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IMPROVED UNIFORM ERROR BOUNDS ON TIME-SPLITTING METHODS FOR THE LONG-TIME DYNAMICS OF THE DIRAC EQUATION WITH SMALL POTENTIALS*

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Abstract. We establish improved uniform error bounds on time-splitting methods for the long-time dynamics of the Dirac equation with small electromagnetic potentials characterized by a dimensionless parameter $\varepsilon \in (0, 1]$ representing the amplitude of the potentials. We begin with a semidiscretization of the Dirac equation in time by a time-splitting method, followed by a full-discretization in space by with the Fourier pseudospectral method in space. By employing the unitary flow property of the second-order time-splitting method for the Dirac equation, we prove uniform error bounds for $\varepsilon \in (0, 1]$ at $C(t)\tau^2$ and $C(t)(h^m + \tau^2)$ for the semidiscretization and full-discretization, respectively, for any time $t \in [0, T_\varepsilon]$ with $T_\varepsilon = T/\varepsilon$ and $T > 0$. In the expressions, τ is the time step, h is the mesh size, $m \geq 2$ depends on the regularity of the solution, and $C(t) = C_0 + C_1\varepsilon t \leq C_0 + C_1 T$ grows at most linearly with respect to t with $C_0 \geq 0$ and $C_1 > 0$ two constants independent of t, h, τ, and ε. Then by adopting the regularity compensation oscillation technique, which controls the high frequency modes by the regularity of the solution and low frequency modes by phase cancellation and energy method, we establish improved uniform error bounds at $O(\varepsilon\tau^2)$ and $O(h^m + \varepsilon\tau^2)$ for the semidiscretization and full-discretization, respectively, up to the long-time T_ε. Numerical results are reported to confirm our error bounds and to demonstrate that they are sharp. Comparisons on the accuracy of different time discretizations for the Dirac equation are also provided.

Key words. Dirac equation, long-time dynamics, time-splitting methods, improved uniform error bound, regularity compensation oscillation (RCO)

MSC codes. 35Q41, 65M70, 65N35, 81Q05

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1. Introduction.

In this paper, we consider the Dirac equation in one or two dimensions (1D or 2D), which can be represented in the two-component form with wave function $\Phi := \Phi(t, \mathbf{x}) = (\phi_1(t, \mathbf{x}), \phi_2(t, \mathbf{x}))^T \in \mathbb{C}^2$ as [18, 19, 38]

$$i\partial_t \Phi = \left(-i \sum_{j=1}^{d} \sigma_j \partial_j + \sigma_3 \right) \Phi + \varepsilon \left(V(\mathbf{x}) I_2 - \sum_{j=1}^{d} A_j(\mathbf{x}) \sigma_j \right) \Phi, \quad \mathbf{x} \in \Omega, \tag{1.1}$$

where $\Omega \subset \mathbb{R}^d$ $(d = 1, 2)$ is a bounded domain imposed with the periodic boundary condition, which is widely used in the study of relativistic quantum mechanics and/or graphene [13, 14]. Here, $i = \sqrt{-1}$, t is time, $\mathbf{x} = (x_1, \ldots, x_d)^T \in \mathbb{R}^d$, $\partial_j = \frac{\partial}{\partial x_j}$ $(j = 1, \ldots, d)$, $\varepsilon \in (0, 1]$ is a dimensionless parameter representing the amplitude of the potential, and $V(\mathbf{x})$ and $A_j(\mathbf{x})$ are given real-valued time-independent electric and

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magnetic potentials, respectively, which are independent of ε. I_2 is the 2×2 identity matrix, and $\sigma_1, \sigma_2, \sigma_3$ are the Pauli matrices defined as

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

In order to study the dynamics of the Dirac equation (1.1), the initial condition is taken as

$$\Phi(t = 0, \mathbf{x}) = \Phi_0(\mathbf{x}), \quad \mathbf{x} \in \overline{\Omega}. \tag{1.2}$$

