INTERNATIONAL JOURNAL OF
NUMERICAL ANALYSIS AND MODELING
Volume 15, Number 3, Pages 405–427

SYMMETRIC HIGH ORDER GAUTSCHI-TYPE EXPONENTIAL WAVE INTEGRATORS PSEUDOSPECTRAL METHOD FOR THE NONLINEAR KLEIN-GORDON EQUATION IN THE NONRELATIVISTIC LIMIT REGIME

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Abstract. A group of high order Gautschi-type exponential wave integrators (EWIs) Fourier pseudospectral method are proposed and analyzed for solving the nonlinear Klein-Gordon equation (KGE) in the nonrelativistic limit regime, where a parameter $0 < \varepsilon \ll 1$ which is inversely proportional to the speed of light, makes the solution propagate waves with wavelength $O(\varepsilon^2)$ in time and $O(1)$ in space. With the Fourier pseudospectral method to discretize the KGE in space, we propose a group of EWIs with designed Gautschi's type quadratures for the temporal integrations, which can offer any intended even order of accuracy provided that the solution is smooth enough, while all the current existing EWIs offer at most second order accuracy. The scheme is explicit, time symmetric and rigorous error estimates show the meshing strategy of the proposed method is time step $\tau = O(\varepsilon^2)$ and mesh size $h = O(1)$ as $0 < \varepsilon \ll 1$, which is 'optimal' among all classical numerical methods towards solving the KGE directly in the limit regime, and which also distinguish our methods from other high order approaches such as Runge-Kutta methods which require $\tau = O(\varepsilon^3)$. Numerical experiments with comparisons are done to confirm the error bound and show the superiority of the proposed methods over existing classical numerical methods.

Key words. Nonlinear Klein-Gordon equation, nonrelativistic limit, exponential wave integrator, high order accuracy, time symmetry, error estimate, meshing strategy, spectral method.

1. Introduction

The Klein-Gordon equation (KGE) is known as the relativistic version of the Schrödinger equation for describing the dynamics of spinless particles [35]. Under proper nondimensionalization, the dimensionless nonlinear KGE in d dimensions ($d = 1, 2, 3$) reads [3, 30, 31, 29, 16, 19, 20, 33]:

$$
\begin{cases}
\varepsilon^2 \partial_{tt} u - \Delta u + \dfrac{1}{\varepsilon^2} u + f(u) = 0, \quad \mathbf{x} \in \mathbb{R}^d, \quad t > 0, \\
u(\mathbf{x}, 0) = \phi_1(\mathbf{x}), \quad \partial_t u(\mathbf{x}, 0) = \dfrac{1}{\varepsilon^2} \phi_2(\mathbf{x}), \quad \mathbf{x} \in \mathbb{R}^d.
\end{cases} \tag{1}
$$

Here t is time, $\mathbf{x}$ is the spatial coordinate, $u := u(\mathbf{x}, t)$ is a real-valued scalar field, $0 < \varepsilon \leq 1$ is a dimensionless parameter which is inversely proportional to the speed of light, ϕ_1 and ϕ_2 are two given real-valued initial data which are independent of ε, and $f(u) : \mathbb{R} \to \mathbb{R}$ is a given nonlinearity independent of ε. It is clear that the

Received by the editors December 29, 2014 and, in revised form, June 19, 2017.
2000 *Mathematics Subject Classification.* 65M12, 65M15, 65M70.

KGE (1) is time symmetric and conserves the *energy* [3, 19, 20, 29]

(2)
$$\begin{aligned}E(t) &:= \int_{\mathbb{R}^d}\left[\varepsilon^2|\partial_t u(\mathbf{x},t)|^2 + |\nabla u(\mathbf{x},t)|^2 + \frac{1}{\varepsilon^2}|u(\mathbf{x},t)|^2 + F(u(\mathbf{x},t))\right]d\mathbf{x}\\ &\equiv \int_{\mathbb{R}^d}\left[\frac{1}{\varepsilon^2}|\phi_2(\mathbf{x})|^2 + |\nabla\phi_1(\mathbf{x})|^2 + \frac{1}{\varepsilon^2}|\phi_1(\mathbf{x})|^2 + F(\phi_1(\mathbf{x}))\right]d\mathbf{x} = E(0),\ t\geq 0,\end{aligned}$$

with $F(u) = 2\int_0^u f(\rho)d\rho$.

For fixed $0 < \varepsilon \leq 1$, i.e. the relativistic regime, the KGE (1) has been well-studied both theoretically and numerically. We refer the readers to [3] for a detailed review on the well-posedness and existing numerical methods for the KGE in this regime. As $\varepsilon \to 0$, which corresponds to the speed of light goes to infinite and is known as the nonrelativistic limit in physics, recent analytical results [30, 31, 29] show that the problem (1) propagates waves with amplitude at $O(1)$, and wavelength at $O(\varepsilon^2)$ and $O(1)$ in time and space, respectively. The small wavelength makes the solution of the KGE highly oscillatory in time as $0 < \varepsilon \ll 1$. Figure 1 shows an example of the profile of the solution under different ε. The high oscillations cause severe numerical burdens in practical computations of the KGE in the nonrelativistic limit regime. For example, in order to capture the solution correctly in the highly oscillatory regime, frequently used finite difference time domain (FDTD) methods, such as the energy conservative type, semi-implicit type and fully explicit type [13, 33], need the meshing strategy requirement (or ε-scalability) $h = O(1)$ but $\tau = O(\varepsilon^3)$ [3], where h andτ denote the spatial mesh size and the time step, respectively. To release the temporal meshing strategy, based on the classical exponential wave integrators (EWIs) established in [23, 26, 27, 32, 17] for solving the oscillatory ODEs arising mainly from molecular dynamics, an EWI with the Gautschi-type quadrature [17] spectral method was proposed for solving the nonlinear KGE in the nonrelativistic limit regime and was shown to improve the ε-scalability to $\tau = O(\varepsilon^2)$ in [3]. This method also finds successful applications in solving the Klein-Gordon-Zakharov (KGZ) system in a similar oscillatory situation [5]. Later on, an EWI with the Deuflhard-type quadrature [14] spectral method, which is equivalent to the time-splitting spectral method, was considered in [12] for the KGE in the nonrelativistic limit regime. It can offer a smaller temporal error bounded but the same ε-scalability. Recent studies turn to utilize multiscale analysis to first derive some sophisticate reformulations or decompositions of the KGE, then based on which one can propose some suitable numerical methods [16, 10, 6, 4] for asymptotic preserving or uniformly accurate property. These multiscale numerical methods are extremely powerful in computations of KGE in the oscillatory regime, however they either require some delicate pre-knowledge of the oscillation structures of the problem [6, 16, 4] or require introducing an extra degree-of-freedom [10]. Very recently, an iterative exponential integrator with optimally uniform accuracy has been proposed in [9]. In view of that the solution to (1) has oscillation wavelength at $O(\varepsilon^2)$ in time, the EWIs could be viewed as the optimal one among all the traditional methods towards integrating the KGE (1) directly in the nonrelativistic limit regime.

However, all the existing EWIs for either solving the oscillatory ODEs from molecular dynamics or solving the KGE offer at most second order accuracy in temporal discretization. Of course, one can apply the Runge-Kutta methods, like the one proposed in [15] for the approximations in time to get higher order temporal