+2j)!(2l+1-2j)!}V^l\\
=&\sqrt{4j+1}(-1)^jV^j\sum_{l=0}^{\infty}\frac{(-1)^l(2l+2j+1)!}{(2l+4j+2)!(2l+1)!}V^l\\
=&\sqrt{4j+1}(-1)^jV^j\sum_{l=0}^{\infty}\frac{(2j+1)!(j+1)_l(j+\frac{3}{2})_l}{(4j+2)!(2j+\frac{3}{2})_l(2j+2)_l(\frac{3}{2})_l}\frac{(\frac{-V}{4})^l}{l!}\\
=&(-1)^j\sqrt{4j+1}\frac{(2j+1)!}{(4j+2)!}V^j{}_2F_3\left[\begin{matrix}j+1,j+\frac{3}{2};\\2j+2,\frac{3}{2},2j+\frac{3}{2};\end{matrix}-\frac{V}{4}\right], \qquad j=0,1,\ldots.
\end{aligned} \tag{15}$$

$I_{1,2j+1}$ can be dealt with similarly:

$$I_{1,2j+1} =(-1)^{j+1}\sqrt{4j+3}\frac{(2j+1)!}{(4j+3)!}V^j{}_2F_3\left[\begin{matrix}j+1,j+\frac{3}{2};\\2j+2,\frac{1}{2},2j+\frac{5}{2};\end{matrix}-\frac{V}{4}\right], \qquad j=0,1,\ldots. \tag{16}$$

Likewise, we can obtain $I_{2,j}$:

$$\begin{aligned}
I_{2,2j} =&(-1)^j\sqrt{4j+1}\frac{(2j)!}{(4j+1)!}V^j{}_2F_3\left[\begin{matrix}j+\frac{1}{2},j+1;\\2j+1,\frac{1}{2},2j+\frac{3}{2};\end{matrix}-\frac{V}{4}\right],\\
I_{2,2j+1} =&(-1)^j\sqrt{4j+3}\frac{(2j+2)!}{(4j+4)!}V^{j+1}{}_2F_3\left[\begin{matrix}j+\frac{3}{2},j+2;\\2j+3,\frac{3}{2},2j+\frac{5}{2};\end{matrix}-\frac{V}{4}\right], \qquad j=0,1,\ldots.
\end{aligned} \tag{17}$$

Based on the formula from MathWorld–A Wolfram Web Resource

$${}_2F_3\left[\begin{matrix}a,a+1/2;\\2a,d,2a-d+1;\end{matrix}z\right] = {}_0F_1\left[\begin{matrix}-;\\d;\end{matrix}\frac{z}{4}\right]{}_0F_1\left[\begin{matrix}-;\\2a-d+1;\end{matrix}\frac{z}{4}\right],$$

the above results can be simplified as

$$\begin{aligned}
I_{1,2j} =&(-1)^j\sqrt{4j+1}\frac{(2j+1)!}{(4j+2)!}V^j{}_0F_1\left[\begin{matrix}-;\\\frac{3}{2};\end{matrix}-\frac{V}{16}\right]{}_0F_1\left[\begin{matrix}-;\\2j+\frac{3}{2};\end{matrix}-\frac{V}{16}\right],\\
I_{1,2j+1} =&(-1)^{j+1}\sqrt{4j+3}\frac{(2j+1)!}{(4j+3)!}V^j{}_0F_1\left[\begin{matrix}-;\\\frac{1}{2};\end{matrix}-\frac{V}{16}\right]{}_0F_1\left[\begin{matrix}-;\\2j+\frac{5}{2};\end{matrix}-\frac{V}{16}\right],\\
I_{2,2j} =&(-1)^j\sqrt{4j+1}\frac{(2j)!}{(4j+1)!}V^j{}_0F_1\left[\begin{matrix}-;\\\frac{1}{2};\end{matrix}-\frac{V}{16}\right]{}_0F_1\left[\begin{matrix}-;\\2j+\frac{3}{2};\end{matrix}-\frac{V}{16}\right],\\
I_{2,2j+1} =&(-1)^j\sqrt{4j+3}\frac{(2j+2)!}{(4j+4)!}V^{j+1}{}_0F_1\left[\begin{matrix}-;\\\frac{3}{2};\end{matrix}-\frac{V}{16}\right]{}_0F_1\left[\begin{matrix}-;\\2j+\frac{5}{2};\end{matrix}-\frac{V}{16}\right], \qquad j=0,1,\ldots.
\end{aligned} \tag{18}$$

It should be noted that $\phi_0(V)$ and $\phi_1(V)$ can also be expressed by the generalized hypergeometric function ${}_0F_1$:

$$\phi_0(V) = {}_0F_1\left[\begin{matrix}-;\\\frac{1}{2};\end{matrix}-\frac{V}{4}\right], \quad \phi_1(V) = {}_0F_1\left[\begin{matrix}-;\\\frac{3}{2};\end{matrix}-\frac{V}{4}\right]. \tag{19}$$

A Bessel function of the first kind can be expressed in terms of function ${}_0F_1$ by (see [39])

$$J_n(x) = \frac{(x/2)^n}{n!}{}_0F_1\left[\begin{matrix}-;\\ n+1;\end{matrix} -\frac{x^2}{4}\right].$$

We also note that ${}_0F_1\left[\begin{matrix}-;\\ \frac{n}{2};\end{matrix} -S\right]$ with $n \in \mathbb{N}$ and any symmetric matrix S also is viewed as a Bessel function of matrix argument (see [44]). The importance of this hypergeometric representation is that most modern software, e.g., Maple, Mathematica, and Matlab, is well equipped to calculate generalized hypergeometric functions. There are also much work concerning the evaluation of generalized hypergeometric functions of a matrix argument, see, e.g. [18, 4, 34, 44].

3.2 Discretization

The key question now is how to deal with $\gamma_j(\tilde{q})$. This can be done by introducing a quadrature formula defined at the abscissae $c_1 \le \ldots \le c_k$, where $0 \le c_1$ and $c_k \le 1$, thus obtaining an approximation of the form

$$\gamma_j(\tilde{q}) \approx \sum_{l=1}^{k} b_l \widehat{P}_j(c_l) f(\tilde{q}(c_l h)), \tag{20}$$

where $b_l,\ l = 1, 2, \ldots, k$, are the quadrature weights. Based on (20) and (12), it is natural to consider the following scheme

$$\begin{aligned} v(h) &= \phi_0(V)q_0 + h\phi_1(V)p_0 + h^2 \sum_{j=0}^{r-1} I_{1,j} \sum_{l=1}^{k} b_l \widehat{P}_j(c_l) f(v(c_l h)),\\ u(h) &= -hM\phi_1(V)q_0 + \phi_0(V)p_0 + h \sum_{j=0}^{r-1} I_{2,j} \sum_{l=1}^{k} b_l \widehat{P}_j(c_l) f(v(c_l h)), \end{aligned}$$

which is the exact solution of the oscillatory initial value problem

$$\begin{aligned} v'(\xi h) &= u(\xi h), & v(0) &= q_0,\\ u'(\xi h) &= -Mv(\xi h) + \sum_{j=0}^{r-1} \widehat{P}_j(\xi) \sum_{l=1}^{k} b_l \widehat{P}_j(c_l) f(v(c_l h)), & u(0) &= p_0. \end{aligned} \tag{21}$$

From (21), it follows that $v(c_i h),\ i = 1, 2, \ldots, k$, can be obtained by solving the following discrete problems:

$$v''(c_i h) + Mv(c_i h) = \sum_{j=0}^{r-1} \widehat{P}_j(c_i) \sum_{l=1}^{k} b_l \widehat{P}_j(c_l) f(v(c_l h)), \quad v(0) = q_0,\ v'(0) = p_0. \tag{22}$$

By setting, as usual, $v_i = v(c_i h)$, $i = 1, 2, \ldots, k$, (22) can be solved by the variation-of-constants formula in the form:

$$\begin{aligned} v_i =& \phi_0(c_i^2 V) q_0 + c_i h \phi_1(c_i^2 V) p_0 \\ &+ (c_i h)^2 \sum_{j=0}^{r-1} \int_0^1 \widehat{P}_j(c_i z)(1-z)\phi_1\big((1-z)^2 c_i^2 V\big) dz \sum_{l=1}^{k} b_l \widehat{P}_j(c_l) f(v_l), \\ i =& 1, 2, \ldots, k. \end{aligned}$$

3.3 The TFC methods

We are now in a position to present our TFC methods for the multi-frequency oscillatory second-order ODEs (1) or the multi-frequency oscillatory Hamiltonian system (2).

