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UNIFORMLY ACCURATE NESTED PICARD ITERATIVE INTEGRATORS FOR THE DIRAC EQUATION IN THE NONRELATIVISTIC LIMIT REGIME*

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Abstract. This paper is devoted to the construction and analysis of uniformly accurate nested Picard iterative integrators (NPI) for the Dirac equation in the nonrelativistic limit regime. In this regime, there is a dimensionless parameter $\varepsilon \in (0, 1]$ inversely proportional to the speed of light and the equation admits propagating waves with $O(1)$ wavelength in space and $O(\varepsilon^2)$ wavelength in time. To overcome the difficulty induced by the temporal ε dependent oscillation, we present the construction of several NPI methods which are uniformly first-, second-, and third-order convergent in time w.r.t. ε. The general idea is applying nested Picard iterations to the integral form of the Dirac equation and using exponential wave integrators to approximate the temporal integrals. Thanks to the nested Picard iterative idea, the NPI method can be extended to arbitrary higher-order in time with optimal and uniform accuracy. The implementation of the second-order in-time NPI method via Fourier pseudospectral discretization is clearly demonstrated, and the corresponding error bounds are rigorously established through the energy method as $h^{m_0} + \tau^2$, where h is the mesh size, τ is the time step, and m_0 depends on the regularity of the solution. Numerical results are reported to confirm the error estimates for the second-order NPI method and show the uniform accurate properties (w.r.t. ε) for the first- and third-order NPI methods as well.

Key words. Dirac equation, nonrelativistic limit regime, error bound, uniformly accurate, high-order accuracy, exponential wave integrator, spectral method

AMS subject classifications. 35Q41, 65M70, 65N35, 81Q05

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1. Introduction.

The dimensionless two-component Dirac equation [4, 12, 13, 14, 18, 19, 29, 32, 34] with external electromagnetic potential in d dimensions ($d = 1, 2$) reads

$$\begin{cases} i\partial_t \Phi(t,\mathbf{x}) = \left[-\frac{i}{\varepsilon} \sum_{j=1}^{d} \sigma_j \partial_j + \frac{1}{\varepsilon^2}\sigma_3 + V(t,\mathbf{x}) I_2 - \sum_{j=1}^{d} A_j(t,\mathbf{x})\sigma_j \right] \Phi(t,\mathbf{x}), \\ \Phi(t=0,\mathbf{x}) = \Phi_0(\mathbf{x}), \quad \mathbf{x} \in \mathbb{R}^d, \end{cases} \tag{1.1}$$

where $i = \sqrt{-1}$, $\varepsilon \in (0, 1]$ is a dimensionless parameter inversely proportional to the speed of light, t is time, $\mathbf{x} = (x_1, \ldots, x_d)^T \in \mathbb{R}^d$ is the spatial coordinate vector, $\partial_k = \frac{\partial}{\partial x_k}$ $(k = 1, \ldots, d)$, and $\Phi := \Phi(t,\mathbf{x}) = (\phi_1(t,\mathbf{x}), \phi_2(t,\mathbf{x}))^T \in \mathbb{C}^2$ is the complex-valued vector wave function of the "spinorfield." I_2 is the 2×2 identity matrix, $V := V(t,\mathbf{x})$ and $\mathbf{A} := \mathbf{A}(t,\mathbf{x}) = (A_1(t,\mathbf{x}), \ldots, A_d(t,\mathbf{x}))^T$ are the real-valued electrical potential and magnetic potential vector, respectively. σ_1, σ_2, σ_3 are the Pauli matrices given by

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$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \qquad \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \qquad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \tag{1.2}$$

The Dirac equation is one of the great triumphs of theoretical physics, and a significant literature on this topic dates back to 1928 [18, 19, 20, 21, 27, 31, 34, 36, 37, 38]. There exist two important regimes for the Dirac equation, i.e., the relativistic case with $\varepsilon = O(1)$ and the nonrelativistic regime with $\varepsilon \ll 1$ (speed of light tends to infinity). Extra difficulties arise in both theoretical analysis and numerical computation in the nonrelativistic limit regime $\varepsilon \ll 1$, due to the fact that the solution to the Dirac equation is highly oscillatory in time with $O(\varepsilon^2)$ wavelength [12, 17, 29, 31, 32, 34]. Numerically, in order to resolve such high frequency in time, the meshing strategy (at least the time step) should depend on ε for traditional finite difference and time splitting methods [4] and this brings a severe numerical burden. In this paper, we intend to develop uniformly accurate numerical methods, i.e., methods that can resolve the solution for all $\varepsilon \in (0, 1]$ without any time step/mesh size restrictions.

Following the ideas for designing uniformly accurate methods for second-order ordinary differential equations [8] and the nonlinear Klein–Gordon equation [6], a uniformly accurate multiscale time integrator Fourier pseudospectral method has been proposed and analyzed in [5] for the Dirac equation in the nonrelativistic limit regime based on a multiscale decomposition of the exact solution. In the multiscale decomposition, the solution is filtered to dominant terms without oscillations and highly oscillatory terms with small amplitudes ($O(\varepsilon^2)$). A similar idea has also been used in [15] for the nonlinear Dirac equations. These multiscale time integrators are based on the preunderstanding of the solution, and they are second-order convergent in time for fixed ε, while these methods can only achieve uniform linear convergence in time w.r.t. $\varepsilon \in (0, 1]$. In addition, the two-scale formulation and exponential-type integrators with "twisted variables" are also possible approaches for designing uniformly accurate methods and we refer to [10, 16, 30] and references therein for more details. To the best of our knowledge, no uniformly accurate methods for the Dirac equation (1.1) (or (1.4)) with cubic (or even higher) convergence rate in time are available in the literature.

The main objective of this work is to propose and analyze uniformly accurate nested Picard iterative integrators (NPI) for solving the Dirac equation (1.1) in the nonrelativistic limit regime. In the NPI method, no multiscale expansion of the solution is needed and no reformulation of the Dirac equation is used, in contrast to the two-scale and "twisted variables" forms [10, 11, 30, 33]. Instead, we write the Dirac equation into the equivalent integral form by Duhamel's principle. Applying a nested Picard iterative idea to the integral equation and using exponential wave integrators (EWIs) [3, 7, 8, 23, 25, 26] for the time integral, we obtain schemes of uniform accuracies with arbitrary orders in time w.r.t. $\varepsilon \in (0, 1]$. We note that the integral form as the starting point of our construction can be replaced by the "twisted variable" formulation [10, 11]. To illustrate the idea clearly, we introduce the "free Dirac operator" $\mathcal{T}$ and the "electromagnetic potential operator" $W(t, \mathbf{x})$ [12, 32]

$$\mathcal{T} = -i\varepsilon \sum_{j=1}^{d} \sigma_j \partial_j + \sigma_3, \quad W(t, \mathbf{x}) = V(t, \mathbf{x}) I_2 - \sum_{j=1}^{d} A_j(t, \mathbf{x}) \sigma_j, \qquad \mathbf{x} \in \mathbb{R}^d, \tag{1.3}$$

and write the Dirac equation (1.1) as

$$i\partial_t \Phi(t, \mathbf{x}) = \frac{1}{\varepsilon^2} \mathcal{T} \Phi(t, \mathbf{x}) + W(t, \mathbf{x}) \Phi(t, \mathbf{x}), \qquad \mathbf{x} \in \mathbb{R}^d. \tag{1.4}$$

The operator $\mathcal{T}$ is diagonalizable in the Fourier space and can be decomposed as

$$\mathcal{T} = \sqrt{I - \varepsilon^2 \Delta}\ \Pi_+ - \sqrt{I - \varepsilon^2 \Delta}\ \Pi_-,$$

where I is the identity operator, Δ is the Laplace operator, $\sqrt{I - \varepsilon^2 \Delta}$ is understood in the Fourier space with the symbol $\lambda(\xi) = \sqrt{1 + \varepsilon^2 |\xi|^2}$ ($\xi \in \mathbb{R}^d$), and $\Pi_\pm$ are the associated projectors defined as

$$\Pi_+ = \frac{1}{2}\left[I + \left(I - \varepsilon^2 \Delta\right)^{-1/2} \mathcal{T}\right], \quad \Pi_- = \frac{1}{2}\left[I - \left(I - \varepsilon^2 \Delta\right)^{-1/2} \mathcal{T}\right]. \tag{1.5}$$

It can be verified that $\Pi_+ + \Pi_- = I$, $\Pi_+ \Pi_- = \Pi_- \Pi_+ = \mathbf{0}$, $\Pi_\pm^2 = \Pi_\pm$, and

$$\mathcal{T}^k = \left(\sqrt{I - \varepsilon^2 \Delta}\right)^k\ \Pi_+ + \left(-\sqrt{I - \varepsilon^2 \Delta}\right)^k\ \Pi_-, \qquad k \in \mathbb{N}.$$

An essential idea/step during the construction of NPI is the splitting of the evolutionary operator

$$e^{i\mathcal{T}t/\varepsilon^2} = e^{it/\varepsilon^2} e^{i\mathcal{A}^\varepsilon t} \Pi_+ + e^{-it/\varepsilon^2} e^{-i\mathcal{A}^\varepsilon t} \Pi_-, \tag{1.6}$$

where $\mathcal{A}^\varepsilon := \frac{\sqrt{I - \varepsilon^2 \Delta} - I}{\varepsilon^2}$ is a bounded operator from $H^s(\mathbb{R}^d)$ to $H^{s-2}(\mathbb{R}^d)$. From (1.6), it is clear that the operator $e^{i\mathcal{T}t/\varepsilon^2}$ causes the rapid oscillation in time and behaves quite differently in the eigenspaces of $\mathcal{T}$. Employing (1.6), we could easily separate and deal with the oscillation induced by the free Dirac operator in different eigenspaces. Introducing the nested Picard iteration idea, we can construct uniformly accurate schemes of arbitrary high-order accuracy (w.r.t. $\varepsilon \in (0, 1]$) in time. In this paper, we focus on the construction of the first-, second-, and third-order uniform in time NPI methods (semidiscrete in time), associated with numerical validations of the uniform accuracies. For the realization of the NPI methods in the fully discrete form, we only present the details for the second-order scheme and its error analysis.

The rest of this paper is organized as follows. Section 2 is devoted to the construction of the NPI methods (up to the third order) and the practical implementation of the second-order accurate NPI method for the Dirac equation (1.1). Then, in section 3 error estimates are rigorously established for the uniform second-order in time NPI method. Numerical results are reported in section 4 to validate the uniformly accurate properties and the error estimates. Last, we draw some conclusions in section 5. Throughout this paper, we adopt standard notation of Sobolev spaces, and the notation $p \lesssim q$ is used to represent that there exists a generic constant $C > 0$, which is independent of time step τ, mesh size h and ε, such that $|p| \le Cq$.

We remark here that

(i) (1.1) is a reduced form of the classical four-component three-dimensional (3D) Dirac equation, and the two forms are quite similar [1, 4, 5]; thus it suffices to consider the Dirac equation (1.1);

ii) for simplicity of notation, the method and analysis for the Dirac equation (1.1) are presented only in one dimension in this paper, while all the notation and results can be easily generalized to (1.1) in a higher dimension (two dimensions) and the classical 3D Dirac equation without any extra work.

2. The NPI method. In this section, we present the details for the uniform first-, second-, and third-order NPI methods in the semidiscrete (in time) form and discuss the implementation in the fully discrete form using Fourier pseudospectral discretization in space. Here we focus on the 1D case, as the methods and the analysis can be easily generalized to two and three dimensions by tensor grids [5].

2.1. Construction of the method. As a common practice for the numerical purpose, we first truncate the whole space 1D Dirac equation (1.4) ($d = 1$) onto a bounded interval $\Omega = (a, b)$ for $\Phi := \Phi(t, x) \in \mathbb{C}^2$,

$$i\partial_t \Phi(t,x) = \frac{1}{\varepsilon^2}\mathcal{T}\Phi(t,x) + W(t,x)\Phi(t,x), \qquad x \in \Omega, \quad t > 0, \tag{2.1}$$

with periodic boundary conditions and initial condition as

$$\Phi(t,x) \text{ is } (b-a) \text{ periodic in } x, \quad t \geq 0; \qquad \Phi(0,x) = \Phi_0(x), \quad x \in \overline{\Omega}. \tag{2.2}$$

Here, we note that $\mathcal{T}$ and $W(t, x)$ are defined in (1.3) with $d = 1$, while the domain of $\mathcal{T}$ becomes $(H_p^1(\Omega))^2$ with $H_p^1(\Omega) = \{u \in H^1(\Omega) | u(a) = u(b)\}$.

Let us discretize the temporal domain as $0 = t_0 < t_1 < \cdots$ with time step $\tau := \Delta t > 0$ and $t_n = n\tau$ for $n \geq 0$. In each time interval $t \in [t_n, t_{n+1}]$, we can apply Duhamel's principle to (2.1) and write the solution $\Phi(t_n + s) := \Phi(t_n + s, x)$ into an integral form as

$$\Phi(t_n+s) = e^{-i\mathcal{T}s/\varepsilon^2}\Phi(t_n) - i\int_0^s e^{-i\mathcal{T}(s-w)/\varepsilon^2}\left(W^n(w)\Phi(t_n+w)\right)dw, \quad 0 \leq s \leq \tau, \tag{2.3}$$

where $W^n(w) := W^n(w, x) = W(t_n + w, x)$.