The Dirac equation (1.1) with (1.2) is dispersive and time symmetric and conserves the total probability [4]

$$\|\Phi(t, \cdot)\|^2 := \int_\Omega |\Phi(t, \mathbf{x})|^2 d\mathbf{x} = \int_\Omega \sum_{j=1}^{2} |\phi_j(t, \mathbf{x})|^2 d\mathbf{x} \equiv \|\Phi(0, \cdot)\|^2 =: \|\Phi_0\|^2, \quad t \geq 0.$$

Since the electromagnetic potentials are both time independent, the energy is also conserved, i. e.,

$$\begin{aligned} E(\Phi(t, \cdot)) &:= \int_\Omega \left(-i \sum_{j=1}^{d} \Phi^* \sigma_j \partial_j \Phi + \Phi^* \sigma_3 \Phi + \varepsilon \left(V(\mathbf{x}) |\Phi|^2 - \sum_{j=1}^{d} A_j(\mathbf{x}) \Phi^* \sigma_j \Phi \right) \right) d\mathbf{x} \\ &\equiv E(\Phi(0, \cdot)) =: E(\Phi_0), \quad t \geq 0, \end{aligned}$$

where $\bar{f}$ denotes the complex conjugate of f and $\Phi^* = \bar{\Phi}^T$.

For the Dirac equation (1.1) with $\varepsilon = 1$, i.e., with $O(1)$-electromagnetic potentials, there are comprehensive analytical and numerical results in the literature. Along the analytical front, for the existence and multiplicity of bound states and/or standing wave solutions, we refer the reader to [22, 27, 29] and references therein. In the numerical aspect, different numerical methods have been proposed, such as the finite difference time domain (FDTD) methods [4, 33], the exponential wave integrator Fourier pseudospectral (EWI-FP) method [4, 5], and the time-splitting Fourier pseudospectral (TSFP) method [7, 10]. Error bounds for these numerical methods have been established for $t \in [0, T]$ with $T > 0$ finite and fixed, i.e., finite-time dynamics, by the energy method. For more details related to the numerical schemes, we refer the reader to [12, 25, 28, 30, 35] and references therein.

Recently, much effort has been devoted to the analysis of different temporal and spatial discretizations for the long-time dynamics of the Dirac equation (1.1) with small electromagnetic potentials, i.e., the dynamics up to the time at $T_\varepsilon := T/\varepsilon$ with $T > 0$ for $\varepsilon \in (0, 1]$, especially when $0 < \varepsilon \ll 1$. The key issue in the analysis is to establish error bounds which depend explicitly on the mesh size h and time step τ as well as the small parameter ε. By adopting the energy method with the help of the discrete Grönwall's inequality, the following error bound was obtained for the second-order FDTD method [23]:

$$\|\Phi(t_n, \cdot) - \Phi^n\|_{l^2} \leq \widetilde{C}(t_n) \left(\frac{h^2}{\varepsilon} + \frac{\tau^2}{\varepsilon} \right), \quad 0 \leq n \leq \frac{T/\varepsilon}{\tau}, \tag{1.3}$$

where $t_n = n\tau$ for $n \geq 0$, Φ^n is the numerical approximation of $\Phi(t_n, x)$ by the FDTD method, and the constant in front of the error bound $\widetilde{C}(t)$ could be growing exponentially with respect to t for $t \in [0, T_\varepsilon]$, i.e.,

$$\widetilde{C}(t) \leq \widetilde{C}_0 e^{\varepsilon \widetilde{C}_1 t} \leq \widetilde{C}_0 e^{\widetilde{C}_1 T}, \qquad 0 \leq t \leq T_\varepsilon = \frac{T}{\varepsilon}, \tag{1.4}$$

with $\widetilde{C}_0$ and $\widetilde{C}_1$ two positive constants independent of h, τ, n, and ε. This suggests that the ε-resolution (or mesh strategy) of the FDTD method for the long-time dynamics, up to the time at $T_\varepsilon = T/\varepsilon$, of the Dirac equation (1.1) with small electromagnetic potentials has to be taken as [23]

$$h = O(\varepsilon^{1/2}), \qquad \tau = O(\varepsilon^{1/2}), \qquad 0 < \varepsilon \leq 1. \tag{1.5}$$