Definition 31 *A trigonometric Fourier collocation (TFC) method for integrating the multi-frequency oscillatory system* (1) *or* (2) *is defined as*

$$\begin{aligned} v_i &= \phi_0(c_i^2 V) q_0 + c_i h \phi_1(c_i^2 V) p_0 + (c_i h)^2 \sum_{j=0}^{r-1} I_{1,j,c_i} \sum_{l=1}^{k} b_l \widehat{P}_j(c_l) f(v_l), \\ & i = 1, 2, \ldots, k, \\ v(h) &= \phi_0(V) q_0 + h \phi_1(V) p_0 + h^2 \sum_{j=0}^{r-1} I_{1,j} \sum_{l=1}^{k} b_l \widehat{P}_j(c_l) f(v_l), \\ u(h) &= -hM \phi_1(V) q_0 + \phi_0(V) p_0 + h \sum_{j=0}^{r-1} I_{2,j} \sum_{l=1}^{k} b_l \widehat{P}_j(c_l) f(v_l), \end{aligned} \tag{23}$$

where h is the stepsize, $\widehat{P}_j$ are defined by (13) *and c_l, b_l, $l = 1, 2, \ldots, k$ are the node points and the quadrature weights of a quadrature formula, respectively. $I_{1,j}$, $I_{2,j}$ can be computed by* (15)–(17) *and the I_{1,j,c_i} are defined as*

$$\begin{aligned} I_{1,j,c_i} :=& \int_0^1 \widehat{P}_j(c_i z)(1-z)\phi_1\big((1-z)^2 c_i^2 V\big) dz \\ =& \sqrt{2j+1} \sum_{l=0}^{\infty} \frac{(-1)^{j+l}}{(2l+2)!} {}_2F_1\left[\begin{matrix} -j, j+1; \\ 2l+3; \end{matrix} c_i\right] (c_i^2 V)^l \\ =& (-1)^j \frac{\sqrt{2j+1}(1-c_i)}{c_i} \sum_{l=0}^{\infty} P_j^{-2l-2}(1-2c_i)\big(c_i(c_i-1)V\big)^l, \end{aligned}$$

where $P_j^{-2l-2}(1-2c_i)$ are associated Legendre functions (see [46]).

Remark 32 *The TFC method* (23) *approximates the solution $q(t)$, $p(t)$ of the system* (2) *in the time interval $[0, h]$. Obviously, the values $v(h)$, $u(h)$ can be*

considered as the initial condition for a new initial value problem approximating $q(t),\ p(t)$ *in the time interval* $[h, 2h]$. *In general, one can extend the TFC methods in the usual time-stepping manner to the interval* $[(i-1)h, ih]$ *for any* $i \geq 2$ *and finally achieve a TFC method for* $q(t),\ p(t)$ *in an arbitrary interval* $[0, Nh]$.

Remark 33 *It can be observed clearly from* (23) *that our TFC methods do not need the symmetry of* M. *Therefore, the method* (23) *can be applied to the system* (1) *with an arbitrary matrix* M. *Moreover, the method* (23) *integrates exactly the linear system* $q'' + Mq = 0$. *Thus it has an additional advantage of energy preservation and quadratic invariant preservation for linear systems.*

Based on (23), we consider Fourier collocation methods for integrating a special and important class of systems of second-order ODEs (5). When $M \to 0$, $I_{1,j}$ and $I_{2,j}$ in (23) become

$$\tilde{I}_{1,j} := \int_0^1 \widehat{P}_j(z)(1-z)\phi_1\big(0\big)dz = (-1)^j \frac{\sqrt{2j+1}}{2} {}_2F_1\left[\begin{matrix}-j, j+1; \\ 3;\end{matrix} 1\right],$$
$$\tilde{I}_{2,j} := \int_0^1 \widehat{P}_j(z)\phi_0\big(0\big)dz = (-1)^j \sqrt{2j+1}\, {}_2F_1\left[\begin{matrix}-j, j+1; \\ 2;\end{matrix} 1\right].$$

In order to simplify the results of $\sum\limits_{j=0}^{r-1} \tilde{I}_{1,j} \sum\limits_{l=1}^{k} b_l \widehat{P}_j(c_l) f(v_l)$ and $\sum\limits_{j=0}^{r-1} \tilde{I}_{2,j} \sum\limits_{l=1}^{k} b_l \widehat{P}_j(c_l) f(v_l)$ with $r \geq 2$, we compute

$$\tilde{I}_{1,j} = \begin{cases} \dfrac{1}{2},\ j = 0, \\ \dfrac{-1}{2\sqrt{3}},\ j = 1, \\ 0,\ j \geq 2, \end{cases} \qquad \tilde{I}_{2,j} = \begin{cases} 1,\ j = 0, \\ 0,\ j \geq 1. \end{cases}$$

Then we have

$$\sum_{j=0}^{r-1} \tilde{I}_{1,j} \sum_{l=1}^{k} b_l \widehat{P}_j(c_l) f(v_l) = \sum_{l=1}^{k} (1-c_l) b_l f(v_l),$$
$$\sum_{j=0}^{r-1} \tilde{I}_{1,j} \sum_{l=1}^{k} b_l \widehat{P}_j(c_l) f(v_l) = \sum_{l=1}^{k} b_l f(v_l).$$

All this can be summed up in the following definition.

Definition 34 *An RKN-type Fourier collocation method for integrating the system* (5) *is defined as*

$$\begin{aligned} v_i &= q_0 + c_i h p_0 + (c_i h)^2 \sum_{j=0}^{r-1} \tilde{I}_{1,j,c_i} \sum_{l=1}^{k} b_l \widehat{P}_j(c_l) f(v_l), \qquad i = 1, 2, \ldots, k, \\ v(h) &= q_0 + h p_0 + h^2 \sum_{l=1}^{k} (1 - c_l) b_l f(v_l), \\ u(h) &= p_0 + h \sum_{l=1}^{k} b_l f(v_l), \end{aligned} \tag{24}$$

where h is the stepsize, $c_l,\ b_l,\ l = 1, 2, \ldots, k$, are the node points and the quadrature weights of a quadrature formula, respectively, and $\tilde{I}_{1,j,c_i}$ are defined by

$$\tilde{I}_{1,j,c_i} := (-1)^j \frac{\sqrt{2j+1}}{2} {}_2F_1 \left[\begin{matrix} -j, j+1; \\ 3; \end{matrix} c_i \right] = (-1)^j \frac{\sqrt{2j+1}(1-c_i)}{c_i} P_j^{-2}(1 - 2c_i). \tag{25}$$

Remark 35 *It can be observed that the method* (24) *is the subclass of k-stage RKN methods with the following Butcher tableau:*

$$\begin{array}{c|c} c & \bar{A} = (\bar{a}_{ij})_{k\times k} \\ \hline & \bar{b}^T \\ \hline & b^T \end{array} \quad = \quad \begin{array}{c|ccc} c_1 & c_1^2 b_1 \sum\limits_{j=0}^{r-1} \tilde{I}_{1,j,c_1} \widehat{P}_j(c_1) & \ldots & c_1^2 b_k \sum\limits_{j=0}^{r-1} \tilde{I}_{1,j,c_1} \widehat{P}_j(c_k) \\ \vdots & \vdots & \ddots & \vdots \\ c_k & c_k^2 b_1 \sum\limits_{j=0}^{r-1} \tilde{I}_{1,j,c_k} \widehat{P}_j(c_1) & \cdots & c_k^2 b_k \sum\limits_{j=0}^{r-1} \tilde{I}_{1,j,c_k} \widehat{P}_j(c_k) \\ \hline & (1-c_1)b_1 & \cdots & (1-c_k)b_k \\ \hline & b_1 & \cdots & b_k \end{array}$$

From the analysis given in next section, it follows that the method (24) *can attain arbitrary algebraic order and is symplectic when choosing a k-point Gauss–Legendre's quadrature and $r = k$. This feature is significant for solving the traditional second-order ODEs* (5). *The point stated above demonstrates the wider applications of the new TFC methods* (23) *and it makes our methods more efficient and competitive. Problem 4 in Section 5 will demonstrate this point clearly.*

4 Properties of the TFC methods

In this section we first analyse the degree of accuracy of the TFC methods in preserving the solution $p(t),\ q(t)$, the quadratic invariant Q and the Hamiltonian H. Other properties including convergence, phase preservation and stability properties are studied as well.