Suitable approximation of the integral term will lead to a numerical scheme. To obtain a uniformly accurate scheme, special attention has to be paid in dealing with the integrand, i.e., the $\Phi(t_n + w)$ term. In the traditional EWI method [4], Taylor expansion for $\Phi(t_n + w)$ has been used and the local error involves $\partial_{ww}\Phi(t_n + w) = O(1/\varepsilon^4)$, which results in the error estimates of $O(\tau^2/\varepsilon^4 + h^{m_0})$, due to the highly oscillatory behavior of $\Phi(t_n + w)$ in time. Thus, to gain a uniformly accurate method, direct use of Taylor expansion and temporal derivatives of $\Phi(t_n + w)$ should be avoided in the numerical approximation. Inspired by the works in [10, 33], we find that this could be done by applying a nested Picard iterative idea to (2.3). As a result, we can construct the following uniformly accurate mth order in time ($m \geq 1$) NPI methods for the Dirac equation in the nonrelativistic limit:

Step 1. In each time interval, i.e., from t_n to t_{n+1}, $n \geq 0$, given $\Phi^n := \Phi^n(x)$ which is the numerical approximation of the exact solution $\Phi(t_n, x)$, let

$$\Phi^{n,0}(s) := \Phi^{n,0}(s,x) = e^{-i\mathcal{T}s/\varepsilon^2}\Phi^n, \qquad 0 \leq s \leq \tau. \tag{2.4}$$

Step 2. Calculate $\Phi^{n,k+1}(s) := \Phi^{n,k+1}(s, x)$ by the following nested Picard iteration:

$$\begin{aligned} &\Phi_*^{n,k+1}(s) = e^{-i\mathcal{T}s/\varepsilon^2}\Phi^n - i\int_0^s e^{-i\mathcal{T}(s-w)/\varepsilon^2}\left(W^n(w)\Phi^{n,k}(w)\right)dw, \\ &\Phi^{n,k+1}(s) \approx \Phi_*^{n,k+1}(s), \qquad 0 \leq s \leq \tau, \quad k = 0, \ldots, m-1. \end{aligned} \tag{2.5}$$

Step 3. Update $\Phi^{n+1}(x)$ by $\Phi^{n+1}(x) = \Phi^{n,m}(\tau) = \Phi^{n,m}(\tau, x)$.

For simplicity of discussion, we simply use $\Phi^n(x) = \Phi(t_n, x)$, which is the case when $n = 0$. According to (2.3), $\Phi^{n,0}(s)$ is an approximation to the exact solution $\Phi(t_n + s)$ with local error $O(\tau)$. $\Phi_*^{n,k+1}(s)$ is an intermedia variable, and $\Phi^{n,k+1}(s)$ is the numerical approximation to the exact solution $\Phi(t_n + s)$ with local error $O(\tau^{k+2})$, which implies that the global accuracy is $O(\tau^{k+1})$. One can simply let $\Phi^{n,k+1}(s) = \Phi_*^{n,k+1}(s)$ in (2.5), but it is not easily computable. Therefore, it is necessary to choose

suitable approximation $\Phi^{n,k+1}(s)$ for numerical convenience and uniform accuracies. Below we discuss this in detail.

$\Phi^{n,k+1}(s)$ will be obtained by approximating the temporal integral term in $\Phi_*^{n,k+1}(s)$ by Gautschi-type quadrature rules or EWI. In the approximation/calculation, we need pay particular attention to the operator $e^{i\mathcal{T}t/\varepsilon^2}$, which can be decomposed as (1.6)

$$e^{i\mathcal{T}t/\varepsilon^2} = e^{it/\varepsilon^2} e^{i\mathcal{A}^\varepsilon t}\Pi_+ + e^{-it/\varepsilon^2} e^{-i\mathcal{A}^\varepsilon t}\Pi_-,$$

and the operators involved are defined on the periodic domain Ω. In order to obtain a uniformly accurate method, we must separate the highly oscillatory frequencies and integrate these $e^{\pm it/\varepsilon^2}$ phases exactly, while only the temporal slowly varying parts (w.r.t. ε) are approximated, e.g., the $\mathcal{A}^\varepsilon$ part.

Now, let us describe the detailed derivation of the uniform first-, second-, and third-order in time NPI methods, respectively.

First-order NPI. First, let us take $k = 0$ in (2.5) and use (1.6); we have

$$\begin{aligned}
\Phi_*^{n,1}(s) &= e^{-i\mathcal{T}s/\varepsilon^2}\Phi^n - i\int_0^s e^{-i\mathcal{T}(s-w)/\varepsilon^2}\left(W^n(w)\Phi^{n,0}(w)\right)dw \\
&= e^{-i\mathcal{T}s/\varepsilon^2}\Phi^n - ie^{-is/\varepsilon^2}\int_0^s e^{-i\mathcal{A}^\varepsilon(s-w)}\Pi_+\left[W^n(w)\left(\left(e^{-i\mathcal{A}^\varepsilon w}\Pi_+ + e^{2iw/\varepsilon^2}e^{i\mathcal{A}^\varepsilon w}\Pi_-\right)\Phi^n\right)\right]dw \\
&\quad - ie^{is/\varepsilon^2}\int_0^s e^{i\mathcal{A}^\varepsilon(s-w)}\Pi_-\left[W^n(w)\left(\left(e^{-2iw/\varepsilon^2}e^{-i\mathcal{A}^\varepsilon w}\Pi_+ + e^{i\mathcal{A}^\varepsilon w}\Pi_-\right)\Phi^n\right)\right]dw. \qquad (2.6)
\end{aligned}$$

Notice that $\Phi_*^{n,1}(s)$ is already an approximation of exact solution at $t_n + s$ with $O(s^2)$ error. It suffices to approximate $\Phi_*^{n,1}(s)$ within $O(s^2)$ error for a linearly convergent scheme. Applying Taylor expansion to the nonoscillatory terms in the integrands in (2.6), e.g., $W^n(w) = W^n(0) + O(w)$, $e^{-i\mathcal{A}^\varepsilon w} = I + O(w)$, the integrals can be approximated via the Gautschi-type quadrature rules or EWI [3, 23, 25] as

$$\begin{aligned}
\Phi_*^{n,1}(s) &= e^{-i\mathcal{T}s/\varepsilon^2}\Phi^n - ie^{-is/\varepsilon^2}\int_0^s \Pi_+\left[W^n(0)\left(\Pi_+\Phi^n + e^{2iw/\varepsilon^2}\Pi_-\Phi^n\right)\right]dw \\
&\quad - ie^{is/\varepsilon^2}\int_0^s \Pi_-\left[W^n(0)\left(e^{-2iw/\varepsilon^2}\Pi_+\Phi^n + \Pi_-\Phi^n\right)\right]dw + O(s^2). \qquad (2.7)
\end{aligned}$$

Neglecting the remainder term $O(s^2)$, the left integrals can be computed exactly, which gives the approximation $\Phi^{n,1}(s)$ of $\Phi_*^{n,1}(s)$ for $0 \le s \le \tau$ as

$$\begin{aligned}
\Phi^{n,1}(s) &= e^{-i\mathcal{T}s/\varepsilon^2}\Phi^n - ie^{-is/\varepsilon^2}\Pi_+\left[sW^n(0)(\Pi_+\Phi^n) + p_1(s)W^n(0)(\Pi_-\Phi^n)\right] \\
&\quad - ie^{is/\varepsilon^2}\Pi_-\left[\overline{p_1(s)}W^n(0)(\Pi_+\Phi^n) + sW^n(0)(\Pi_-\Phi^n)\right] \\
&= e^{-is/\varepsilon^2}\left[e^{-i\mathcal{A}^\varepsilon s}\Phi_+^n - is\Pi_+\left(W^n(0)\Phi_+^n\right) - ip_1(s)\Pi_+\left(W^n(0)\Phi_-^n\right)\right] \\
&\quad + e^{is/\varepsilon^2}\left[e^{i\mathcal{A}^\varepsilon s}\Phi_-^n - is\Pi_-\left(W^n(0)\Phi_-^n\right) - i\overline{p_1(s)}\Pi_-\left(W^n(0)\Phi_+^n\right)\right], \qquad (2.8)
\end{aligned}$$

where we denote $\Phi_\pm^n := \Pi_\pm\Phi^n = \Pi_\pm\Phi^n(x)$ for simplicity of notation and

$$p_1(s) = \int_0^s e^{2iw/\varepsilon^2}\,dw = \frac{\varepsilon^2}{2i}\left(e^{2is/\varepsilon^2} - 1\right) = se^{is/\varepsilon^2}\mathrm{sinc}\left(\frac{s}{\varepsilon^2}\right) = O(s) \qquad (2.9)$$

with $\mathrm{sinc}(s) = \sin(s)/s$ ($s \in \mathbb{R}, \mathrm{sinc}(0) = 1$).

If we use $\Phi^{n,1}$ in (2.8) as the numerical approximation for the exact solution, i.e., choose $\Phi^{n+1}(x) = \Phi^{n,1}(\tau, x) = \Phi^{n,1}(\tau)$ given in (2.8) by setting s to τ, we could obtain the linear NPI method, which is uniformly accurate in time with linear convergence rate. The key observation is that $\Phi_*^{n,1}(s)$ in (2.6) deviates from the exact solution with an error of $O(\tau^2)$, and the local errors induced by numerical approximation in (2.7) are of $O(\tau^2)$. The global convergence rate for this scheme would be first-order $O(\tau)$ which is independent of ε.

Second-order NPI. To obtain a second-order in time NPI scheme, let us substitute $\Phi^{n,1}(s)$ back into the integral in (2.5) and arrive at

$$\begin{aligned}
\Phi_*^{n,2}(s) = e^{-i\mathcal{T}s/\varepsilon^2}\Phi^n - ie^{-is/\varepsilon^2}\Bigg[& \int_0^s \left(e^{-i\mathcal{A}^\varepsilon s} g_+^{1,n}(w) - ip_1(w) e^{-i\mathcal{A}^\varepsilon(s-w)} g_+^{2,n}(w)\right) dw \\
& + \int_0^s e^{2iw/\varepsilon^2}\left(e^{-i\mathcal{A}^\varepsilon s} g_+^{3,n}(w) - i\overline{p_1(w)} e^{-i\mathcal{A}^\varepsilon(s-w)} g_+^{4,n}(w)\right) dw\Bigg] \\
& - ie^{is/\varepsilon^2}\Bigg[\int_0^s \left(e^{i\mathcal{A}^\varepsilon s} g_-^{1,n}(w) - i\overline{p_1(w)} e^{i\mathcal{A}^\varepsilon(s-w)} g_-^{2,n}(w)\right) dw \\
& + \int_0^s e^{-2iw/\varepsilon^2}\left(e^{i\mathcal{A}^\varepsilon s} g_-^{3,n}(w) - ip_1(w) e^{i\mathcal{A}^\varepsilon(s-w)} g_-^{4,n}(w)\right) dw\Bigg],
\end{aligned}$$

where

$$\begin{cases}
g_\pm^{1,n}(w) = e^{\pm i\mathcal{A}^\varepsilon w}\Pi_\pm\left[W^n(w)\left(e^{\mp i\mathcal{A}^\varepsilon w}\Phi_\pm^n - iw\Pi_\pm\left(W^n(0)\Phi_\pm^n\right)\right)\right], \\
g_\pm^{3,n}(w) = e^{\pm i\mathcal{A}^\varepsilon w}\Pi_\pm\left[W^n(w)\left(e^{\pm i\mathcal{A}^\varepsilon w}\Phi_\mp^n - iw\Pi_\mp\left(W^n(0)\Phi_\mp^n\right)\right)\right], \\
g_\pm^{2,n}(w) = \Pi_\pm\left[W^n(w)\left(\Pi_\pm\left(W^n(0)\Phi_\mp^n\right)\right)\right], \\
g_\pm^{4,n}(w) = \Pi_\pm\left[W^n(w)\left(\Pi_\mp\left(W^n(0)\Phi_\pm^n\right)\right)\right].
\end{cases} \tag{2.10}$$

As $\Phi^{n,1}(s)$ is an approximation of $O(s^2)$ error, $\Phi_*^{n,2}(s)$ is already an approximation of exact solution at $t_n + s$ with $O(s^3)$ error. It remains to find a proper numerical approximation of $\Phi_*^{n,2}(s)$ with $O(s^3)$ error for a quadratically convergent scheme. Again, applying the midpoint rule for $g_\pm^{1,n}(w)$ terms and Taylor expansion and EWI for other nonoscillatory terms in the integrands (the oscillatory terms are only those $e^{\pm 2iw/\varepsilon^2}$, $p_1(w)$ terms), we can approximate $\Phi_*^{n,2}(s)$ as

$$\begin{aligned}
\Phi_*^{n,2}(s) = e^{-i\mathcal{T}s/\varepsilon^2}\Phi^n - e^{-is/\varepsilon^2}\Bigg[& ise^{-i\mathcal{A}^\varepsilon s} g_+^{1,n}(s/2) + \int_0^s p_1(w)\left(g_+^{2,n}(0) + g_+^{4,n}(0)\right) dw \\
& + ie^{-i\mathcal{A}^\varepsilon s}\int_0^s e^{2iw/\varepsilon^2}\left(g_+^{3,n}(0) + w\dot{g}_+^{3,n}(0)\right) dw\Bigg] - e^{is/\varepsilon^2}\Bigg[ise^{i\mathcal{A}^\varepsilon s} g_-^{1,n}(s/2) \\
& + \int_0^s \overline{p_1(w)}\left(g_-^{2,n}(0) + g_-^{4,n}(0)\right) dw \\
& + ie^{i\mathcal{A}^\varepsilon s}\int_0^s e^{-2iw/\varepsilon^2}\left(g_-^{3,n}(0) + w\dot{g}_-^{3,n}(0)\right) dw\Bigg] + O(s^3),
\end{aligned}$$

where

$$\begin{aligned}
\dot{g}_\pm^{3,n}(w) = e^{\pm i\mathcal{A}^\varepsilon w}\Pi_\pm\Big[& \partial_w W^n(w)\left(e^{\pm i\mathcal{A}^\varepsilon w}\Phi_\mp^n - iw\Pi_\mp\left(W^n(0)\Phi_\mp^n\right)\right) \\
& + W^n(w)\left(\pm i\mathcal{A}_*^\varepsilon e^{\pm i\mathcal{A}^\varepsilon w}\Phi_\mp^n - i\Pi_\mp\left(W^n(0)\Phi_\mp^n\right)\right)\Big] \pm i\mathcal{A}_*^\varepsilon g_\pm^{3,n}(w),
\end{aligned} \tag{2.11}$$

with $\mathcal{A}_*^\varepsilon = \sin(\mathcal{A}^\varepsilon\tau)/\tau$. Here, in $\dot g_\pm^{3,n}(w)$, we use a filtered version $\mathcal{A}_*^\varepsilon$ instead of $\mathcal{A}^\varepsilon$ itself. The purpose is to match the regularity loss of time derivative in $\dot g_\pm^{3,n}$ with time step τ instead of spatial mesh size h for $\mathcal{A}^\varepsilon$ (see proofs of Lemmas 3.2 and 3.3 when estimating $\|P_M(\partial_s g_+^{3,n}(0)) - I_M(\dot g_+^{3,n}(0))\|_{L^2}$ and $\|\dot G_+^{3,n}(\cdot)\|_{L^2}$). Filters of other types may be employed also [5, 8, 15].

