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# High order closed Newton–Cotes trigonometrically-fitted formulae for the numerical solution of the Schrödinger equation

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ABSTRACT

In this paper, we investigate the connection between

- closed Newton–Cotes formulae,
- trigonometrically-fitted methods,
- symplectic integrators and
- efficient integration of the Schrödinger equation.
The study of multistep symplectic integrators is very poor although in the last decades several one step symplectic integrators have been produced based on symplectic geometry (see the relevant literature and the references here). In this paper we study the closed Newton–Cotes formulae and we write them as symplectic multilayer structures. Based on the closed Newton–Cotes formulae, we also develop trigonometrically-fitted symplectic methods. An error analysis for the one-dimensional Schrödinger equation of the new developed methods and a comparison with previous developed methods is also given. We apply the new symplectic schemes to the well-known radial Schrödinger equation in order to investigate the efficiency of the proposed method to these type of problems.



## 1. Introduction

It is of great interest the research area of development of numerical integration methods for ordinary differential equations that preserve qualitative properties of the analytic solution. In this paper, we consider Hamilton's equations of motion which are linear in position $p$ and momentum $q$

$$\begin{aligned} \dot{q} &= mp, \\ \dot{p} &= -mq, \end{aligned} \tag{1}$$

where $m$ is a constant scalar or matrix. The Eq. (1) is an important one in the field of molecular dynamics.

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In order to preserve the characteristics of the Hamiltonian system in the numerical approximation, it is necessary to use symplectic integrators.

In the recent years work has been done mainly in the production of one step symplectic integrators (see [3]). Zhu et al. [1] have studied the symplectic integrators and the well-known open Newton–Cotes differential methods. They have presented the open Newton–Cotes differential methods as multilayer symplectic integrators.

The construction of multistep symplectic integrators based on the open Newton–Cotes integration methods was investigated by Chiou and Wu [2].

The last decades much work has been done on exponential – trigonometrically fitting and the numerical solution of periodic initial value problems (see [4–112] and references therein).

In this paper:

- We try to present closed Newton–Cotes differential methods as multilayer symplectic integrators.
- We apply the closed Newton–Cotes methods on the Hamiltonian system (1) and we obtain the result that the Hamiltonian energy of the system remains almost constant as the integration proceeds.
- The trigonometrically-fitted methods are developed.
- An error analysis for the one-dimensional Schrödinger equation of the new developed methods and a comparison with previous developed methods is also given.

We note that the aim of this paper is to generate methods that can be used for non-linear differential equations as well as linear ones.

In Section 2 the results about symplectic matrices and schemes are presented. In Section 3 closed Newton–Cotes integral rules and differential methods are described and the new trigonometrically-fitted methods are developed. In Section 4 the conversion of the closed Newton–Cotes differential methods into multilayer symplectic structures is presented. The error analysis for the one-dimensional Schrödinger equation of the new developed methods and a comparison with previous developed methods is presented in Section 5. Finally, numerical results are presented in Section 6.

## 2. Basic theory on symplectic schemes and numerical methods

Zhu et al. [1] have obtained a theory on symplectic numerical schemes and symplectic matrices in which the following basic theory is based.

Dividing an interval $[a, b]$ with $N$ points we have

$$x_0 = a, \quad x_n = x_0 + nh = b, \quad n = 1, 2, \dots, N. \tag{2}$$

We note that $x$ is the independent variable and $a$ and $b$ in the equation for $x_0$ (Eq. (2)) are different than the $a$ and $b$ in Eq. (3). The above division leads to the following discrete scheme:

$$\begin{pmatrix} p_{n+1} \\ q_{n+1} \end{pmatrix} = M_{n+1} \begin{pmatrix} p_n \\ q_n \end{pmatrix}, \quad M_{n+1} = \begin{pmatrix} a_{n+1} & b_{n+1} \\ c_{n+1} & d_{n+1} \end{pmatrix}. \tag{3}$$

Based on the above we can write the $n$-step approximation to the solution as

$$\begin{pmatrix} p_n \\ q_n \end{pmatrix} = \begin{pmatrix} a_n & b_n \\ c_n & d_n \end{pmatrix} \begin{pmatrix} a_{n-1} & b_{n-1} \\ c_{n-1} & d_{n-1} \end{pmatrix} \cdots \begin{pmatrix} a_1 & b_1 \\ c_1 & d_1 \end{pmatrix} \begin{pmatrix} p_0 \\ q_0 \end{pmatrix} = M_n, M_{n-1}, \dots, M_1 \begin{pmatrix} p_0 \\ q_0 \end{pmatrix}.$$

Defining

$$S = M_n, M_{n-1}, \dots, M_1 = \begin{pmatrix} A_n & B_n \\ C_n & D_n \end{pmatrix}$$

the discrete transformation can be written as

$$\begin{pmatrix} p_n \\ q_n \end{pmatrix} = S \begin{pmatrix} p_0 \\ q_0 \end{pmatrix}.$$

A discrete scheme (3) is a symplectic scheme if the transformation matrix $S$ is symplectic.

A matrix $A$ is symplectic if $A^{\mathrm{T}} J A = J$ where

$$J = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}.$$

The product of symplectic matrices is also symplectic. Hence, if each matrix $M_n$ is symplectic the transformation matrix $S$ is symplectic. Consequently, the discrete scheme (2) is symplectic if each matrix $M_n$ is symplectic.