The following result is needed in our analysis and its proof can be found in [2].

Lemma 41 *Let $g : [0,h] \to \mathbb{R}^d$ have j continuous derivatives in the interval $[0,h]$. Then $\int_0^1 \widehat{P}_j(\tau) g(\tau h) d\tau = \mathcal{O}(h^j)$. As a consequence, $\gamma_j(v) = \mathcal{O}(h^j)$.*

Let the quadrature formula in (23) have order $m-1$, i.e., be exact for polynomials of degree less than or equal to $m-1$ (we note that $m \geq k \geq r$). Then we have

$$\Delta_j(h) := \gamma_j(v) - \sum_{l=1}^{k} b_l \widehat{P}_j(c_l) f(v_l) = \mathcal{O}(h^{m-j}), \qquad j = 0, 1, \ldots, r-1.$$

For the exact solution of (2), let $\mathbf{y}(h) = \left(q^T(h), p^T(h)\right)^T$. Then the oscillatory Hamiltonian system (2) can be rewritten in the form

$$\mathbf{y}'(\xi h) = F(\mathbf{y}(\xi h)) := \begin{pmatrix} p(\xi h) \\ -Mq(\xi h) + \sum_{j=0}^{\infty} \widehat{P}_j(\xi) \gamma_j(q) \end{pmatrix}, \quad \mathbf{y}_0 = \begin{pmatrix} q_0 \\ p_0 \end{pmatrix}. \tag{26}$$

The Hamiltonian is

$$H(\mathbf{y}) = \frac{1}{2} p^T p + \frac{1}{2} q^T M q + U(q). \tag{27}$$

On the other hand, for the TFC method (23), denoting $\omega(h) = \left(v^T(h), u^T(h)\right)^T$, the numerical solution satisfies

$$\omega'(\xi h) = \begin{pmatrix} u(\xi h) \\ -Mv(\xi h) + \sum_{j=0}^{r-1} \widehat{P}_j(\xi) \sum_{l=1}^{k} b_l \widehat{P}_j(c_l) f(v(c_l h)) \end{pmatrix}, \quad \omega_0 = \begin{pmatrix} q_0 \\ p_0 \end{pmatrix}. \tag{28}$$

4.1 The order

To express the dependence of the solutions of $\mathbf{y}'(t) = F(\mathbf{y}(t))$ on the initial values, for any given $\tilde{t} \in [0,h]$, we denote by $\mathbf{y}(\cdot, \tilde{t}, \tilde{\mathbf{y}})$ the solution satisfying the initial condition $\mathbf{y}(\tilde{t}, \tilde{t}, \tilde{\mathbf{y}}) = \tilde{\mathbf{y}}$ and set

$$\Phi(s, \tilde{t}, \tilde{\mathbf{y}}) = \frac{\partial \mathbf{y}(s, \tilde{t}, \tilde{\mathbf{y}})}{\partial \tilde{\mathbf{y}}}. \tag{29}$$

Recalling the elementary theory of ODEs, we have the following standard result (see, e.g. [24])

$$\frac{\partial \mathbf{y}(s, \tilde{t}, \tilde{\mathbf{y}})}{\partial \tilde{t}} = -\Phi(s, \tilde{t}, \tilde{\mathbf{y}}) F(\tilde{\mathbf{y}}). \tag{30}$$

The following theorem states the result on the order of our TFC methods.

Theorem 42 *Let the quadrature formula in* (23) *have order $m-1$. Then for the TFC method* (23)

$$\mathbf{y}(h) - \omega(h) = \mathcal{O}(h^{n+1}) \text{ with } n = \min\{m, 2r\}.$$

The RKN-type Fourier collocation method (24) *is also of order n.*

Proof. It follows from Lemma 41, (29) and (30) that

$$\begin{aligned}
&\mathbf{y}(h)-\omega(h)=\mathbf{y}(h,0,\mathbf{y}_0)-\mathbf{y}\big(h,h,\omega(h)\big)=-\int_0^h \frac{d\mathbf{y}\big(h,\tau,\omega(\tau)\big)}{d\tau}d\tau\\
=&-\int_0^h \Big[\frac{\partial \mathbf{y}\big(h,\tau,\omega(\tau)\big)}{\partial \tilde{t}}+\frac{\partial \mathbf{y}\big(h,\tau,\omega(\tau)\big)}{\partial \tilde{\mathbf{y}}}\omega'(\tau)\Big]d\tau\\
=&h\int_0^1 \Phi\big(h,\xi h,\omega(\xi h)\big)\Big[F\big(\omega(\xi h)\big)-\omega'(\xi h)\Big]d\xi\\
=&h\int_0^1 \Phi\big(h,\xi h,\omega(\xi h)\big)\begin{pmatrix}\mathbf{0}\\ \sum\limits_{j=0}^{r-1}\widehat{P}_j(\xi)\Delta_j(h)+\sum\limits_{j=r}^{\infty}\widehat{P}_j(\xi)\gamma_j(v)\end{pmatrix}d\xi.
\end{aligned}$$

We rewrite $\Phi(h,\xi h,\omega(\xi h))$ as a block matrix,

$$\Phi(h,\xi h,\omega(\xi h))=\begin{pmatrix}\Phi_{11}(\xi h)\ \Phi_{12}(\xi h)\\ \Phi_{21}(\xi h)\ \Phi_{22}(\xi h)\end{pmatrix},$$

where Φ_{ij} $(i,j=1,2)$ are all $d\times d$ matrices. Then we obtain

$$\begin{aligned}
\mathbf{y}(h)-\omega(h)=&h\begin{pmatrix}\int_0^1\Phi_{12}(\xi h)\Big(\sum\limits_{j=0}^{r-1}\widehat{P}_j(\xi)\Delta_j(h)+\sum\limits_{j=r}^{\infty}\widehat{P}_j(\xi)\gamma_j(v)\Big)d\xi\\ \int_0^1\Phi_{22}(\xi h)\Big(\sum\limits_{j=0}^{r-1}\widehat{P}_j(\xi)\Delta_j(h)+\sum\limits_{j=r}^{\infty}\widehat{P}_j(\xi)\gamma_j(v)\Big)d\xi\end{pmatrix}\\
=&h\begin{pmatrix}\sum\limits_{j=0}^{r-1}\int_0^1\Phi_{12}(\xi h)\widehat{P}_j(\xi)d\xi\Delta_j(h)+\sum\limits_{j=r}^{\infty}\int_0^1\Phi_{12}(\xi h)\widehat{P}_j(\xi)d\xi\gamma_j(v)\\ \sum\limits_{j=0}^{r-1}\int_0^1\Phi_{22}(\xi h)\widehat{P}_j(\xi)d\xi\Delta_j(h)+\sum\limits_{j=r}^{\infty}\int_0^1\Phi_{22}(\xi h)\widehat{P}_j(\xi)d\xi\gamma_j(v)\end{pmatrix}\\
=&h\Big(\sum_{j=0}^{r-1}\mathcal{O}(h^j\times h^{m-j})+\sum_{j=r}^{\infty}\mathcal{O}(h^j\times h^j)\Big)=\mathcal{O}(h^{m+1})+\mathcal{O}(h^{2r+1}),
\end{aligned}$$

which completes the proof. □

4.2 The order of energy preservation and quadratic invariant preservation

In what follows we are concerned with the order of preserving the Hamiltonian energy by our TFC method.