Evaluating the integrals above and neglecting the $O(s^3)$ remainder term, we find the approximation $\Phi^{n,2}(s)$ of $\Phi_*^{n,2}$ as

$$
\begin{aligned}
\Phi^{n,2}(s) = e^{-is/\varepsilon^2}\Big[& e^{-i\mathcal{A}^\varepsilon s}\left(\Phi_+^n - is g_+^{1,n}\left(\frac{s}{2}\right) - ip_1(s) g_+^{3,n}(0) - iq_1(s)\dot g_+^{3,n}(0)\right) \\
& - p_2(s)\left(g_+^{2,n}(0) + g_+^{4,n}(0)\right)\Big] \\
& + e^{is/\varepsilon^2}\Big[e^{i\mathcal{A}^\varepsilon s}\left(\Phi_-^n - is g_-^{1,n}\left(\frac{s}{2}\right) - i\overline{p_1(s)} g_-^{3,n}(0) - i\overline{q_1(s)}\dot g_-^{3,n}(0)\right) \\
& - \overline{p_2(s)}\left(g_-^{2,n}(0) + g_-^{4,n}(0)\right)\Big],
\end{aligned} \tag{2.12}
$$

with

$$
\begin{aligned}
p_2(s) &= \int_0^s p_1(w)\,dw = \frac{\varepsilon^2}{2i}(p_1(s) - s) = \frac{\varepsilon^2 s}{2i}\left(e^{is/\varepsilon^2}\mathrm{sinc}\left(\frac{s}{\varepsilon^2}\right) - 1\right) = O(s^2), \\
q_1(s) &= \int_0^s w e^{2iw/\varepsilon^2}\,dw = \frac{\varepsilon^2}{2i}\left(s e^{2is/\varepsilon^2} - p_1(s)\right) = e^{2is/\varepsilon^2}\overline{p_2(s)} = O(s^2).
\end{aligned} \tag{2.13}
$$

Thus, letting $\Phi^{n+1}(x) = \Phi^{n,2}(\tau, x)$ with $\Phi^{n,2}(\tau, x) = \Phi^{n,2}(\tau)$ given in (2.12) by setting s to τ, we have gained a second-order in time NPI method.

Third-order NPI. Analogously, in order to obtain a higher-order NPI scheme, we employ (2.5) once more (i.e., $k = 2$) and get

$$
\begin{aligned}
&\Phi_*^{n,3}(s) \\
&= e^{-is/\varepsilon^2}\Bigg\{ e^{-i\mathcal{A}^\varepsilon s}\Phi_+^n - ie^{-i\mathcal{A}^\varepsilon s}\int_0^s \left(f_+^{1,n}(w) + e^{2iw/\varepsilon^2} f_+^{2,n}(w) - ip_1(w) f_+^{3,n}(w)\right) dw \\
&\qquad + i\int_0^s e^{-i\mathcal{A}^\varepsilon(s-w)}\left(q_1(w) f_+^{4,n}(w) + p_2(w) f_-^{4,n}(w)\right) dw\Bigg\} \\
&\quad + e^{is/\varepsilon^2}\Bigg\{ e^{i\mathcal{A}^\varepsilon s}\Phi_-^n - ie^{i\mathcal{A}^\varepsilon s}\int_0^s \left(f_-^{1,n}(w) + e^{-2iw/\varepsilon^2} f_-^{2,n}(w) - i\overline{p_1(w)} f_-^{3,n}(w)\right) dw \\
&\qquad + i\int_0^s e^{i\mathcal{A}^\varepsilon(s-w)}\left(\overline{q_1(w)} f_-^{4,n}(w) + \overline{p_2(w)} f_+^{4,n}(w)\right) dw\Bigg\},
\end{aligned}
$$

with

$$
\begin{aligned}
f_\pm^{1,n}(w) &:= e^{\pm\mathcal{A}^\varepsilon w}\Pi_\pm\left[W^n(w)\left(e^{\mp i\mathcal{A}^\varepsilon w}\left(\Phi_\pm^n - iw g_\pm^{1,n}(w/2)\right)\right)\right], \\
f_\pm^{2,n}(w) &:= e^{\pm\mathcal{A}^\varepsilon w}\Pi_\pm\left[W^n(w)\left(e^{\pm i\mathcal{A}^\varepsilon w}\left(\Phi_\mp^n - iw g_\mp^{1,n}(w/2)\right)\right)\right], \\
f_\pm^{3,n}(w) &:= e^{\pm\mathcal{A}^\varepsilon w}\Pi_\pm\left[W^n(w)\left(e^{-i\mathcal{A}^\varepsilon w} g_+^{3,n}(0) + e^{i\mathcal{A}^\varepsilon w} g_-^{3,n}(0)\right)\right], \\
f_\pm^{4,n}(w) &= \Pi_\pm\left[W^n(w)\left(ie^{\mp i\mathcal{A}^\varepsilon w}\dot g_\pm^{3,n}(0) + g_\mp^{2,n}(0) + g_\mp^{4,n}(0)\right)\right].
\end{aligned}
$$

As $\Phi^{n,2}(s)$ is an approximation of $O(s^3)$ error, $\Phi_*^{n,3}(s)$ is an approximation of exact solution at $t_n + s$ with $O(s^4)$ error. Thus, we only need a numerical approximation of $\Phi_*^{n,3}(s)$ with $O(s^4)$ error for a third-order scheme. Applying Simpson's rule for the $f_\pm^{n,1}(w)$ terms and Taylor expansion and EWI for the rest of the terms, we could derive an approximation $\Phi^{n,3}(s) = \Phi_*^{n,3}(s) + O(s^4)$ as

$$\begin{aligned}
\Phi^{n,3}(s) = e^{-is/\varepsilon^2}\Bigg\{ & e^{-i\mathcal{A}^\varepsilon s}\Bigg[\Phi_+^n - i\frac{s}{6}\left(f_+^{1,n}(0) + 4f_+^{1,n}\left(\frac{s}{2}\right) + f_+^{1,n}(s)\right) \\
& - i\Big(p_1(s)f_+^{2,n}(0) + q_1(s)\dot{f}_+^{2,n}(0) + \frac{1}{2}r_1(s)\ddot{f}_+^{2,n}(0)\Big) \\
& - \Big(p_2(s)f_+^{3,n}(0) + r_2(s)\dot{f}_+^{3,n}(0)\Big)\Bigg] + i\left(q_2(s)f_+^{4,n}(0) + p_3(s)f_-^{4,n}(0)\right)\Bigg\} \\
& + e^{is/\varepsilon^2}\Bigg\{ e^{i\mathcal{A}^\varepsilon s}\Bigg[\Phi_-^n - i\frac{s}{6}\left(f_-^{1,n}(0) + 4f_-^{1,n}(\frac{s}{2}) + f_-^{1,n}(s)\right) \\
& - i\Big(\overline{p_1(s)}f_-^{2,n}(0) + \overline{q_1(s)}\dot{f}_-^{2,n}(0) + \frac{1}{2}\overline{r_1(s)}\ddot{f}_-^{2,n}(0)\Big) \\
& - \Big(\overline{p_2(s)}f_-^{3,n}(0) + \overline{r_2(s)}\dot{f}_-^{3,n}(0)\Big)\Bigg] + i\left(\overline{q_2(s)}f_-^{4,n}(0) + \overline{p_3(s)}f_+^{4,n}(0)\right)\Bigg\},
\end{aligned}$$

where

(2.14)

$$\begin{aligned}
& p_3(s) = \int_0^s p_2(w)\,dw = \frac{\varepsilon^2}{2i}\left(p_2(s) - \frac{s^2}{2}\right), \quad q_2(s) = \int_0^s q_1(w)\,dw = \frac{\varepsilon^2}{2i}(q_1(s) - p_2(s)), \\
& r_1(s) = \int_0^s w^2 e^{2iw/\varepsilon^2}\,dw = \frac{\varepsilon^2}{2i}(s^2 e^{2is/\varepsilon^2} - 2q_1(s)), \\
& r_2(s) = \int_0^s w p_1(w)\,dw = \frac{\varepsilon^2}{2i}\left(q_1(s) - \frac{s^2}{2}\right),
\end{aligned}$$

and $\dot{f}_\pm^{2,n}, \ddot{f}_\pm^{2,n}, \dot{f}_\pm^{3,n}$ are approximations to $\partial_w f_\pm^{2,n}(w), \partial_{ww} f_\pm^{2,n}(w), \partial_w f_\pm^{3,n}(w)$, respectively, with only $\mathcal{A}^\varepsilon$ from differentiation being replaced by $\mathcal{A}_*^\varepsilon$.

It is straightforward to check that $p_3(s), q_2(s), r_1(s), r_2(s)$ are all of $O(s^3)$. Finally, the third-order in time NPI method is given by $\Phi^{n+1}(x) = \Phi^{n,3}(\tau, x)$ with $\Phi^{n,3}(\tau, x) = \Phi^{n,3}(\tau)$.

Remark 2.1. For simplicity, we only present the first- to third-order in time NPI methods. While in principle it can be extended to arbitrary order in time by continuing the iteration, the success of the NPI methods relies on the fact that the operators $\mathcal{A}^\varepsilon$ and $\Pi_\pm$ can be easily computed in the Fourier domain by fast Fourier transform (FFT). The uniform accurate properties of the NPI methods can be seen from the derivation that the errors introduced in numerical approximations do not depend on ε.

2.2. Fourier spectral discretization. We have presented the construction of semidiscrete in time NPI schemes, and in this and the next subsections we take the second-order NPI scheme for example to discuss spatial discretization and the implementation, respectively. As indicated in Remark 2.1, the operators $\mathcal{T}, \Pi_\pm$, and $\mathcal{A}^\varepsilon$ can be easily computed in the Fourier domain, which is crucial to the success of the numerical scheme. Thus, we adopt the Fourier spectral discretization in space [35].

Let us discretize the space domain as $a = x_0 < x_1 < \cdots < x_M = b$ with mesh size $h := \Delta x = (b-a)/M$ and grid points $x_j := a + j\,h$ for $j \in \mathcal{T}_M := \{0, 1, \ldots, M\}$, where M is a positive even integer. Define the spaces

$$X_M = \{U = (U_0, U_1, \ldots, U_M)^T \mid U_j \in \mathbb{C}^2, j \in \mathcal{T}_M,\ U_0 = U_M\}$$
$$\text{with} \quad \|U\|_{l^2} = h \sum\nolimits_{j=0}^{M-1} |U_j|^2,$$
$$Y_M = Z_M \times Z_M \text{ with}$$
$$Z_M = \text{span}\left\{\phi_l(x) = e^{i\mu_l(x-a)},\ \mu_l = \frac{2l\pi}{b-a}, \quad l = -\frac{M}{2}, \ldots, \frac{M}{2} - 1\right\}.$$

Denote $[C_p(a,b)]^2$ as the function space consisting of all periodic vector function $U(x) : [a,b] \to \mathbb{C}^2$. Then, for any $U(x) \in [L^2(a,b)]^2$ and $U \in X_M$, let $P_M :\ [L^2(a,b)]^2 \to Y_M$ be the standard projection operator, and let $I_M :\ [C_p(a,b)]^2 \to Y_M$ or $I_M : X_M \to Y_M$ be the standard interpolation operator, i.e.,

(2.15)
$$(P_M U)(x) = \sum_{l=-M/2}^{M/2-1} \widehat{U}_l\, e^{i\mu_l(x-a)}, \quad (I_M U)(x) = \sum_{l=-M/2}^{M/2-1} \widetilde{U}_l\, e^{i\mu_l(x-a)}, \qquad a \le x \le b,$$

with

(2.16)
$$\widehat{U}_l = \frac{1}{b-a}\int_a^b U(x)\, e^{-i\mu_l(x-a)}\, dx, \quad \widetilde{U}_l = \frac{1}{M}\sum_{j=0}^{M-1} U_j\, e^{-2ijl\pi/M}, \quad l = -\frac{M}{2}, \ldots, \frac{M}{2} - 1,$$

where $U_j = U(x_j)$ when U is a function. The Parseval's identity implies that

$$\|I_M(U)(\cdot)\|_{L^2} = \|U\|_{l^2} \quad \forall U \in X_M. \tag{2.17}$$

The Fourier spectral discretization for (2.1) reads as follows: Find $\Phi_M^n := \Phi_M^n(s) = \Phi_M(t_n + s) = \Phi_M(t_n + s, x) \in Y_M$, i.e.,

$$\Phi_M(t_n + s, x) = \sum_{l=-M/2}^{M/2-1} \widehat{(\Phi^n)}_l(s)\, e^{i\mu_l(x-a)}, \qquad a \le x \le b, \qquad 0 \le s \le \tau, \tag{2.18}$$

such that

$$i\partial_s \Phi_M^n(s) = \frac{1}{\varepsilon^2}\mathcal{T}\Phi_M^n(s) + P_M(W^n(s)\Phi_M^n(s)), \qquad a < x < b, \qquad 0 \le s \le \tau, \tag{2.19}$$

with $\Phi_M^n(0) = P_M\left(\Phi(t_n, x)\right)$.