In addition, if the second-order finite difference spatial discretization is replaced by the Fourier pseudospectral method, i.e., the FDFP method, the error bound in (1.3) is improved to $C(t_n)(h^m + \tau^2/\varepsilon)$ with $m \geq 2$ depending on the regularity of the solution [23], and thus the ε-resolution of the FDFP method is improved to $h = O(1)$ and $\tau = O(\varepsilon^{1/2})$ [23]. Very recently, similar to the proof for the FDTD and FDFP methods, by adopting the energy method with the help of the discrete Grönwall's inequality, for the EWI-FP method as well as the TSFP method, the error bound in (1.3) is further improved to [4, 24]

$$\|\Phi(t_n, \cdot) - I_h \Phi^n\|_{L^2} \leq C(t_n)(h^m + \tau^2), \quad 0 \leq n \leq \frac{T/\varepsilon}{\tau}, \tag{1.6}$$

where Φ^n is the numerical approximation of $\Phi(t_n, x)$ by either the EWI-FP method or the TSFP method, I_h is the standard interpolation operator, and $C(t)$ behaves the same as $\widetilde{C}(t)$ in (1.4), i.e., it could grow exponentially with respect to t. Thus, the ε-resolution of the EWI-FP and TSFP methods for simulating the long-time dynamics, up to the time at $T_\varepsilon = T/\varepsilon$, of the the Dirac equation (1.1) is improved to [24]

$$h = O(1), \qquad \tau = O(1). \tag{1.7}$$

The time-splitting methods have been widely used to numerically solve dispersive partial differential equations (PDEs) [1, 26, 31, 34], and they show better performance in terms of resolution for high oscillatory dispersive PDEs. The main aims of this paper fall into two aspects: (i) by employing the unitary flow property of the second-order time-splitting method for the Dirac equation, we show that $C(t)$ in (1.6) grows at most linearly with respect to t for $t \in [0, T_\varepsilon]$, i.e., there exist two constants $C_0 \geq 0$ and $C_1 > 0$ independent of t, h, τ, and ε, such that

$$C(t) \leq C_0 + C_1 \varepsilon t \leq C_0 + C_1 T, \qquad 0 \leq t \leq T_\varepsilon = \frac{T}{\varepsilon}; \tag{1.8}$$

and (ii) by adopting the regularity compensation oscillation (RCO) technique, which controls high frequency modes by the regularity of the solution and low frequency modes by phase cancellation and energy method [2, 3], we establish improved uniform error bounds for the second-order TSFP method for the long-time dynamics of the Dirac equation (1.1) as

$$\|\Phi(t_n, \cdot) - I_h \Phi^n\|_{L^2} \lesssim h^m + \varepsilon \tau^2, \quad 0 \leq n \leq \frac{T/\varepsilon}{\tau}. \tag{1.9}$$

It is clear that the error bound with the term $\varepsilon\tau^2$ in (1.9) is much better than the term τ^2 in (1.6) for $\varepsilon \in (0, 1)$, especially when $0 < \varepsilon \ll 1$, i.e., the Dirac equation (1.1) with small electromagnetic potentials. We remark here that the linear growth of the constant $C(t)$ in error bounds for the time-splitting methods has been established for the Maxwell equations [16, 17] and the Schrödinger equation [2] in the literature. The long-time error estimates for the nonlinear Klein-Gordon equation [3, 8, 9] and the Korteweg–De Vries equation [15] were recently established.

The rest of this paper is organized as follows. In section 2, the second-order time-splitting methods including the semidiscretization and full-discretization for the long-time dynamics of the Dirac equation with small potentials are presented. In section 3, uniform error bounds for the time-splitting methods are established up to the time at $O(1/\varepsilon)$ and the errors are shown to grow linearly with respect to the time t. In section 4, we prove the improved uniform error bounds rigorously by adopting the RCO technique. Extensive numerical results are reported in section 5. Finally, some conclusions are drawn in section 6. Throughout this paper, we adopt the notation $A \lesssim B$ to represent that there exists a generic constant $C > 0$, which is independent of h, τ, and ε such that $|A| \leq CB$.