Theorem 43 *Under the condition in Theorem 42, we have*

$$H(\omega(h))-H(\mathbf{y}_0)=\mathcal{O}(h^{n+1})\ \textit{with}\ n=\min\{m,2r\}.$$

The RKN-type Fourier collocation method (24) *has the same order in preserving the Hamiltonian energy as the TFC methods.*

We then consider the quadratic invariant $Q(\mathbf{y}) = q^T Dp$ of (1). The following result states the degree of accuracy of the TFC method (23) in its preservation.

Theorem 44 *Under the condition in Theorem 42, we have*

$$Q(\omega(h)) - Q(\mathbf{y}_0) = \mathcal{O}(h^{n+1}) \text{ with } n = \min\{m, 2r\}.$$

The proofs of these two theorems are given in Appendix A and Appendix B, respectively. It is well-known that nth order numerical methods can preserve the Hamiltonian energy or the quadratic invariant with at least nth degree of accuracy but unfortunately it follows from the proofs of these two theorems that our methods preserve the Hamiltonian energy and the quadratic invariant only with nth degree of accuracy. However, we prove in the next theorem that when $M \to 0$, the Fourier collocation methods can be symplectic, i.e., they exactly preserve the quadratic invariant.

A better result in preserving the quadratic invariant can be obtained for the RKN-type Fourier collocation method (24) and we state it in the following theorem.

Theorem 45 *Under the condition that $c_l,\ l = 1, 2, \ldots, k$ are chosen as the node points of a k-point Gauss–Legendre's quadrature over the integral $[0, 1]$ and $r = k$, the RKN-type Fourier collocation method* (24) *is symplectic, i.e., it preserves the quadratic invariant of* (5) *exactly.*

Proof. For any $m \in (1, 2, \ldots, k)$, let

$$h(x) := x^2 \sum_{j=0}^{k-1} \widehat{P}_j(c_m)\tilde{I}_{1,j,x} - c_m^2 \sum_{j=0}^{k-1} \tilde{I}_{1,j,c_m} \widehat{P}_j(x) - x + c_m.$$

By the formulas (13), (25) and the fact that c_l are the node points of a Gauss–Legendre's quadrature, it is true that

$$h(x) = (ax + b)\widehat{P}_k(x),$$

where

$$a = \frac{(-1)^k}{\sqrt{2k+1}}\Big[c_m^2 \sum_{j=0}^{k-1}(-1)^j \sqrt{2j+1}\tilde{I}_{1,j,c_m}(j^2 + j - k^2 - k) + k(k+1)c_m - 1\Big],$$

$$b = \frac{(-1)^k}{\sqrt{2k+1}}\Big[c_m - c_m^2 \sum_{j=0}^{k-1}(-1)^j \sqrt{2j+1}\tilde{I}_{1,j,c_m}\Big].$$

From the fact that $\widehat{P}_k(c_n) \equiv 0,\ n = 1, 2, \ldots, k$, it follows that $h(c_n) \equiv 0$ and thus

$$c_m^2 \sum_{j=0}^{k-1} \tilde{I}_{1,j,c_m} \widehat{P}_j(c_n) - c_n^2 \sum_{j=0}^{k-1} \tilde{I}_{1,j,c_n} \widehat{P}_j(c_m) = c_m - c_n.$$

Therefore, we have

$$b_m(\bar{b}_n - \bar{a}_{mn}) - b_n(\bar{b}_m - \bar{a}_{nm}) = b_m\big((1-c_n)b_n - \bar{a}_{mn}\big) - b_n\big((1-c_m)b_m - \bar{a}_{nm}\big)$$
$$= b_m b_n\Big(c_m - c_n - c_m^2 \sum_{j=0}^{k-1} \tilde{I}_{1,j,c_m} \widehat{P}_j(c_n) + c_n^2 \sum_{j=0}^{k-1} \tilde{I}_{1,j,c_n} \widehat{P}_j(c_m)\Big) = b_m b_n 0 = 0.$$

The symplecticity conditions of RKN methods (see [23, 21]) ensure the conclusion immediately. □

Remark 46 *This result means that choosing a suitable k-point Gauss–Legendre's quadrature formula as well as $r = k$ in* (24) *yields a symplectic method of arbitrary order. This manipulation is very simple and convenient and it opens up the possibility of using high-order symplectic methods to solve the second-order ODEs* (5).

4.3 Convergence analysis of the iteration

It can be observed that usually the TFC method (23) constitutes of a system of implicit equations for the determination of v_i and it requires iterative computation. In this paper, we use the fixed-point iteration in practical computation. The maximum norm for a matrix or a vector is denoted by $\|\cdot\|$. Insofar as the convergence of the fixed-point iteration for the TFC method (23) is concerned, we have the following result.

Theorem 47 *Assume that M is symmetric and positive semi-definite and that f satisfies a Lipschitz condition in the variable q, i.e., there exists a constant L with the property that $\|f(q_1) - f(q_2)\| \le L\|q_1 - q_2\|$. If*

$$0 < h < \frac{1}{\sqrt{Lr^2 \max\limits_{i=1,\cdots,k} c_i^2 \max\limits_{j=1,\cdots,k} |b_j|}}, \tag{31}$$

then the fixed-point iteration for the TFC method (23) *is convergent. For a quadrature formula, generally speaking, not all of the node points c_i $(i = 1, 2, \ldots, k)$ are equal to zero and this ensures that $\max\limits_{i=1,\cdots,k} c_i^2 \max\limits_{j=1,\cdots,k} |b_j| \neq 0$.*

Proof. Following Definition 31, the first formula of (23) can be rewritten as

$$Q = \phi_0(c^2V)q_0 + c\phi_1(c^2V)hp_0 + h^2A(V)f(Q), \tag{32}$$

where $c = (c_1, c_2, \ldots, c_k)^T$, $Q = (v_1, v_2, \ldots, v_k)^T$, $A(V) = (a_{ij}(V))_{k\times k}$ and $a_{ij}(V)$ are defined as

$$a_{ij}(V) := c_i^2 b_j \sum_{l=0}^{r-1} I_{1,l,c_i} \widehat{P}_l(c_j).$$

From (13), it follows that $|\widehat{P}_j| \leq \sqrt{2j+1}$. We then obtain

$$\begin{aligned}\|a_{ij}(V)\| &\leq c_i^2|b_j| \sum_{l=0}^{r-1} \sqrt{2l+1} \int_0^1 |\widehat{P}_l(c_i z)| \left\|(1-z)\phi_1\big((1-z)^2 c_i^2 V\big)\right\| dz \\ &\leq c_i^2|b_j| \sum_{l=0}^{r-1} (2l+1) \int_0^1 \left\|(1-z)\phi_1\big((1-z)^2 c_i^2 V\big)\right\| dz.\end{aligned}$$

By Proposition 2.1 in [37], we know that $\left\|\phi_1\big((1-z)^2 c_i^2 V\big)\right\| \leq 1$ and then we get

$$\|a_{ij}(V)\| \leq c_i^2|b_j| \sum_{l=0}^{r-1} (2l+1) = r^2 c_i^2 |b_j|,$$

which yields $\|A(V)\| \leq r^2 \max\limits_{i=1,\cdots,k} c_i^2 \max\limits_{j=1,\cdots,k} |b_j|$. Let

$$\varphi(x) = \phi_0(c^2 V) q_0 + c\phi_1(c^2 V) h p_0 + h^2 A(V) f(x).$$

Then

$$\begin{aligned}\|\varphi(x) - \varphi(y)\| &= \left\|h^2 A(V) f(x) - h^2 A(V) f(y)\right\| \leq h^2 L \|A(V)\| \|x-y\| \\ &\leq h^2 L r^2 \max_{i=1,\cdots,k} c_i^2 \max_{j=1,\cdots,k} |b_j| \|x-y\|,\end{aligned}$$

which means that $\varphi(x)$ is a contraction from the assumption (31). The well-known Contraction Mapping Theorem then ensures the convergence of the fixed-point iteration. □

If the matrix M is not symmetric, it can be observed that the restriction on h becomes $0 < h^2 \|A(V)\| < \dfrac{1}{L}$. For the RKN-type Fourier collocation method (24), the restriction on h is $0 < h < \dfrac{1}{\sqrt{L \max\limits_{1\leq i,j\leq k}\{\bar{a}_{ij}\}}}$. If the assumption on f in Theorem 47 is only satisfied in a neighbourhood of the initial value then further restrictions on h are required in order that the argument of f remains in this neighbourhood.