Substituting (2.18) into (2.19), we obtain the equations for the Fourier coefficients as

(2.20)
$$i\partial_s \widehat{(\Phi^n)}_l(s) = \frac{1}{\varepsilon^2}\mathcal{T}_l \widehat{(\Phi^n)}_l(s) + (\widehat{W^n\Phi_M^n})_l(s), \qquad 0 \le s \le \tau, \quad l = -\frac{M}{2}, \ldots, \frac{M}{2} - 1,$$

with $\mathcal{T}_l = \left(\begin{smallmatrix} 1 & \varepsilon\mu_l \\ \varepsilon\mu_l & -1 \end{smallmatrix}\right)$ the Fourier representation of $\mathcal{T}$. Equivalently, it can be written in the integral form by the variation-of-constant formula as

(2.21)
$$\widehat{(\Phi^n)}_l(s) = e^{-i\mathcal{T}_l s/\varepsilon^2}\widehat{(\Phi^n)}_l(0) - i\int_0^s e^{-i\mathcal{T}_l(s-w)/\varepsilon^2}(\widehat{W^n\Phi_M^n})_l(w)\, dw, \quad 0 \le s \le \tau.$$

Combined with the derived second-order NPI method, we introduce

$$\Phi_M^{n,k}(s) = \sum_{l=-M/2}^{M/2-1} \widehat{(\Phi^{n,k})}_l(s) e^{i\mu_l(x-a)}, \qquad k = 0, 1, 2,$$

where $\widehat{(\Phi^{n,0})}_l(s) = e^{-i\mathcal{T}_l s/\varepsilon^2}\widehat{(\Phi^n)}_l(0)$, and $\widehat{(\Phi^{n,k})}_l(s), k = 1, 2$, $l = -\frac{M}{2}, \ldots, \frac{M}{2} - 1$ can be obtained by nested Picard iteration based on (2.21) as

$$\begin{aligned}
\widehat{(\Phi^{n,1})}_l(s) = e^{-is/\varepsilon^2}\Big[& e^{-i\mathcal{A}_l^\varepsilon s}\Pi_l^+\widehat{(\Phi^n)}_l(0) - is\Pi_l^+(W^n\widehat{(\Pi_+\Phi_M^n)})_l(0) \\
& - ip_1(s)\Pi_l^+(W^n\widehat{(\Pi_-\Phi_M^n)})_l(0)\Big] \\
+ e^{is/\varepsilon^2}\Big[& e^{i\mathcal{A}_l^\varepsilon s}\Pi_l^-\widehat{(\Phi^n)}_l(0) - is\Pi_l^-(W^n\widehat{(\Pi_-\Phi_M^n)})_l(0) \\
& - i\overline{p_1(s)}\Pi_l^-(W^n\widehat{(\Pi_+\Phi_M^n)})_l(0)\Big],
\end{aligned} \tag{2.22}$$

$$\begin{aligned}
\widehat{(\Phi^{n,2})}_l(s) = e^{-is/\varepsilon^2}\Big[& e^{-i\mathcal{A}_l^\varepsilon s}\Big(\Pi_l^+\widehat{(\Phi^n)}_l(0) - is\widehat{(g_+^1)}_l(s/2) - ip_1(s)\widehat{(g_+^3)}_l(0) \\
& - iq_1(s)\widehat{(\dot g_+^3)}_l(0)\Big) - p_2(s)\Big(\widehat{(g_+^2)}_l(0) + \widehat{(g_+^4)}_l(0)\Big)\Big] \\
+ e^{is/\varepsilon^2}\Big[& e^{i\mathcal{A}_l^\varepsilon s}\Big(\Pi_l^-\widehat{(\Phi^n)}_l(0) - is\widehat{(g_-^1)}_l(s/2) - i\overline{p_1(s)}\widehat{(g_-^3)}_l(0) \\
& - i\overline{q_1(s)}\widehat{(\dot g_-^3)}_l(0)\Big) - \overline{p_2(s)}\Big(\widehat{(g_-^2)}_l(0) + \widehat{(g_-^4)}_l(0)\Big)\Big],
\end{aligned} \tag{2.23}$$

where $\mathcal{A}_l^\varepsilon$ and $\Pi_l^\pm$ are the corresponding Fourier representations of $\mathcal{A}^\varepsilon$ and the projectors $\Pi_\pm$ as

$$\mathcal{A}_l^\varepsilon = \frac{\delta_l - 1}{\varepsilon^2} I_2, \quad \Pi_l^+ = \begin{pmatrix} \frac{1+\delta_l}{2\delta_l} & \frac{\varepsilon\mu_l}{2\delta_l} \\ \frac{\varepsilon\mu_l}{2\delta_l} & \frac{\varepsilon^2\mu_l^2}{2\delta_l(\delta_l+1)} \end{pmatrix}, \quad \Pi_l^- = \begin{pmatrix} \frac{\varepsilon^2\mu_l^2}{2\delta_l(\delta_l+1)} & -\frac{\varepsilon\mu_l}{2\delta_l} \\ -\frac{\varepsilon\mu_l}{2\delta_l} & \frac{1+\delta_l}{2\delta_l} \end{pmatrix} \tag{2.24}$$

with $\delta_l = \sqrt{1 + \varepsilon^2\mu_l^2}$, and $g_\pm^k(\cdot), k = 1, 2, 3, 4$ and $\dot g_\pm^3(\cdot)$ are defined the same as $g_\pm^{k,n}(\cdot)$ and $\dot g_\pm^{3,n}(\cdot)$ in (2.10)–(2.11), respectively, by replacing $\Phi_\pm^n$ with $\Pi_\pm\Phi_M^n(0)$. Finally, taking $s = \tau$ in $\widehat{(\Phi^{n,2})}_l(s)$ immediately gives the approximation of $\widehat{(\Phi^n)}_l(\tau)$ that we want. One can continue to obtain a fully discrete third-order NPI scheme. We note that the above process is equivalent to discretizing the second-order NPI (2.12) in space via Fourier spectral discretization.

2.3. Second-order NPI method. As to implementation, we need to further approximate the integrals for computing the Fourier transform coefficients in (2.16), (2.22), and (2.23) by numerical quadratures. Let Φ_j^n be the numerical approximation of the exact solution $\Phi(t_n, x_j)$ to the Dirac equation (2.1) for $n \geq 0$ and $j \in \mathcal{T}_M$, and denote $\Phi^n \in X_M$ as the numerical solution vector at time $t = t_n$. In addition, denote $W^n = W(t_n, x) = V(t_n, x)I_2 - A_1(t_n, x)\sigma_1$, $W^{n+\frac{1}{2}} = W(t_n + \frac{\tau}{2}, x) = V(t_n + \frac{\tau}{2}, x)I_2 - A_1(t_n + \frac{\tau}{2}, x)\sigma_1$, $\dot W^n = \partial_t W(t_n, x)$ for $n \geq 0$. Choosing $\Phi_j^0 = \Phi_0(x_j)$ for $j \in \mathcal{T}_M$, then the Fourier pseudospectral discretization of the second-order NPI scheme for the Dirac equation (1.4) in one dimension reads for $n \geq 0$ and $j \in \mathcal{T}_M$ as

$$\Phi_j^{n+1} = \sum_{l=-M/2}^{M/2-1} \widetilde{(\Phi^{n+1})}_l e^{i\mu_l(x_j-a)} \tag{2.25}$$

with

$$\begin{aligned}
\widetilde{(\Phi^{n+1})}_l = {} & e^{-i\tau/\varepsilon^2}\Big[e^{-i\mathcal{A}_l^\varepsilon\tau}\Big(\Pi_l^+\widetilde{(\Phi^n)}_l - i\tau\widetilde{\big(g_+^1\big)}_l - ip_1(\tau)\widetilde{\big(g_+^3\big)}_l - iq_1(\tau)\widetilde{\big(\dot g_+^3\big)}_l\Big) \\
& - p_2(\tau)\Big(\widetilde{\big(g_+^2\big)}_l + \widetilde{\big(g_+^4\big)}_l\Big)\Big] \\
& + e^{i\tau/\varepsilon^2}\Big[e^{i\mathcal{A}_l^\varepsilon\tau}\Big(\Pi_l^-\widetilde{(\Phi^n)}_l - i\tau\widetilde{\big(g_-^1\big)}_l - i\overline{p_1(\tau)}\widetilde{\big(g_-^3\big)}_l - i\overline{q_1(\tau)}\widetilde{\big(\dot g_-^3\big)}_l\Big) \\
& - \overline{p_2(\tau)}\Big(\widetilde{\big(g_-^2\big)}_l + \widetilde{\big(g_-^4\big)}_l\Big)\Big],
\end{aligned} \tag{2.26}$$

where

$$\begin{cases}
\widetilde{\big(g_\pm^1\big)}_l = e^{\pm i\mathcal{A}_l^\varepsilon\tau/2}\Pi_l^\pm\Big[\Big(\widetilde{W^{n+\frac12}(e^{\mp i\mathcal{A}^\varepsilon\tau/2}\Pi_\pm\Phi^n)}\Big)_l - i\tfrac{\tau}{2}\Big(\widetilde{W^{n+\frac12}(\Pi_\pm\widetilde{(W^n(\Pi_\pm\Phi^n))})}\Big)_l\Big], \\
\widetilde{\big(g_\pm^2\big)}_l = \Pi_l^\pm(W^n(\Pi_\pm\widetilde{(W^n}(\Pi_\mp\Phi^n))))_l, \qquad \widetilde{\big(g_\pm^3\big)}_l = \Pi_l^\pm(W^n\widetilde{(\Pi_\mp\Phi^n)})_l, \\
\widetilde{\big(\dot g_\pm^3\big)}_l = \Pi_l^\pm\Big[\Big(\dot W^n\widetilde{(\Pi_\mp\Phi^n)}\Big)_l \pm i(W^n(\widetilde{\mathcal{A}_*^\varepsilon\Pi_\mp}\Phi^n))_l - i(W^n(\Pi_\mp\widetilde{(W^n}(\Pi_\mp\Phi^n))))_l\Big] \\
\qquad \pm i(\mathcal{A}_*^\varepsilon)_l\widetilde{\big(g_\pm^3\big)}_l, \qquad\qquad (\mathcal{A}_*^\varepsilon)_l = \sin((\delta_l-1)\tau/\varepsilon^2)/\tau I_2, \\
\widetilde{\big(g_\pm^4\big)}_l = \Pi_l^\pm(W^n(\Pi_\mp\widetilde{(W^n}(\Pi_\pm\Phi^n))))_l, \qquad l = -\frac{M}{2},\dots,\frac{M}{2}-1.
\end{cases} \tag{2.27}$$

Here, we remark that (i) $\dot W^n$ can also be chosen as a suitable finite difference approximation of $\partial_t W(t_n,x)$; (ii) for simplicity of notation, we denote $\Pi_\pm\Phi^n := \Pi_\pm I_M(\Phi^n)$.

The first- and third-order NPI schemes can be implemented similarly. It can be seen that the NPI method (2.25)–(2.27) for the Dirac equation (1.4) is explicit, efficient, and easy to implement with the discrete FFT. The computational cost is $O(M\log M)$ per time step and the memory cost is $O(M)$. In the next section, we will show that it is uniformly accurate in both space and time w.r.t. $\varepsilon\in(0,1]$.

3. A uniform error bound for second-order NPI method. In this section, we analyze the second-order NPI method in the fully discrete form (2.25)–(2.27) to establish the uniform error bound via the energy method. The analysis presented below could be extended to other NPI methods.

Let $0<T<\infty$ be any fixed time. We first make the following assumptions [12, 17] on the electromagnetic potentials and the exact solution $\Phi := \Phi(t) = \Phi(t,x)$ to the Dirac equation (2.1):

$$(A) \qquad \|V\|_{W^{2,\infty}([0,T];W_p^{m_0,\infty})} + \|A_1\|_{W^{2,\infty}([0,T];W_p^{m_0,\infty})} \lesssim 1,$$

$$(B) \qquad \|\Phi\|_{L^\infty([0,T];(H_p^{m_0})^2)} \lesssim 1, \qquad m_0 \ge 4,$$

where $H_p^m(\Omega) = \{u \mid u\in H^m(\Omega),\ \partial_x^l u(a) = \partial_x^l u(b),\ l=0,\dots,m-1\}$ and $W_p^{m,\infty}(\Omega) = \{u \mid u\in W^{m,\infty}(\Omega),\ \partial_x^l u(a) = \partial_x^l u(b),\ l=0,\dots,m-1\}$ for $m\in\mathbb{N}$. It should be noted that a higher temporal regularity of $V(t,x)$ and $A_1(t,x)$ is needed for a higher-order

scheme. In the rest of this paper, all the functions and norms are taken in certain H_p^m spaces, and we will omit the subscript p for brevity. We remark here that assumption (B) is equivalent to that $\Phi_0(x) \in (H_p^{m_0})^2$ [12] under assumption (A). We also note that assumption (A) is for the spatial spectral accuracy under the periodic truncation of the whole space problem, and the periodic assumptions in (A) can be dropped in practice as long as the solution to the whole space problem (1.1) is well localized.

THEOREM 3.1. *Let $\Phi^n \in X_M$ be the numerical approximation obtained from the NPI method (2.25)–(2.27) and denote $\Phi_I^n(x) = I_M(\Phi^n)(x) \in Y_M$. Under assumptions (A) and (B), there exist constants $0 < \tau_0, h_0 \le 1$ sufficiently small and independent of ε such that for any $0 < \varepsilon \le 1$, when $0 < \tau \le \tau_0$ and $0 < h \le h_0$, we have*

$$\|\Phi(t_n,\cdot) - \Phi_I^n(\cdot)\|_{L^2} \lesssim h^{m_0} + \tau^2, \quad 0 \le n \le \frac{T}{\tau}. \tag{3.1}$$

By the triangle inequality, we have

$$\|\Phi(t_n,\cdot) - \Phi_I^n(\cdot)\|_{L^2} \le \|\Phi(t_n,\cdot) - P_M(\Phi(t_n))(\cdot)\|_{L^2} + \|P_M(\Phi(t_n))(\cdot) - \Phi_I^n(\cdot)\|_{L^2} \tag{3.2}$$

with $\|\Phi(t_n,\cdot) - P_M(\Phi(t_n))(\cdot)\|_{L^2} \lesssim h^{m_0}$ from standard Fourier projection properties [35] under assumption (B). Thus, we only need to estimate $\|P_M(\Phi(t_n))(\cdot) - \Phi_I^n(\cdot)\|_{L^2}$. Therefore, we introduce the error function $\mathbf{e}^n(x) = \sum_{l=-M/2}^{M/2-1} \widehat{(\mathbf{e}^n)}_l e^{i\mu_l(x-a)} \in Y_M$ as

$$\mathbf{e}^n(x) = P_M(\Phi(t_n))(x) - \Phi_I^n(x), \qquad x \in \Omega, \quad n \ge 0, \tag{3.3}$$

where $\widetilde{(\mathbf{e}^n)}_l = \widehat{\Phi}_l(t_n) - \widetilde{(\Phi^n)}_l$.

Taking $s = \tau$ in (2.3) and computing the Fourier coefficients for both sides, we have

$$\begin{aligned}
&\widehat{\Phi}_l(t_n+\tau)\\
&= e^{-i\tau/\varepsilon^2}\left[e^{-i\mathcal{A}_l^\varepsilon\tau}\Pi_l^+\widehat{\Phi}_l(t_n) - i\int_0^\tau e^{is/\varepsilon^2}e^{-i\mathcal{A}_l^\varepsilon(\tau-s)}\Pi_l^+\widehat{(W^n(s)\Phi(t_n+s))}_l\,ds\right]\\
&\quad + e^{i\tau/\varepsilon^2}\left[e^{i\mathcal{A}_l^\varepsilon\tau}\Pi_l^-\widehat{\Phi}_l(t_n) - i\int_0^\tau e^{-is/\varepsilon^2}e^{i\mathcal{A}_l^\varepsilon(\tau-s)}\Pi_l^-\widehat{(W^n(s)\Phi(t_n+s))}_l\,ds\right].
\end{aligned} \tag{3.4}$$

Subtracting (2.26) from it, we can get the error equation

$$\widetilde{(\mathbf{e}^{n+1})}_l = e^{-i\mathcal{T}_l\tau/\varepsilon^2}\widetilde{(\mathbf{e}^n)}_l + e^{-i\tau/\varepsilon^2}\left(\widetilde{(\xi_+^n)}_l + \widetilde{(F_+^n)}_l\right) + e^{i\tau/\varepsilon^2}\left(\widetilde{(\xi_-^n)}_l + \widetilde{(F_-^n)}_l\right), \tag{3.5}$$

where $\xi_\pm^n(x) = \sum_{l=-M/2}^{M/2-1}\widehat{(\xi_\pm^n)}_l e^{i\mu_l(x-a)}$ and $F_\pm^n(x) = \sum_{l=-M/2}^{M/2-1}\widetilde{(F_\pm^n)}_l e^{i\mu_l(x-a)}$ ($x \in \Omega$, $n \ge 0$) are, respectively, the local truncation error and the error for the electromagnetic part defined as ($l = -M/2, \ldots, M/2-1$),

(3.6)
$$\begin{cases}\widehat{(\xi_+^n)}_l = -i\displaystyle\int_0^\tau e^{is/\varepsilon^2}e^{-i\mathcal{A}_l^\varepsilon(\tau-s)}\Pi_l^+(W^n(\widehat{s)\Phi(t_n}+s))_l\,ds + ie^{-i\mathcal{A}_l^\varepsilon\tau}\Big[\tau\widetilde{\Big(g_+^{1,n}(\frac{\tau}{2})\Big)}_l \\ \qquad\qquad + p_1(\tau)\widetilde{\Big(g_+^{3,n}(0)\Big)}_l + q_1(\tau)\widetilde{\Big(\dot g_+^{3,n}(0)\Big)}_l\Big] + p_2(\tau)\left[\widetilde{\Big(g_+^{2,n}(0)\Big)}_l + \widetilde{\Big(g_+^{4,n}(0)\Big)}_l\right], \\ \widehat{(\xi_-^n)}_l = -i\displaystyle\int_0^\tau e^{-is/\varepsilon^2}e^{i\mathcal{A}_l^\varepsilon(\tau-s)}\Pi_l^-(W^n(\widehat{s)\Phi(t_n}+s))_l\,ds + ie^{i\mathcal{A}_l^\varepsilon\tau}\Big[\tau\widetilde{\Big(g_-^{1,n}(\frac{\tau}{2})\Big)}_l \\ \qquad\qquad + \overline{p_1(\tau)}\widetilde{\Big(g_-^{3,n}(0)\Big)}_l + \overline{q_1(\tau)}\widetilde{\Big(\dot g_-^{3,n}(0)\Big)}_l\Big] + \overline{p_2(\tau)}\left[\widetilde{\Big(g_-^{2,n}(0)\Big)}_l + \widetilde{\Big(g_-^{4,n}(0)\Big)}_l\right],\end{cases}$$

and

(3.7)
$$\begin{cases}\widetilde{(F_+^n)}_l = ie^{-i\mathcal{A}_l^\varepsilon\tau}\Big[\tau\widetilde{(G_+^{1,n})}_l + p_1(\tau)\widetilde{(G_+^{3,n})}_l + q_1(\tau)\widetilde{\Big(\dot G_+^{3,n}\Big)}_l\Big] + p_2(\tau)\Big[\widetilde{(G_+^{2,n})}_l + \widetilde{(G_+^{4,n})}_l\Big], \\ \widetilde{(F_-^n)}_l = ie^{i\mathcal{A}_l^\varepsilon\tau}\Big[\tau\widetilde{(G_-^{1,n})}_l + \overline{p_1(\tau)}\widetilde{(G_-^{3,n})}_l + \overline{q_1(\tau)}\widetilde{\Big(\dot G_-^{3,n}\Big)}_l\Big] + \overline{p_2(\tau)}\Big[\widetilde{(G_-^{2,n})}_l + \widetilde{(G_-^{4,n})}_l\Big],\end{cases}$$

with $g_\pm^{k,n}(s), k = 1,2,3,4$, defined in (2.10), $G_\pm^{k,n}(x) = \sum_{l=-M/2}^{M/2-1}\widetilde{(G_\pm^{k,n})}e^{i\mu_l(x-a)}$, $k = 1,2,3,4$, and $\dot G_\pm^{3,n}(x) = \sum_{l=-M/2}^{M/2-1}\widetilde{(\dot G_\pm^{3,n})}e^{i\mu_l(x-a)}$ defined as

$$\begin{cases}\widetilde{\Big(G_\pm^{1,n}\Big)}_l = \widetilde{(g_\pm^1)}_l - \widetilde{\Big(g_\pm^{1,n}(\frac{\tau}{2})\Big)}_l, \qquad \widetilde{\Big(\dot G_\pm^{3,n}\Big)}_l = \widetilde{(\dot g_\pm^3)}_l - \widetilde{\Big(\dot g_+^{3,n}(0)\Big)}_l, \\ \widetilde{\Big(G_\pm^{k,n}\Big)}_l = \widetilde{(g_\pm^k)}_l - \widetilde{\Big(g_\pm^{k,n}(0)\Big)}_l, \qquad k = 2,3,4,\end{cases} \tag{3.8}$$

where $\widetilde{(g_\pm^k)}_l$ $(k = 1,2,3,4)$ and $\widetilde{(\dot g_\pm^3)}$ are given in (2.27).

We first establish the following two lemmas, providing the error bounds for $\|\xi_\pm^n(\cdot)\|_{L^2}$ and $\|F_\pm^n(\cdot)\|_{L^2}$, which can finally lead to the error bound (3.1).

LEMMA 3.2. *Under the assumptions* (A) *and* (B)*, there exist constants* $0 < \tau_0$, $h_0 \le 1$ *sufficiently small and independent of* ε *such that for any* $0 < \varepsilon \le 1$*, when* $0 < \tau \le \tau_0$ *and* $0 < h \le h_0$*, we have the error estimates for the local truncation error* $\xi_\pm^n \in Y_M$ *in* (3.6)*,*

$$\|\xi_\pm^n(\cdot)\|_{L^2} \lesssim \tau\left(h^{m_0} + \tau^2\right), \qquad 0 \le n < \frac{T}{\tau}. \tag{3.9}$$

LEMMA 3.3. *Under the assumptions* (A) *and* (B)*, the error for the electromagnetic part* $F_\pm^n(x) \in Y_M$ *satisfies the bounds*

$$\|F_\pm^n(\cdot)\|_{L^2} \lesssim \tau(h^{m_0} + \|\mathbf{e}^n(\cdot)\|_{L^2}), \quad 0 \le n \le \frac{T}{\tau}. \tag{3.10}$$

Proof of Lemma 3.2. Reviewing the iteration scheme (2.5) and the derivation of the method when $\Phi^n(x)$ is replaced by $\Phi(t_n, x)$, it can be found that the local truncation error mainly comes from the approximation of $\Phi(t_n + w)$ by $\Phi^{n,0}(w), \Phi^{n,1}(w)$ and the use of numerical quadrature rules for time integrals. Therefore, let us first calculate the accuracies of the approximation.

Recalling the integral form of $\Phi(t_n+s)$ in (2.3) and the definition of $\Phi^{n,0}(s)$ in (2.4), we have

$$\mathcal{R}_0(s) := \Phi(t_n+s) - \Phi^{n,0}(s) = -i\int_0^s e^{-i\mathcal{T}(s-w)/\varepsilon^2}\left(W^n(w)\Phi(t_n+w)\right)\,dw, \quad 0\le s\le\tau.$$

With assumptions (A) and (B), we can immediately obtain

$$\|\mathcal{R}_0\|_{L^\infty([0,\tau];(H^{m_0})^2)} \lesssim \tau\|\Phi\|_{L^\infty([0,\tau];(H^{m_0})^2)} \lesssim \tau, \qquad n\ge 0. \tag{3.11}$$

Following the construction of the scheme from (2.3) and (2.6) to (2.8) and under assumptions (A) and (B), we can obtain the estimate for

$$\mathcal{R}_1(s) := \Phi(t_n+s) - \Phi^{n,1}(s) = \Phi(t_n+s) - \Phi_*^{n,1}(s) + \Phi_*^{n,1}(s) - \Phi^{n,1}(s), \quad 0\le s\le\tau, \tag{3.12}$$

with

$$\Phi(t_n+s) - \Phi_*^{n,1}(s) = -i\int_0^s e^{-i\mathcal{T}(s-w)/\varepsilon^2}\left(W^n(w)\mathcal{R}_0(w)\right)\,dw, \quad 0\le s\le\tau, \tag{3.13}$$

as

$$\begin{aligned}&\|\mathcal{R}_1\|_{L^\infty([0,\tau];(H^{m_0-2})^2)}\\ &\quad\lesssim \tau\left(\|\mathcal{R}_0\|_{L^\infty([0,\tau];(H^{m_0-2})^2)} + \tau\|\Phi\|_{L^\infty([0,\tau];(H^{m_0})^2)}\right) \lesssim \tau^2, \qquad n\ge 0.\end{aligned} \tag{3.14}$$