4.4 Stability

In this part we are concerned with the stability.. As stated in [14], the linear stability of RKN methods is generally analysed by the test equation

$$y''(t) = -\lambda^2 y(t) \quad \text{with } \lambda > 0. \tag{33}$$

Applying the RKN-type Fourier collocation method (24) to (33) yields the recursion

$$\begin{pmatrix} v_1 \\ hu_1 \end{pmatrix} = Q(\vartheta) \begin{pmatrix} q_0 \\ hp_0 \end{pmatrix},$$

where

$$Q(\vartheta) = \begin{pmatrix} 1 - \vartheta^2 \bar{b}^T N^{-1} e & 1 - \vartheta^2 \bar{b}^T N^{-1} c \\ -\vartheta^2 b^T N^{-1} e & 1 - \vartheta^2 b^T N^{-1} c \end{pmatrix}$$

with $N = I + \vartheta^2 \bar{A},\ \vartheta = \lambda h,\ e = (1, \ldots, 1)^T$.

For an RKN method, we have the following definitions:

- $I_s = \{\vartheta > 0 |\ \rho(Q) < 1\}$ is called the *interval of stability*.
- $I_p = \{\vartheta > 0 |\ \rho(Q) = 1$ and $\mathrm{tr}(Q)^2 < 4\det(Q)\}$ is called the *interval of periodicity*.

For the TFC method (23), following [49], we use the scalar revised test equation:

$$q''(t) + \omega^2 q(t) = -\epsilon q(t) \text{ with } \omega^2 + \epsilon > 0, \tag{34}$$

where ω represents an estimation of the dominant frequency λ and $\epsilon = \lambda^2 - \omega^2$ is the error of that estimation. Applying (23) to (34) produces

$$\begin{aligned} Q &= \phi_0(c^2 V) q_0 + c\phi_1(c^2 V) h p_0 - z A(V) Q, \qquad z = \epsilon h^2, \qquad V = h^2 \omega^2, \\ v_1 &= \phi_0(V) q_0 + \phi_1(V) h p_0 - z \bar{b}^T(V) Q, \\ h u_1 &= -V \phi_1(V) q_0 + \phi_0(V) h p_0 - z b^T(V) Q, \end{aligned} \tag{35}$$

where $c,\ Q,\ A(V)$ are defined in Subsection 4.3 and

$$\bar{b}(V) = \Big(b_1 \sum_{j=0}^{r-1} I_{1,j} \widehat{P}_j(c_1), \ldots, b_k \sum_{j=0}^{r-1} I_{1,j} \widehat{P}_j(c_k) \Big)^T,$$

$$b(V) = \Big(b_1 \sum_{j=0}^{r-1} I_{2,j} \widehat{P}_j(c_1), \ldots, b_k \sum_{j=0}^{r-1} I_{2,j} \widehat{P}_j(c_k) \Big)^T.$$

From (35), it follows that

$$\begin{pmatrix} v_1 \\ h u_1 \end{pmatrix} = S(V, z) \begin{pmatrix} q_0 \\ h p_0 \end{pmatrix},$$

where the stability matrix $S(V, z)$ is given by

$$S(V,z) = \begin{pmatrix} \phi_0(V) - z\bar{b}^T(V) N^{-1} \phi_0(c^2 V) & \phi_1(V) - z\bar{b}^T(V) N^{-1} (c \cdot \phi_1(c^2 V)) \\ -V\phi_1(V) - z b^T(V) N^{-1} \phi_0(c^2 V) & \phi_0(V) - z b^T(V) N^{-1} (c \cdot \phi_1(c^2 V)) \end{pmatrix}$$

with $N = I + zA(V)$.

Accordingly, we have the following definitions of stability for our method (23).

Definition 48 *$R_s = \{(V, z) |\ V > 0$ and $\rho(S) < 1\}$ is called the stability region of the method* (23)*. $R_p = \{(V, z) |\ V > 0,\ \rho(S) = 1$ and $\mathrm{tr}(S)^2 < 4\det(S)\}$ is called the periodicity region of the method* (23)*.*

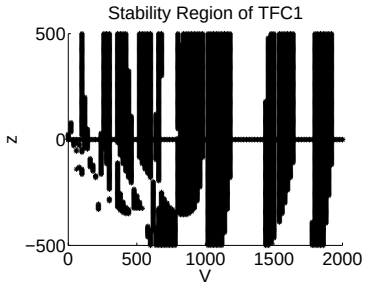


Fig. 1. Stability region of the method TFC1.

Remark 49 *In the previous analysis, we choose the shifted Legendre polynomials as an example of orthonormal basis. It is noted that a different choice of the orthonormal basis can be made and then the above analysis is accordingly modified. We do not discuss this point further in this paper and different choices of the basis will be considered in future investigations.*

Remark 410 *In this paper, we do not discuss the non-autonomous problem* $q''(t) + Mq(t) = f(t, q(t))$ *because by appending the equation* $t'' = 0$*, it can be turned into the autonomous form*

$$u''(t) + \widetilde{M}u(t) = g(u(t)).$$

where $u(t) = \left(t, q^T(t)\right)^T$, $g(u(t)) = \left(t, f^T(t, q(t))\right)^T$ *and* $\widetilde{M} = \begin{pmatrix} 1 & 0_{1\times d} \\ 0_{d\times 1} & M \end{pmatrix}$. *Therefore, our TFC methods and the whole analysis presented in the paper are applicable to the non-autonomous problem* $q''(t) + Mq(t) = f(t, q(t))$.

5 Numerical experiments

As an example of the TFC methods, we choose a Gauss–Legendre's quadrature that is exact for all polynomials of degree ≤ 5 as the quadrature formula in (23), which means that

$$\begin{aligned} c_1 &= \frac{5-\sqrt{15}}{10}, \quad c_2 = \frac{1}{2}, \quad c_3 = \frac{5+\sqrt{15}}{10}, \\ b_1 &= \frac{5}{18}, \qquad b_2 = \frac{4}{9}, \quad b_3 = \frac{5}{18}. \end{aligned} \tag{36}$$

Then we choose $r = 3$ in (23) and denote the corresponding trigonometric Fourier collocation methods as TFC1. According to the analysis given in Section 4, we have the following result for the method TFC1.

Theorem 51 *Let $t_{\text{end}} = Nh$ and apply the method TFC1 with the step size h to* (1) *in the interval $[0, t_{\text{end}}]$. We denote the numerical solution at Nh by $\omega_N(h)$ and then we have*

$$\omega_N(h) - \mathbf{y}(Nh) = \mathcal{O}(h^6),$$
$$Q(\omega_N(h)) - Q(\mathbf{y}_0) = \mathcal{O}(h^6),$$
$$H(\omega_N(h)) - H(\mathbf{y}_0) = \mathcal{O}(h^6).$$

Here all the constants implicit in $\mathcal{O}$ are independent of N and h but depend on t_{end}. When $M \to 0$, the method TFC1 is symplectic and it exactly preserves the quadratic invariant of (5).