Now we can prove the estimate for $\|\xi_+^n\|_{L^2}$. For $l=-M/2,\dots,M/2-1$, we have

$$\begin{aligned}\widehat{\left(\xi_+^n\right)}_l =& -i\int_0^\tau e^{is/\varepsilon^2}e^{-i\mathcal{A}_l^\varepsilon(\tau-s)}\Pi_l^+\Big[\widehat{(W^n(s)\Phi(t_n+s))}_l\\ &-\widehat{(W^n\Phi^{n,1})}_l(s) + \widehat{(W^n\Phi^{n,1})}_l(s)\Big]\,ds\\ &+ ie^{-i\mathcal{A}_l^\varepsilon\tau}\left[\tau\widehat{\left(g_+^{1,n}(\frac{\tau}{2})\right)}_l + p_1(\tau)\widehat{\left(g_+^{3,n}(0)\right)}_l + q_1(\tau)\widehat{\left(\partial_s g_+^{3,n}(0)\right)}_l\right]\\ &+ p_2(\tau)\left[\widehat{\left(g_+^{2,n}(0)\right)}_l + \widehat{\left(g_+^{4,n}(0)\right)}_l\right] + \widehat{\left(\eta_+^n\right)}_l\\ =& -i\int_0^\tau e^{is/\varepsilon^2}e^{-i\mathcal{A}_l^\varepsilon(\tau-s)}\Pi_l^+\Big[\widehat{(W^n(s)\Phi(t_n+s))}_l - \widehat{(W^n\Phi^{n,1})}_l(s)\Big]\,ds + \widehat{\left(\eta_+^n\right)}_l\\ &-i\int_0^\tau\Bigg\{e^{-i\mathcal{A}_l^\varepsilon\tau}\Big[\int_{\tau/2}^s\int_{\tau/2}^{s_1}\partial_{s_2s_2}\widehat{\left(g_+^{1,n}(s_2)\right)}_l\,ds_2ds_1\\ &+e^{2is/\varepsilon^2}\int_0^s\int_0^{s_1}\partial_{s_2s_2}\widehat{\left(g_+^{3,n}(s_2)\right)}_l\,ds_2ds_1\Big]\\ &-ip_1(s)\Big[\int_s^\tau -i\mathcal{A}_l^\varepsilon e^{-i\mathcal{A}_l^\varepsilon(s_1-s)}\widehat{\left(g_+^{2,n}+g_+^{4,n}\right)}_l(s)\,ds_1\\ &+\int_0^s\partial_{s_1}\widehat{\left(g_+^{2,n}(s_1)+g_+^{4,n}(s_1)\right)}_l\,ds_1\Big]\Bigg\}ds,\end{aligned} \tag{3.15}$$

where $\eta_+^n(x) = \sum_{l=-M/2}^{M/2-1} \widehat{(\eta_+^n)}_l e^{i\mu_l(x-a)}$ with

$$\begin{aligned}\widehat{(\eta_+^n)}_l = ie^{-i\mathcal{A}_l^\varepsilon\tau}\Big(&\tau\Big[\Big(\widetilde{g_+^{1,n}(\frac{\tau}{2})}\Big)_l - \Big(\widehat{g_+^{1,n}(\frac{\tau}{2})}\Big)_l\Big] + p_1(\tau)\Big[\Big(\widetilde{g_+^{3,n}(0)}\Big)_l - \Big(\widehat{g_+^{3,n}(0)}\Big)_l\Big]\\ &+ q_1(\tau)\Big[\Big(\widetilde{\dot g_+^{3,n}(0)}\Big)_l - \Big(\widehat{\partial_s g_+^{3,n}(0)}\Big)_l\Big]\Big) + p_2(\tau)\Big[\Big(\widetilde{g_+^{2,n}(0)}\Big)_l - \Big(\widehat{g_+^{2,n}(0)}\Big)_l\\ &+\Big(\widetilde{g_+^{4,n}(0)}\Big)_l - \Big(\widehat{g_+^{4,n}(0)}\Big)_l\Big].\end{aligned} \tag{3.16}$$

Recalling the definition of $g_\pm^{k,n}(w)$ $(k = 1, 2, 3, 4)$ in (2.10) and assumptions (A) and (B), we have

$$\begin{aligned}&\|g_\pm^{k,n}(\cdot)\|_{H^{m_0}} \lesssim 1, \qquad \|\partial_{ss} g_\pm^{l,n}(s)\|_{H^{m_0-4}} + \|\partial_s g_\pm^{l,n}(s)\|_{H^{m_0-2}} \lesssim 1,\\ &\|\partial_{ss} g_\pm^{m,n}(s)\|_{H^{m_0}} + \|\partial_s g_\pm^{m,n}(s)\|_{H^{m_0}} \lesssim 1, \qquad k = 1, 2, 3, 4, \quad l = 1, 3, \quad m = 2, 4.\end{aligned}$$

As a consequence of the standard Fourier interpolation and projection properties, using Parseval's identity and Holder's inequality, in view of the above facts and the bounds for $p_1(\tau)$, $p_2(\tau), q_1(\tau)$ in (2.9) and (2.13),

$$|p_1(\tau)| \lesssim \tau, \quad |p_2(\tau)| \lesssim \tau^2, \quad |q_1(\tau)| \lesssim \tau^2, \tag{3.17}$$

and $m_0 \geq 4$, we can bound the L^2 norm of $\eta_+^n(x)$ from (3.16) as

$$\begin{aligned}\|\eta_+^n(\cdot)\|_{L^2} \lesssim\ & \tau\Big(\|P_M\Big(g_+^{1,n}\Big(\frac{\tau}{2}\Big)\Big) - I_M\Big(g_+^{1,n}\Big(\frac{\tau}{2}\Big)\Big)\|_{L^2}\\ &+ \|P_M(g_+^{3,n}(0)) - I_M(g_+^{3,n}(0))\|_{L^2}\Big)\\ &+ \tau^2\|P_M(\partial_s g_+^{3,n}(0)) - I_M(\dot g_+^{3,n}(0))\|_{L^2}\\ &+ \tau^2\sum_{k=2,4}\|P_M(g_+^{k,n}(0)) - I_M(g_+^{k,n}(0))\|_{L^2}\\ \lesssim\ & \tau h^{m_0} + \tau^2\|P_M(\partial_s g_+^{3,n}(0)) - I_M(\dot g_+^{3,n}(0))\|_{L^2} + \tau^2 h^{m_0}\\ \lesssim\ & \tau(h^{m_0} + \tau^2) + \tau^2\|P_M(\partial_s g_+^{3,n}(0)) - I_M(\dot g_+^{3,n}(0))\|_{L^2}.\end{aligned} \tag{3.18}$$

According to the definition of $g_+^{3,n}(w)$ and $\dot g_+^{3,n}(w)$ in (2.10)–(2.11), we have

$$\begin{aligned}&\Big(\widetilde{\dot g_+^{3,n}(0)}\Big)_l - \Big(\widehat{\partial_s g_+^{3,n}(0)}\Big)_l\\ &= i(\mathcal{A}_*^\varepsilon)_l\Big[\Big(\widetilde{g_+^{3,n}(0)}\Big)_l - \Big(\widehat{g_+^{3,n}(0)}\Big)_l\Big] + i\left((\mathcal{A}_*^\varepsilon)_l - \mathcal{A}_l^\varepsilon\right)\Big(\widehat{g_+^{3,n}(0)}\Big)_l\\ &\quad + i\Pi_l^+\Big[\big(W^n\widetilde{(\mathcal{A}_*^\varepsilon\Phi_-^n)}\big)_l - \big(W^n\widehat{(\mathcal{A}^\varepsilon\Phi_-^n)}\big)_l\Big]\\ &+ \Pi_l^+\left[\Big(\widetilde{\dot W^n\Phi_-^n}\Big)_l - \Big(\widehat{\dot W^n\Phi_-^n}\Big)_l - i\left(\big(W^n\widetilde{(\Pi_-(W^n\Phi_-^n))}\big)_l - \big(W^n\widehat{(\Pi_-(W^n\Phi_-^n))}\big)_l\right)\right],\end{aligned}$$

where $W^n := W^n(0)$, $\dot{W}^n := \partial_s W^n(0)$. Noting the definition of $\mathcal{A}_*^\varepsilon$ in (2.27), it can be found that $\|(\mathcal{A}_*^\varepsilon)_l\|_{l^2} \le \frac{1}{\tau}$ and

$$\begin{aligned}\mathcal{A}_l^\varepsilon - (\mathcal{A}_*^\varepsilon)_l &= \left[\delta_l^- - \frac{\sin(\delta_l^-\tau)}{\tau}\right] I_2 \\ &= \left[\delta_l^- - \frac{\delta_l^-\tau + \frac{1}{2}(\delta_l^-\tau)^2\sin(\theta\delta_l^-\tau)}{\tau}\right] I_2 = \frac{\tau(\delta_l^-)^2\sin(\theta\delta_l^-\tau)}{2} I_2\end{aligned}$$

with $\delta_l^- = (\delta_l - 1)/\varepsilon^2 = \mu_l^2/(1+\delta_l) \in (0, \mu_l^2)$, $\theta \in (0,1)$. Then, with standard Fourier interpolation and projection properties and Parseval's identity, we obtain

$$\begin{aligned}&\|P_M(\partial_s g_+^{3,n}(0)) - I_M(\dot{g}_+^{3,n}(0))\|_{L^2} \\ &\quad\lesssim \frac{h^{m_0}}{\tau} + \tau\|P_M(g_+^{3,n}(0))\|_{H^4} + \|I_M(W^n(\mathcal{A}_*^\varepsilon\Phi_-^n)) - P_M(W^n(\mathcal{A}^\varepsilon\Phi_-^n))\|_{L^2} + h^{m_0} \\ &\quad\lesssim \frac{h^{m_0}}{\tau} + \tau + h^{m_0} + \|I_M(W^n(\mathcal{A}_*^\varepsilon\Phi_-^n)) - I_M(W^n(\mathcal{A}^\varepsilon\Phi_-^n))\|_{L^2}\end{aligned}$$

with

$$\begin{aligned}&\|I_M(W^n(\mathcal{A}_*^\varepsilon\Phi_-^n)) - I_M(W^n(\mathcal{A}^\varepsilon\Phi_-^n))\|_{L^2}^2 \\ &\quad= h\sum_{j=0}^{M-1}\left|W_j^n\left[\left(\mathcal{A}_*^\varepsilon\Phi_-^n\right)(x_j) - \left(\mathcal{A}^\varepsilon\Phi_-^n\right)(x_j)\right]\right|^2 \\ &\quad\lesssim \|I_M(\mathcal{A}_*^\varepsilon\Phi_-^n) - I_M(\mathcal{A}^\varepsilon\Phi_-^n)\|_{L^2}^2 \lesssim h^{2m_0} + \|P_M(\mathcal{A}_*^\varepsilon\Phi_-^n) - P_M(\mathcal{A}^\varepsilon\Phi_-^n)\|_{L^2}^2 \\ &\quad\lesssim h^{2m_0} + \sum_{l=-M/2}^{M/2-1}\left|((\mathcal{A}_*^\varepsilon)_l - \mathcal{A}_l^\varepsilon)\Pi_l^-(\widehat{\Phi(t_n)})_l\right|^2 \lesssim h^{2m_0} + \tau^2\|\Phi(t_n)\|_{H^4}^2 \lesssim h^{2m_0} + \tau^2,\end{aligned}$$

where $(\mathcal{A}_*^\varepsilon\Phi_-^n)(x) = \sum_{l\in\mathbb{Z}}(\mathcal{A}_*^\varepsilon)_l\Pi_l^-(\widehat{\Phi(t_n)})_l e^{i\mu_l(x-a)}$, $(\mathcal{A}^\varepsilon\Phi_-^n)(x) = \sum_{l\in\mathbb{Z}}\mathcal{A}_l^\varepsilon\Pi_l^-(\widehat{\Phi(t_n)})_l e^{i\mu_l(x-a)}$.

Thus, we get

$$\|\eta_+^n(\cdot)\|_{L^2} \lesssim \tau(h^{m_0} + \tau^2) + \tau^2(h^{m_0}/\tau + \tau + h^{m_0}) \lesssim \tau(h^{m_0} + \tau^2).$$

Under assumptions (A) and (B), combining the above estimates and the estimate for $\|\mathcal{R}_1\|_{L^\infty([0,\tau];(L^2)^2)}$ in (3.14), using Holder's inequality and Parseval's identity, from (3.15) we get

(3.19)

$$\begin{aligned}\|\xi_+^n(\cdot)\|_{L^2} &\lesssim \tau\|(W^n(s)\Phi(t_n+s,\cdot) - (W^n\Phi^{n,1})(s,\cdot)\|_{L^\infty([0,\tau];(L^2)^2)} \\ &\quad+ \tau^3\sum_{k=1,3}\|\partial_{ss}g_+^{k,n}(s)\|_{L^\infty([0,\tau];(L^2)^2)} \\ &\quad+ \tau^3\sum_{k=2,4}\left(\|g_+^{k,n}(s)\|_{L^\infty([0,\tau];(H^2)^2)} + \|\partial_s g_+^{k,n}(s)\|_{L^\infty([0,\tau];(L^2)^2)}\right) + \|\eta_+^n(\cdot)\|_{L^2} \\ &\lesssim \tau(h^{m_0} + \tau^2).\end{aligned}$$

Estimates on ξ_-^n can be derived similarly as in (3.19). Therefore, we conclude that (3.9) holds true. ∎

Proof of Lemma 3.3. According to the definitions of $\widetilde{\left(F_{\pm}^{n}\right)_l}$ in (3.7) and the bounds for coefficients (3.17), we have for $l=-M/2,-M/2+1,\ldots,M/2$,

$$\left|\widetilde{(F_{\pm}^{n})_l}\right| \lesssim \tau\left(\left|\widetilde{\left(G_{\pm}^{1,n}\right)_l}\right| + \left|\widetilde{\left(G_{\pm}^{3,n}\right)_l}\right|\right) + \tau^2\left(\left|\widetilde{\left(\dot{G}_{\pm}^{3,n}\right)_l}\right| + \left|\widetilde{\left(G_{\pm}^{2,n}\right)_l}\right| + \left|\widetilde{\left(G_{\pm}^{4,n}\right)_l}\right|\right).$$

The Parseval's identity implies

$$\|F_{\pm}^{n}\|_{L^2} \lesssim \tau\left(\|G_{\pm}^{1,n}\|_{L^2} + \|G_{\pm}^{3,n}\|_{L^2}\right) + \tau^2\left(\|\dot{G}_{\pm}^{3,n}\|_{L^2} + \|G_{\pm}^{2,n}\|_{L^2} + \|G_{\pm}^{4,n}\|_{L^2}\right).$$

Then it is enough to estimate the bounds for $\|G_{\pm}^{k,n}\|_{L^2}$ and $\|\dot{G}_{\pm}^{3,n}\|_{L^2}, k=1,2,3,4$.

Let us first analyze $G_{+}^{1,n}$. Comparing (2.27) with (2.10)–(2.11), applying $\|\Pi_{\pm}^{l}\|_{l^2}\le 1$, the triangle inequality, and the Parseval's identity, we can obtain

(3.20)
$$\begin{aligned}\|G_{+}^{1,n}(\cdot)\|_{L^2}^2 \lesssim{}& \|I_M(W^{n+\frac{1}{2}}(e^{-i\mathcal{A}^{\varepsilon}\tau/2}\Pi_{+}\Phi(t_n))) - I_M(W^{n+\frac{1}{2}}(e^{-i\mathcal{A}^{\varepsilon}\tau/2}\Pi_{+}\Phi^n))\|_{L^2}^2\\ &+\tau^2\|I_M(W^{n+\frac{1}{2}}(\Pi_{+}(W^n(\Pi_{+}\Phi(t_n))))) - I_M(W^{n+\frac{1}{2}}(\Pi_{+}(W^n(\Pi_{+}\Phi^n))))\|_{L^2}^2,\end{aligned}$$

Recalling assumptions (A) and (B), and using the Parseval's identity several times, we have

$$\begin{aligned}&\|I_M(W^{n+\frac{1}{2}}(e^{-i\mathcal{A}^{\varepsilon}\tau/2}\Pi_{+}\Phi(t_n))) - I_M(W^{n+\frac{1}{2}}(e^{-i\mathcal{A}^{\varepsilon}\tau/2}\Pi_{+}\Phi^n))\|_{L^2}^2\\ &\quad= h\sum_{j=0}^{M-1}\left|W_j^{n+\frac{1}{2}}\left[\left(e^{-i\mathcal{A}^{\varepsilon}\tau/2}\Pi_{+}\Phi(t_n)\right)(x_j) - \left(e^{-i\mathcal{A}^{\varepsilon}\tau/2}\Pi_{+}\Phi^n\right)_j\right]\right|^2\\ &\quad\lesssim h\sum_{j=0}^{M-1}\left|\left(e^{-i\mathcal{A}^{\varepsilon}\tau/2}\Pi_{+}\Phi(t_n)\right)(x_j) - \left(e^{-i\mathcal{A}^{\varepsilon}\tau/2}\Pi_{+}\Phi^n\right)_j\right|^2\\ &\quad\lesssim \|P_M(e^{-i\mathcal{A}^{\varepsilon}\tau/2}\Pi_{+}\Phi(t_n)) - I_M(e^{-i\mathcal{A}^{\varepsilon}\tau/2}\Pi_{+}\Phi^n)\|_{L^2}^2 + h^{2m_0}\\ &\quad\lesssim \sum_{l=-M/2}^{M/2-1}\left|e^{-i\mathcal{A}_l^{\varepsilon}\tau/2}\Pi_l^{+}\widehat{(\Phi(t_n))}_l - e^{-i\mathcal{A}_l^{\varepsilon}\tau/2}\Pi_l^{+}\widetilde{(\Phi^n)}_l\right|^2 + h^{2m_0}\\ &\quad\lesssim \sum_{l=-M/2}^{M/2-1}\left|\widehat{(\Phi(t_n))}_l - \widetilde{(\Phi^n)}_l\right|^2 + h^{2m_0} \lesssim \|P_M(\Phi(t_n)) - I_M(\Phi^n)\|_{L^2}^2 + h^{2m_0},\end{aligned}$$

where

$$\begin{cases}\left(e^{-i\mathcal{A}^{\varepsilon}\tau/2}\Pi_{+}\Phi(t_n)\right)(x) = \sum_{l\in\mathbb{Z}} e^{-i\mathcal{A}_l^{\varepsilon}\tau/2}\Pi_l^{+}\widehat{(\Phi(t_n))}_l e^{i\mu_l(x-a)},\\ \left(e^{-i\mathcal{A}^{\varepsilon}\tau/2}\Pi_{+}\Phi^n\right)_j = \sum_{l=-M/2}^{M/2-1} e^{-i\mathcal{A}_l^{\varepsilon}\tau/2}\Pi_l^{+}\widetilde{(\Phi^n)}_l e^{i\mu_l(x_j-a)}.\end{cases}$$

By a similar procedure, we can obtain

$$\begin{aligned}&\|I_M(W^{n+\frac{1}{2}}(\Pi_{+}(W^n(\Pi_{+}\Phi(t_n))))) - I_M(W^{n+\frac{1}{2}}(\Pi_{+}(W^n(\Pi_{+}\Phi^n))))\|_{L^2}^2\\ &\quad\lesssim h^{2m_0} + \|P_M(\Phi(t_n)) - I_M(\Phi^n)\|_{L^2}^2.\end{aligned}$$

Therefore, we have $\|G_+^{1,n}(\cdot)\|_{L^2} \lesssim h^{m_0} + \|\mathbf{e}^n(\cdot)\|_{L^2}$. We can similarly prove that

$$\begin{aligned}
&\|G_+^{k,n}(\cdot)\|_{L^2} \lesssim h^{m_0} + \|\mathbf{e}^n(\cdot)\|_{L^2}, \qquad k = 2,3,4,\\
&\|\dot{G}_+^{3,n}(\cdot)\|_{L^2} \lesssim \frac{1}{\tau}\|G_+^{3,n}(\cdot)\|_{L^2} + \|I_M(W^n(\Pi_-(W^n(\Pi_-\Phi(t_n)))))\\
&\qquad\qquad - I_M(W^n(\Pi_-(W^n(\Pi_-\Phi^n))))\|_{L^2}\\
&\qquad\qquad + \|I_M(W^n(\mathcal{A}_*^\varepsilon\Pi_-\Phi(t_n))) - I_M(W^n(\mathcal{A}_*^\varepsilon\Pi_-\Phi^n))\|_{L^2}\\
&\qquad\qquad + \|I_M(\dot{W}^n(\Pi_-\Phi(t_n))) - I_M(\dot{W}^n(\Pi_-\Phi^n))\|_{L^2} \lesssim \frac{1}{\tau}\left(h^{m_0} + \|\mathbf{e}^n(\cdot)\|_{L^2}\right).
\end{aligned}$$

Thus, (3.10) holds true for F_+^n. F_-^n can be estimated in the same way and the details are omitted for brevity. ∎

Remark 3.1. If the filter $\mathcal{A}_*^\varepsilon$ is not applied, the estimates for the local errors $\|\xi_+\|_{L^2}$, i.e., (3.19), do not change for smooth solutions although the proof differs a little bit. However, when estimating $\|\mathbf{e}^n(\cdot)\|_{L^2}$ via controlling the error term $\|\dot{G}_+^{3,n}(\cdot)\|_{L^2}$, $\|\mathbf{e}^n(\cdot)\|_{H^2}$ is involved, since we will have $\|I_M(W^n(\mathcal{A}^\varepsilon\Pi_-\Phi(t_n))) - I_M(W^n(\mathcal{A}^\varepsilon\Pi_-\Phi^n))\|_{L^2}$ instead of $\|I_M(W^n(\mathcal{A}_*^\varepsilon\Pi_-\Phi(t_n))) - I_M(W^n(\mathcal{A}_*^\varepsilon\Pi_-\Phi^n))\|_{L^2}$. This would require a certain CFL-type condition $\tau \lesssim h^2$ to complete the estimates on $\|\mathbf{e}^n(\cdot)\|_{L^2}$.

Proof of Theorem 3.1. Taking the l^2 norm of the vectors on (3.5), we have

$$\begin{aligned}
\left|\widetilde{(\mathbf{e}^{n+1})}_l\right|^2 &= \left|e^{-i\mathcal{T}_l\tau/\varepsilon^2}\widetilde{(\mathbf{e}^n)}_l + \widetilde{(\chi^n)}_l\right|^2 = \left|\widetilde{(\mathbf{e}^n)}_l\right|^2 + \left|\widetilde{(\chi^n)}_l\right|^2\\
&\quad + 2\mathrm{Re}\left((e^{-i\mathcal{T}_l\tau/\varepsilon^2}\widetilde{(\mathbf{e}^n)}_l)^*\widetilde{(\chi^n)}_l\right),
\end{aligned}$$

which gives (with Young's inequality)

$$\left|\widetilde{(\mathbf{e}^{n+1})}_l\right|^2 - \left|\widetilde{(\mathbf{e}^n)}_l\right|^2 \lesssim \tau\left|\widetilde{(\mathbf{e}^n)}_l\right|^2 + \frac{1}{\tau}\left|\widetilde{(\chi^n)}_l\right|^2, \qquad l = -\frac{M}{2},\ldots,\frac{M}{2}-1, \tag{3.21}$$

where $\chi^n(x) = \sum_{l=-M/2}^{M/2-1}\widetilde{(\chi^n)}_l e^{i\mu_l(x-a)} \in Y_M$ is defined as

$$\widetilde{(\chi^n)}_l = e^{-i\tau/\varepsilon^2}\left(\widehat{(\xi_+^n)}_l + \widetilde{(F_+^n)}_l\right) + e^{i\tau/\varepsilon^2}\left(\widehat{(\xi_-^n)}_l + \widetilde{(F_-^n)}_l\right), \quad l = -\frac{M}{2},\ldots,\frac{M}{2}-1.$$

Using Parseval's identity, Lemma 3.2, and Lemma 3.3, we get

$$\|\chi^n\|_{L^2}^2 \lesssim \|\xi_+^n\|_{L^2}^2 + \|\xi_-^n\|_{L^2}^2 + \|F_+^n\|_{L^2}^2 + \|F_-^n\|_{L^2}^2 \lesssim \tau^2\|\mathbf{e}^n\|_{L^2}^2 + \tau^2(h^{m_0}+\tau^2)^2. \tag{3.22}$$

Similarly, let us sum up (3.21) for l and utilize Parseval's identity and (3.22); we can obtain

$$\begin{aligned}
\|\mathbf{e}^{n+1}\|_{L^2}^2 - \|\mathbf{e}^n\|_{L^2}^2 &\lesssim \tau\|\mathbf{e}^n\|_{L^2}^2 + \frac{1}{\tau}\|\chi^n\|_{L^2}^2\\
&\lesssim \tau\|\mathbf{e}^n\|_{L^2}^2 + \tau(h^{m_0}+\tau^2)^2, \quad 0 \le n \le \frac{T}{\tau} - 1.
\end{aligned} \tag{3.23}$$

Summing up (3.23) for n, we get

$$\|\mathbf{e}^n(\cdot)\|_{L^2}^2 - \|\mathbf{e}^0(\cdot)\|_{L^2}^2 \lesssim \tau\sum_{m=0}^{n-1}\|\mathbf{e}^m(\cdot)\|_{L^2}^2 + n\tau\left(h^{m_0}+\tau^2\right)^2, \quad 0 < n \le \frac{T}{\tau}. \tag{3.24}$$

Since $\|\mathbf{e}^0(\cdot)\|_{L^2} = \|P_M(\Phi_0) - I_M(\Phi_0)\| \lesssim h^{m_0}$, the discrete Gronwall's inequality will lead to the conclusion when $0 < \tau \le \tau_0 \le 1$ and $0 < h \le h_0 \le 1$ sufficiently small,

$$\|\mathbf{e}^n(\cdot)\|_{L^2} \lesssim h^{m_0} + \tau^2, \quad 0 \le n \le \frac{T}{\tau}. \tag{3.25}$$

Together with (3.2), we conclude that (3.1) holds. ∎

4. Numerical results. In this section, we present numerical results to demonstrate the performance of our NPI methods. We solve the Dirac equation (2.1) in one dimension, using the first-, second-, and third-order NPI methods, on a bounded interval $\Omega = (-16, 16)$ with periodic boundary conditions and the electromagnetic potentials

$$A_1(t,x) = \frac{(x+1)^2}{1+x^2}, \quad V(t,x) = \frac{1-x}{1+x^2}, \qquad x \in \mathbb{R}, \quad t \ge 0, \tag{4.1}$$

and the initial data $\Phi_0(x) = (\phi_1(x),\ \phi_2(x))^T$ with $\phi_1(x) = e^{-x^2/2}, \phi_2(x) = e^{-(x-1)^2/2}$.