For the method TFC1, the stability region is shown in Fig. 1. When $M \to 0$, the interval of periodicity of RNK-type TFC1 is

$$\left(0, \sqrt{54 - 2\sqrt{489}}\right] \bigcup \left[\sqrt{10}, 4\sqrt{15/7}\right] \bigcup \left[2\sqrt{15}, \sqrt{54 + 2\sqrt{489}}\right].$$

In order to show the efficiency and robustness of the method TFC1, the integrators we select for comparison are:

- AAVF–GL: a high precision energy-preserving integrator AAVF–GL using the Gauss–Legendre's rule (36) in [52];
- EPCM1: the "extended Labatto IIIA method of order four" in [30], which is an energy-preserving collocation method (the case $s = 2$ in [19]);
- EPRKM1: the energy-preserving Runge–Kutta method (formula (19) in [2]) using $r = 3$ and the Gauss–Legendre's rule (36);
- SRKM1: the symplectic Runge–Kutta method of order 5 in [48] based on Radau quadrature;
- TFC1: the TFC method derived in this section.

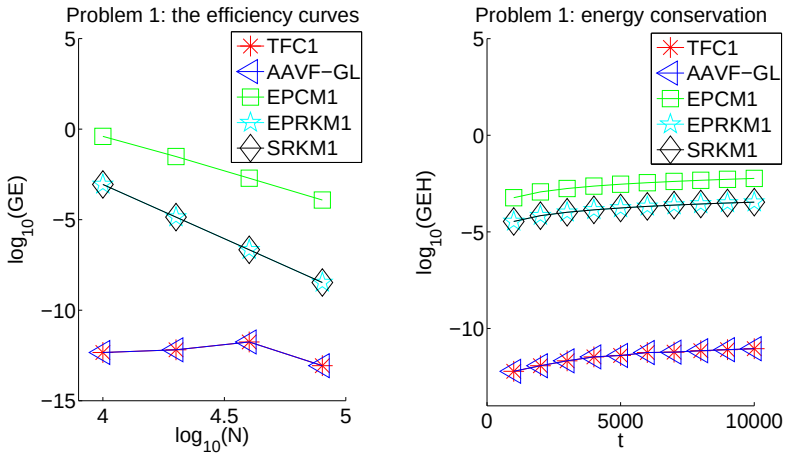
It is noted that these five methods are all implicit and we use a fixed-point iteration in the practical computations. In all the problems, we set 10^{-16} as the error tolerance and 10 as the maximum number of each iteration for showing the efficiency curve as well as energy conservation for a Hamiltonian system. For each problem we also present the requisite total numbers of iterations for each method when choosing different error tolerances in the fixed-point iteration.

Problem 1. Consider the oscillatory nonlinear system

$$q'' + \begin{pmatrix} 13 & -12 \\ -12 & 13 \end{pmatrix} q = -\frac{\partial U}{\partial q}, \qquad q(0) = \begin{pmatrix} -1 \\ 1 \end{pmatrix}, \qquad q'(0) = \begin{pmatrix} -5 \\ 5 \end{pmatrix}$$

with $U(q) = q_1 q_2 (q_1 + q_2)^3$. Its analytic solution is $q = \begin{pmatrix} -\cos(5t) - \sin(5t) \\ \cos(5t) + \sin(5t) \end{pmatrix}$ and the Hamiltonian

$$H(q, q') = \frac{1}{2} q'^T q' + \frac{1}{2} q^T \begin{pmatrix} 13 & -12 \\ -12 & 13 \end{pmatrix} q + U(q).$$



(i) (ii)

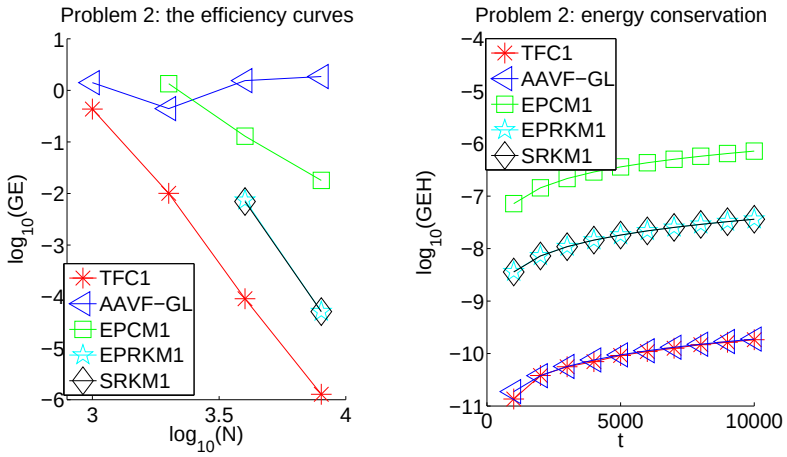
Fig. 2. Results for Problem 1. (i): The logarithm of the global error (GE) over the integration interval against the logarithm of $N = t_{\text{end}}/h$. (ii): The logarithm of the global error of Hamiltonian $GEH = |H_n - H_0|$ against t.

First we solve the problem in the interval $[0, 1000]$ with different stepsizes $h = 0.1/2^i,\ i = 0, 1, 2, 3$. The global errors ($GE = \|q(t_{\text{end}}) - v(t_{\text{end}})\|$) are presented in Fig. 2 (i). Then we integrate this problem with the stepsize $h = 0.1$ in the interval $[0, 10000]$. See Fig. 2 (ii) for the energy conservation of different methods. We also solve the problem in the interval $[0, 10]$ with the stepsize $h = 0.01$ and display the total numbers of iterations in Table 1 for different error tolerances (tol) chosen in the fixed-point iteration.

Methods	$tol = 1.0e-006$	$tol = 1.0e-008$	$tol = 1.0e-010$	$tol = 1.0e-012$
TFC1	1000	1000	1000	1000
AAVF–GL	1000	1000	1000	1000
EPCM1	4000	5000	6000	7545
EPRKM1	3600	4547	5331	6000
SRKM1	3756	4733	5629	6433

Table 1. Results for Problem 1: The total numbers of iterations for different error tolerances (tol).

Problem 2. Fermi–Pasta–Ulam problem is an important model for simulations in statistical mechanics which is considered in [20, 21, 11, 52, 57]. It is a Hamil-



(i) (ii)

Fig. 3. Results for Problem 2. (i): The logarithm of the global error (GE) over the integration interval against the logarithm of $N = t_{\text{end}}/h$. (ii): The logarithm of the global error of Hamiltonian $GEH = |H_n - H_0|$ against t.

tonian system with the Hamiltonian

$$H(x,y) = \frac{1}{2}\sum_{i=1}^{2m} y_i^2 + \frac{\omega^2}{2}\sum_{i=1}^{m} x_{m+i}^2 + \frac{1}{4}\Big[(x_1 - x_{m+1})^4 + \sum_{i=1}^{m-1}(x_{i+1} - x_{m+i-1} - x_i - x_{m+i})^4 + (x_m + x_{2m})^4\Big].$$

This results in

$$x''(t) + Mx(t) = -\nabla U(x), \qquad t \in [0, t_{\text{end}}],$$

where

$$M = \begin{pmatrix} \mathbf{0}_{m\times m} & \mathbf{0}_{m\times m} \\ \mathbf{0}_{m\times m} & \omega^2 I_{m\times m} \end{pmatrix},$$

$$U(x) = \frac{1}{4}\Big[(x_1 - x_{m+1})^4 + \sum_{i=1}^{m-1}(x_{i+1} - x_{m+i-1} - x_i - x_{m+i})^4 + (x_m + x_{2m})^4\Big].$$

We choose

$$m = 3,\ \omega = 50,\ x_1(0) = 1,\ y_1(0) = 1,\ x_4(0) = \frac{1}{\omega},\ y_4(0) = 1,$$

and choose zero for the remaining initial values. The system is integrated in the interval $[0, 100]$ with the stepsizes $h = 0.1/2^k$, $k = 0, 1, 2, 3$. We plot the logarithm of the global errors in Fig. 3 (i). Here it is noted that for EPCM1, EPRKM1 and SRKM1, the global errors are too large for some values of h,

thus we do not plot the corresponding points in Fig. 3 (i). Then we solve this problem in the interval $[0, 10000]$ with the stepsize $h = 0.005$ and present the energy conservation in Fig. 3 (ii). Besides, we solve the problem in the interval $[0, 10]$ with the stepsize $h = 0.01$ to show the convergence rate of iterations for different methods. Table 2 lists the total numbers of iterations for different error tolerances.

Methods	$tol = 1.0e-006$	$tol = 1.0e-008$	$tol = 1.0e-010$	$tol = 1.0e-012$
TFC1	1164	2000	2036	2992
AAVF–GL	1631	2000	2706	3000
EPCM1	9937	11925	14844	16945
EPRKM1	6353	8529	10789	12821
SRKM1	6625	8682	10862	12888

Table 2. Results for Problem 2: The total numbers of iterations for different error tolerances (tol).

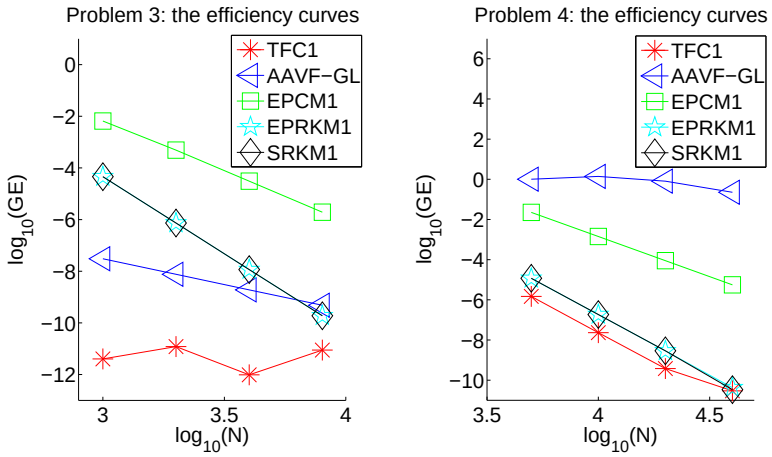
Problem 3. Consider a nonlinear wave equation (see [49])

$$\frac{\partial^2 u}{\partial^2 t} - gd(x)\frac{\partial^2 u}{\partial^2 x} = \frac{1}{4}\lambda^2(x,u)u, \qquad 0 < x \leq b, \qquad t > 0,$$
$$\frac{\partial u}{\partial x}(t,0) = \frac{\partial u}{\partial x}(t,b) = 0, \quad u(0,x) = \sin\Big(\frac{\pi x}{b}\Big), \quad u_t(0,x) = -\frac{\pi}{b}\sqrt{gd(x)}\cos\Big(\frac{\pi x}{b}\Big),$$

where $d(x)$ is the depth function given by $d(x) = d_0\Big[2+\cos(\frac{2\pi x}{b})\Big]$, g denotes the acceleration of gravity, and $\lambda(x,u)$ is the coefficient of bottom friction defined by $\lambda(x,u) = \dfrac{g|u|}{C^2 d(x)}$ with Chezy coefficient C.

By using second-order symmetric differences, this problem is converted into a system of ODEs in time

$$\frac{d^2 u_i}{dt^2} - gd(x_i)\frac{u_{i+1} - 2u_i + u_{i-1}}{\Delta x^2} = \frac{1}{4}\lambda^2(x_i,u_i)u_i, \quad 0 < t \leq t_{end},$$
$$u_i(0) = \sin\Big(\frac{\pi x_i}{b}\Big), \quad u_i'(0) = -\frac{\pi}{b}\sqrt{gd(x_i)}\cos\Big(\frac{\pi x_i}{b}\Big), \quad i = 1, 2\ldots., N,$$



(i) (ii)

Fig. 4. Results for Problem 3 (i) and Problem 4 (ii). The logarithm of the global error (GE) over the integration interval against the logarithm of $N = t_{\text{end}}/h$.

where $\Delta x = \frac{1}{N}$ is the spatial mesh step and $x_i = i\Delta x$. This semi-discrete oscillatory system has the form

$$\frac{d^2U}{dt^2} + MU = F(t,U), \quad 0 < t \leq t_{end}.$$

$$U(0) = \left(\sin\left(\frac{\pi x_1}{b}\right), \ldots, \sin\left(\frac{\pi x_N}{b}\right)\right)^T, \tag{37}$$

$$U'(0) = \left(-\frac{\pi}{b}\sqrt{gd(x_1)}\cos\left(\frac{\pi x_1}{b}\right), \ldots, -\frac{\pi}{b}\sqrt{gd(x_N)}\cos\left(\frac{\pi x_N}{b}\right)\right)^T,$$

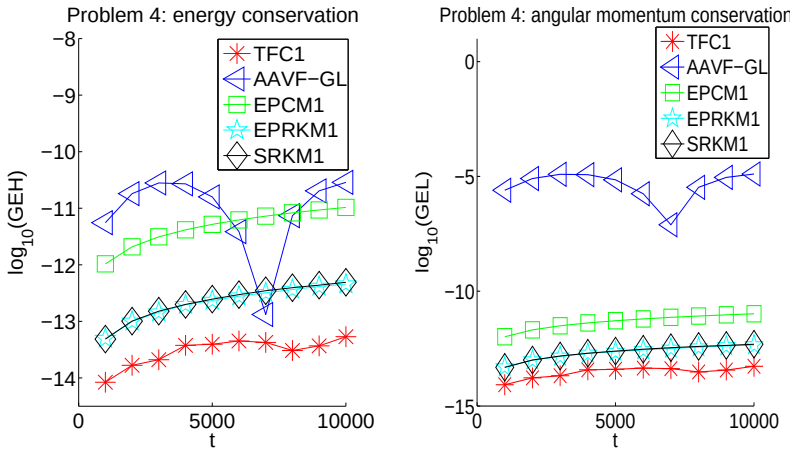
where $U(t)$ denotes the N-dimensional vector with entries $u_i(t) \approx u(x_i,t)$,

$$M = \frac{g}{\Delta x^2}\begin{pmatrix} -2d(x_1) & d(x_2) & & & \\ d(x_2) & -2d(x_2) & d(x_2) & & \\ & \ddots & \ddots & \ddots & \\ & & d(x_{N-1}) & -2d(x_{N-1}) & d(x_{N-1}) \\ & & & d(x_N) & -2d(x_N) \end{pmatrix},$$

and

$$F(t,U) = \left(\frac{1}{4}\lambda^2(x_1,u_1)u_1, \ldots, \frac{1}{4}\lambda^2(x_N,u_N)u_N\right)^T.$$

For the parameters in this problem we choose $b = 100, g = 9.81, d_0 = 10, C = 50$. The system is integrated in the interval $[0, 100]$ with $N = 32$ and the integration stepsizes $h = 0.1/2^j$ for $j = 0, 1, 2, 3$. The global errors are shown in Fig. 4



(i) (ii)

Fig. 5. Results for Problem 4. (i): The logarithm of the global error of Hamiltonian $GEH = |H_n - H_0|$ against t. (ii): The logarithm of the global error of angular momentum $GEL = |L_n - L_0|$ against t.

(i). Table 3 gives the total numbers of iterations when applying the different methods to this problem in the interval $[0, 10]$ with the stepsize $h = 0.01$ and different error tolerances in the fix-point iteration. Since the matrix M in this problem is not symmetric, (37) is not equivalent to a Hamiltonian system and thus there is no Hamiltonian energy to conserve. However, this problem can still be used to compare the accuracy of the numerical solution produced by each method. It also provides an example for supporting the assertion that our TFC methods are still applicable to (1) with a nonsymmetric matrix M. This is the reason why we apply these numerical methods to this non-Hamiltonian problem.

Methods	$tol = 1.0e-006$	$tol = 1.0e-008$	$tol = 1.0e-010$	$tol = 1.0e-012$
TFC1	1000	1000	1000	1000
AAVF–GL	1000	1000	1000	1000
EPCM1	4000	5000	6163	8000
EPRKM1	3000	4000	5000	6217
SRKM1	3000	4000	5455	6940

Table 3. Results for Problem 3: The total numbers of iterations for different error tolerances (tol).