Denote $\Phi^n_{h,\tau}$ as the numerical solution obtained by the NPI method with mesh size h and time step τ, and the "reference" solution $\Phi(t,x) = (\phi_1(t,x), \phi_2(t,x))$ is obtained numerically by the third-order NPI method with very fine mesh $h = 1/32$ and time step $\tau = 1 \times 10^{-4}$. To quantify the convergence, we use the numerical error function $e_{h,\tau}(t_n) = \|\Phi^n_{h,\tau} - \Phi(t_n,\cdot)\|_{l^2} = \sqrt{h\sum_{j=0}^{M-1}|(\Phi^n_{h,\tau})_j - \Phi(t_n,x_j)|^2}$.

In Tables 1 and 2, we list the spatial and temporal errors for the second-order NPI method at $T = 1$, i.e., $e_{h,\tau}(t = 1.0)$, respectively. τ is fixed to be 10^{-6} for the spatial error analysis, and h is fixed to be $1/8$ when testing the temporal error. To a clear visual perception of the uniformly accurate property and the convergence rate in time of the NPI method, we plot the temporal errors of the first- to third-order NPI methods in Figure 1. From Tables 1–2 and Figure 1, we can make the following observations:

(i) In space, the NPI method is uniformly spectrally accurate for all $\varepsilon \in (0, 1]$ (cf. Table 1).

(ii) In time, the NPI method is also uniformly accurate for all $\varepsilon \in (0, 1]$ and it can achieve at least uniform $O(\tau), O(\tau^2)$ and $O(\tau^3)$ accuracies with different schemes (cf. Table 2 and Figure 1).

Therefore, the NPI method is uniformly accurate for all $\varepsilon \in (0, 1]$ without any restriction on the time or space step sizes, i.e., the mesh strategy (or ε-scalability) is $\tau = O(1)$ and $h = O(1)$.

We also compare the efficiency of the first-, second-, and third-order NPI methods for $\varepsilon = 1$ with the same mesh size $h = 1/8$. For schemes with different orders, roughly speaking, after one iteration, the terms to be evaluated at each time step will double (two eigenspaces of free Dirac operator to separate the oscillation) with some terms involving an extra FFT operation (for $\mathcal{A}^\varepsilon$). As a result, the computational costs

TABLE 1
Spatial error analysis of the second-order NPI method for the Dirac equation in one dimension.

$e_{h,\tau}(1.0)$	$h_0 = 2$	$h_0/2$	$h_0/2^2$	$h_0/2^3$	$h_0/2^4$
$\varepsilon_0 = 1$	1.29	4.38E-1	3.63E-2	7.59E-5	2.64E-10
$\varepsilon_0/2$	8.60E-1	2.22E-1	5.23E-3	4.75E-6	1.77E-10
$\varepsilon_0/2^2$	5.82E-1	1.40E-1	1.49E-3	1.20E-6	1.71E-10
$\varepsilon_0/2^3$	5.46E-1	9.62E-2	9.45E-4	6.58E-7	1.07E-10
$\varepsilon_0/2^4$	5.67E-1	1.04E-1	8.68E-4	4.30E-7	1.50E-10

TABLE 2

Temporal error analysis of the second-order NPI method for the Dirac equation in one dimension. The convergence order is calculated as $\log_4(e_{h,4\tau}/e_{h,\tau})$. $e^{\infty}_{\tau,h}$ *is the maximum error in each column.*

$e_{h,\tau}(1.0)$	$\tau_0 = 0.2$	$\tau_0/2^2$	$\tau_0/2^4$	$\tau_0/2^6$	$\tau_0/2^8$	$\tau_0/2^{10}$	$\tau_0/2^{12}$
$\varepsilon_0 = 1$	7.84E-02	4.92E-03	3.08E-04	1.93E-05	1.20E-06	7.53E-08	4.71E-09
order	-	2.00	2.00	2.00	2.00	2.00	2.00
$\varepsilon_0/2$	6.17E-02	4.02E-03	2.52E-04	1.58E-05	9.85E-07	6.16E-08	3.85E-09
order	-	1.97	2.00	2.00	2.00	2.00	2.00
$\varepsilon_0/2^2$	4.89E-02	3.23E-03	2.08E-04	1.30E-05	8.12E-07	5.07E-08	3.17E-09
order	-	1.96	1.98	2.00	2.00	2.00	2.00
$\varepsilon_0/2^3$	1.82E-02	2.47E-03	1.80E-04	1.14E-05	7.15E-07	4.47E-08	2.79E-09
order	-	1.44	1.89	1.99	2.00	2.00	2.00
$\varepsilon_0/2^4$	1.56E-02	1.08E-03	1.44E-04	1.07E-05	6.73E-07	4.22E-08	2.64E-09
order	-	1.93	1.45	1.88	1.99	2.00	2.00
$\varepsilon_0/2^5$	1.51E-02	9.41E-04	6.66E-05	8.81E-06	6.58E-07	4.13E-08	2.60E-09
order	-	2.00	1.91	1.46	1.87	2.00	2.00
$\varepsilon_0/2^6$	1.50E-02	9.21E-04	5.82E-05	4.13E-06	5.50E-07	4.10E-08	2.57E-09
order	-	2.01	1.99	1.91	1.45	1.87	2.00
$\varepsilon_0/2^7$	1.50E-02	9.15E-04	5.72E-05	3.63E-06	2.57E-07	3.45E-08	2.56E-09
order	-	2.02	2.00	1.99	1.91	1.45	1.88
$\varepsilon_0/2^8$	1.49E-02	9.14E-04	5.69E-05	3.57E-06	2.26E-07	1.61E-08	2.16E-09
order	-	2.02	2.00	2.00	1.99	1.91	1.45
$\varepsilon_0/2^9$	1.49E-02	9.13E-04	5.69E-05	3.55E-06	2.23E-07	1.41E-08	1.01E-09
order	-	2.02	2.00	2.00	2.00	1.99	1.91
$e^{\infty}_{\tau,h}$	7.84E-02	4.92E-03	3.08E-04	1.93E-05	1.20E-06	7.53E-08	4.71E-09
Order	-	2.00	2.00	2.00	2.00	2.00	2.00

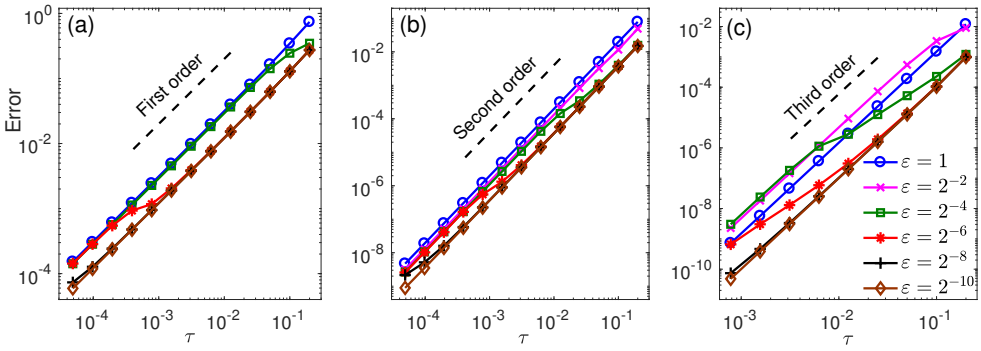

FIG. 1. *Temporal errors of the* (a) *first-,* (b) *second-, and* (c) *third-order NPI methods for the Dirac equation in one dimension.*

TABLE 3

Numerical comparison of the first-, second-, and third-order NPI methods with respect to the accuracy and efficiency.

$e_{h,\tau}(1.0)$ and CPU time	First-order NPI	Second-order NPI	Third-order NPI
$\tau = 0.01$	3.15E-2 (0.043s)	1.97E-4 (0.14s)	1.49E-6 (0.21s)
$\tau = 0.001$	3.12E-3 (0.24s)	1.97E-6 (0.75s)	1.49E-9 (1.74s)

at each time step will roughly double if the order of the scheme increases by one. As shown in Table 3, the CPU time doubles or triples when the convergence order

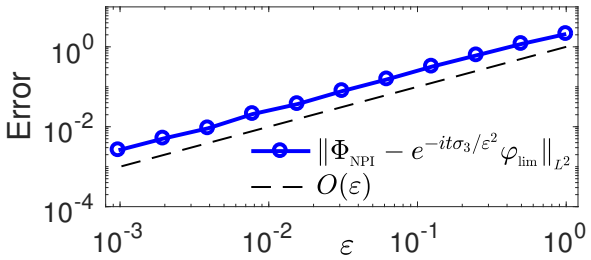

FIG. 2. *Convergence order of the (third-order) NPI scheme to the Schrödinger-type limit system.*

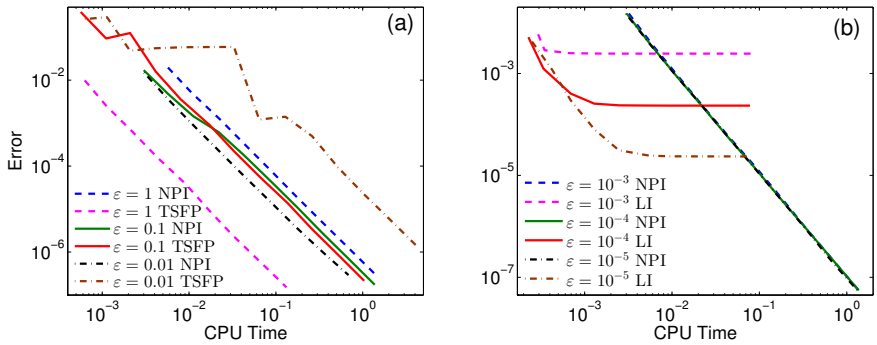

FIG. 3. *Numerical comparison of the second-order NPI method with* (a) *TSFP for* $\varepsilon = 1, 0.1, 0.01$, (b) *LI for* $\varepsilon = 10^{-3}, 10^{-4}, 10^{-5}$ *with respect to the accuracy and efficiency.*

increases by one, and it costs nearly the same time for the first-order method with $\tau = 0.001$ and the third-order method with $\tau = 0.01$, while the latter one is much more accurate. Therefore, it is feasible to apply high-order schemes when $\varepsilon = O(1)$.

Furthermore, we investigate the convergency of the NPI schemes toward the limit system [5] of (2.1) as $\varepsilon \to 0^+$, i.e., $\phi(t,x) \to e^{-it\sigma_3/\varepsilon^2}\varphi(t,x)$, where $\varphi(t,x)$ satisfies $\varphi(0,x) = \Phi_0(x)$ and

$$i\partial_t\varphi = -\frac{1}{2}\sigma_3\Delta\varphi + V(t,x)\varphi, \qquad x \in \mathbb{R}, \quad t > 0. \tag{4.2}$$

Figure 2 shows the error between $\Phi_{\rm NPI}$ and $e^{-it\sigma_3/\varepsilon^2}\varphi_{\rm lim}$, where $\Phi_{\rm NPI}$ is obtained by the (third-order) NPI method with time step $\tau = 10^{-4}$ and $\varphi_{\rm lim}$ is obtained by the time-splitting Fourier pseudospectral (TSFP) method [2] with time step $\tau = 10^{-6}$ ($h = 1/8, t = 1.0$). As shown in Figure 2, the (third-order) NPI scheme converges to the Schrödinger-type limit system at order $O(\varepsilon)$.

In the regime $\varepsilon \ll 1$, a limit integrator (LI) for the Dirac equation can be designed by solving the Schrödinger-type limit system (4.2) using TSFP; for $\varepsilon = O(1)$, classical solvers for the Dirac equation have demonstrated their efficiencies [4]. Here we compare the efficiency of the NPI method with that of the classical TSFP method (for the Dirac equation) [4] and the LI for different ε, and the temporal discretizations involved are all second-order accurate, with mesh size $h = 1/8$ (fine enough for Fourier spectral methods) and final time $T = 1$. The CPU times and the errors at $t = 1.0$ for different methods are shown in Figure 3, and we find the following: (i) In the classical regime (i.e., $\varepsilon = 1$), TSFP is about 10 times faster than NPI. However, as ε becomes smaller, the efficiency of TSFP soon decreases since a smaller time step

is required to resolve the temporal oscillation of the solution. It is observed that NPI is more efficient than TSFP when $\varepsilon < 0.1$. (ii) In the nonrelativistic limit regime (i.e., $\varepsilon \ll 1$), LI is about 15 times faster than NPI till an accuracy of $O(\varepsilon)$, due to the fact that the limit system is an $O(\varepsilon)$ approximation to the Dirac equation. Figure 3 depicts that the efficiency of NPI is almost uniform w.r.t. ε, while the performances of TSFP and LI are quite different for varying ε.

5. Conclusion. We have proposed and rigorously analyzed a class of uniformly accurate NPIs for the Dirac equation with a dimensionless parameter $\varepsilon \in (0, 1]$, which is inversely proportional to the speed of light. Our method utilizes a nested Picard iterative idea associated with exponential wave integrators for the integral form of the Dirac equation. It is simple and efficient and does not rely on preknowledge of the solution. More importantly, the NPI method could easily achieve uniform high-order convergence in time. Rigorous error analysis has been established for the second-order NPI method and it showed that the method is uniformly accurate in space with spectral accuracy and in time with quadratic convergence rate for all $\varepsilon \in (0, 1]$. We also provided numerical results to validate the uniformly accurate properties and the convergence rates of the first-, second-, and third-order NPI methods. The NPI approach could be employed to develop uniformly accurate schemes for other systems, which will be the subject of future studies.

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