Now we use the next problem to show that our TFC methods exhibit good performance for a special and important class of second-order ODEs $q'' = f(q)$ ($M = 0$ in (1)).

Problem 4. A perturbed Kepler's problem is given by

$$q_1'' = -\frac{q_1}{(q_1^2+q_2^2)^{3/2}} - \frac{(2\epsilon+\epsilon^2)q_1}{(q_1^2+q_2^2)^{5/2}}, \quad q_1(0)=1, \quad q_1'(0)=0,$$
$$q_2'' = -\frac{q_2}{(q_1^2+q_2^2)^{3/2}} - \frac{(2\epsilon+\epsilon^2)q_2}{(q_1^2+q_2^2)^{5/2}}, \quad q_2(0)=0, \quad q_2'(0)=1+\epsilon.$$

The exact solution is $q_1(t)=\cos(t+\epsilon t),\ q_2(t)=\sin(t+\epsilon t)$. The Hamiltonian is

$$H = \frac{1}{2}(q_1'^2+q_2'^2) - \frac{1}{\sqrt{q_1^2+q_2^2}} - \frac{(2\epsilon+\epsilon^2)}{3(q_1^2+q_2^2)^{3/2}}.$$

The system also has the angular momentum $L = q_1q_2' - q_2q_1'$ as a first integral. We take the parameter value $\epsilon = 10^{-3}$.

First we solve the problem in the interval $[0, 1000]$ with different stepsizes $h = 0.1/2^{i-1},\ i = 0, 1, 2, 3$ and present the global errors in Fig. 4 (ii). Then we integrate this problem with the stepsize $h = 0.1$ in the interval $[0, 10000]$ and devote Fig. 5 for the energy conservation and angular momentum conservation. This problem is also solved in the interval $[0, 10]$ with the stepsize $h = 0.01$ and Table 4 lists the total numbers of iterations for different error tolerances.

Methods	$tol = 1.0e-006$	$tol = 1.0e-008$	$tol = 1.0e-010$	$tol = 1.0e-012$
TFC1	1000	2000	2000	2000
AAVF–GL	1000	2000	2000	3000
EPCM1	2999	3000	4000	5000
EPRKM1	2000	3000	4000	5000
SRKM1	2000	3000	4000	5000

Table 4. Results for Problem 4: The total numbers of iterations for different error tolerances (tol).

By the results of the numerical experiments, it can be observed clearly that our method provides a considerably more accurate numerical solution than other methods and preserves well the Hamiltonian energy. Moreover, our method requires less fixed-point iterations than other methods, which is significant in long-term computations.

6 Conclusions

This paper presents a framework for the derivation and analysis of a novel class of TFC methods (23) for the multi-frequency oscillatory system (1) or (2). These new collocation methods are based on the variation-of-constants formula and a local Fourier expansion of the problem. Based on the TFC methods (23),

a special RKN-type Fourier collocation method (24) is designed for solving a special and important class of second-order ODEs (5). It has been shown that the new TFC methods can have arbitrary order and we can obtain symplectic RKN-type Fourier collocation methods (24) with arbitrary order of accuracy for (5) in a very convenient and simple way. Numerical experiments carried out in this paper demonstrate clearly that the novel TFC methods have excellent numerical behaviour in comparison with some existing methods in the scientific literature.

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Appendix A. Proof of Theorem 43

By virtue of Lemma 41, (27) and (28), one has

$$
\begin{aligned}
&H(\omega(h)) - H(\mathbf{y}_0) = h\int_0^1 \nabla H(\omega(\xi h))^T \omega'(\xi h) d\xi \\
=&h\int_0^1 \Big(\big(Mv(\xi h) - \sum_{j=0}^{\infty} \widehat{P}_j(\xi)\gamma_j(v)\big)^T,\ u(\xi h)^T\Big) \\
&\cdot \begin{pmatrix} u(\xi h) \\ -Mv(\xi h) + \sum\limits_{j=0}^{r-1} \widehat{P}_j(\xi) \sum\limits_{l=1}^{k} b_l \widehat{P}_j(c_l) f(v(c_l h)) \end{pmatrix} d\xi \\
=&h\int_0^1 u(\xi h)^T \Big(\sum_{j=0}^{r-1} \widehat{P}_j(\xi) \sum_{l=1}^{k} b_l \widehat{P}_j(c_l) f(v(c_l h)) - \sum_{j=0}^{\infty} \widehat{P}_j(\xi)\gamma_j(v)\Big) d\xi \\
=&h\int_0^1 u(\xi h)^T \Big(- \sum_{j=0}^{r-1} \widehat{P}_j(\xi) \Delta_j(h) - \sum_{j=r}^{\infty} \widehat{P}_j(\xi)\gamma_j(v)\Big) d\xi \\
=&-h\sum_{j=0}^{r-1} \int_0^1 u(\xi h)^T \widehat{P}_j(\xi) d\xi \Delta_j(h) - h\sum_{j=r}^{\infty} \int_0^1 u(\xi h)^T \widehat{P}_j(\xi) d\xi \gamma_j(v) \\
=&h\sum_{j=0}^{r-1} \mathcal{O}(h^j \times h^{m-j}) + h\sum_{j=r}^{\infty} \mathcal{O}(h^j \times h^j) = \mathcal{O}(h^{m+1}) + \mathcal{O}(h^{2r+1}).
\end{aligned}
$$

□

Appendix B. Proof of Theorem 44

From $Q(\mathbf{y}) = q^T Dp$ and $D^T = -D$, it follows that

$$
\begin{aligned}
&Q(\omega(h)) - Q(\mathbf{y}_0) = h\int_0^1 \nabla Q(\omega(\xi h))^T \omega'(\xi h) d\xi \\
=&h\int_0^1 \Big(-u(\xi h)^T D,\ v(\xi h)^T D\Big) \begin{pmatrix} u(\xi h) \\ -Mv(\xi h) + \sum\limits_{j=0}^{r-1} \widehat{P}_j(\xi) \sum\limits_{l=1}^{k} b_l \widehat{P}_j(c_l) f(v(c_l h)) \end{pmatrix} d\xi.
\end{aligned}
$$

Since $q^T D(f(q) - Mq) = 0$ for any $q \in \mathbb{R}^d$, we obtain

$$
\begin{aligned}
&Q(\omega(h)) - Q(\mathbf{y}_0) = h\int_0^1 v(\xi h)^T D\Big(-Mv(\xi h) + \sum_{j=0}^{r-1} \widehat{P}_j(\xi) \sum_{l=1}^{k} b_l \widehat{P}_j(c_l) f(v(c_l h))\Big) d\xi \\
=&h\int_0^1 v(\xi h)^T D\Big(\sum_{j=0}^{r-1} \widehat{P}_j(\xi) \sum_{l=1}^{k} b_l \widehat{P}_j(c_l) f(v(c_l h)) - \sum_{j=0}^{\infty} \widehat{P}_j(\xi)\gamma_j(v)\Big) d\xi \\
=&h\int_0^1 v(\xi h)^T D\Big(-\sum_{j=0}^{r-1} \widehat{P}_j(\xi)\Delta_j(h) - \sum_{j=r}^{\infty} \widehat{P}_j(\xi)\gamma_j(v)\Big) d\xi \\
=&-h\sum_{j=0}^{r-1} \int_0^1 v(\xi h)^T D\widehat{P}_j(\xi) d\xi \Delta_j(h) - h\sum_{j=r}^{\infty} \int_0^1 v(\xi h)^T D\widehat{P}_j(\xi) d\xi \gamma_j(v) \\
=&h\sum_{j=0}^{r-1} \mathcal{O}(h^j \times h^{m-j}) + h\sum_{j=r}^{\infty} \mathcal{O}(h^j \times h^j) = \mathcal{O}(h^{m+1}) + \mathcal{O}(h^{2r+1}).
\end{aligned}
$$

□

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