2. The time-splitting methods. For simplicity, in the following sections, we focus on the Dirac equation (1.1) in 1D, i.e., $d = 1$ in (1.1), for the numerical methods and corresponding analysis. The methods and results can be easily generalized to (1.1) in 2D, i.e., $d = 2$, and to the four-component Dirac equation given in [4, 5].

The Dirac equation (1.1) in 1D on the bounded computational domain $\Omega = (a, b)$ with periodic boundary condition collapses to

$$i\partial_t \Phi = (-i\sigma_1\partial_x + \sigma_3)\Phi + \varepsilon(V(x)I_2 - A_1(x)\sigma_1)\Phi, \qquad x \in \Omega, \quad t > 0, \tag{2.1}$$

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

where $\Phi := \Phi(t, x)$ and $\Phi_0(a) = \Phi_0(b)$.

2.1. The semidiscretization. Define the operators

$$\mathbf{T} := -\sigma_1\partial_x - i\sigma_3, \quad \mathbf{V} := -i(V(x)I_2 - A_1(x)\sigma_1); \tag{2.3}$$

then (2.1) can be expressed by

$$\partial_t \Phi(t, x) = (\mathbf{T} + \varepsilon\mathbf{V})\Phi(t, x), \quad x \in \Omega, \ t > 0. \tag{2.4}$$

Take a time step size $\tau > 0$ and denote the time grids as $t_n = n\tau$ for $n = 0, 1, \ldots$. As both $\mathbf{T}$ and $\mathbf{V}$ are time independent, the solution to (2.4) with (2.2) can be propagated through

$$\Phi(t_{n+1}, x) = e^{\tau(\mathbf{T}+\varepsilon\mathbf{V})}\Phi(t_n, x), \quad n = 0, 1, \ldots. \tag{2.5}$$

To approximate the operator $e^{\tau(\mathbf{T}+\varepsilon\mathbf{V})}$, we apply the second-order time-splitting (Strang splitting) [37], which gives

$$e^{\tau(\mathbf{T}+\varepsilon\mathbf{V})} \approx e^{\frac{\tau}{2}\mathbf{T}} e^{\varepsilon\tau\mathbf{V}} e^{\frac{\tau}{2}\mathbf{T}}. \tag{2.6}$$

Therefore, the semidiscretization of the Dirac equation (2.1) via Strang splitting can be expressed as

$$\Phi^{[n+1]}(x) = \mathcal{S}_\tau(\Phi^{[n]}(x)) := e^{\frac{\tau}{2}\mathbf{T}} e^{\varepsilon\tau\mathbf{V}} e^{\frac{\tau}{2}\mathbf{T}} \Phi^{[n]}(x), \quad n = 0, 1, \ldots, \tag{2.7}$$

where we take the initial condition $\Phi^{[0]}(x) := \Phi_0(x)$ for $x \in \overline{\Omega}$. Here, $\Phi^{[n]}(x)$ is the approximation of $\Phi(t_n, x)$.

Remark 2.1. We could also apply the first-order Lie–Trotter splitting as [39]

$$e^{\tau(\mathbf{T}+\varepsilon\mathbf{V})} \approx e^{\tau\mathbf{T}} e^{\varepsilon\tau\mathbf{V}},$$

another composition of the second-order Strang splitting as

$$e^{\tau(\mathbf{T}+\varepsilon\mathbf{V})} \approx e^{\frac{\tau}{2}\varepsilon\mathbf{V}} e^{\tau\mathbf{T}} e^{\frac{\tau}{2}\varepsilon\mathbf{V}},$$

and the fourth-order partitioned Runge–Kutta splitting (PRK4) as [11]

$$\begin{aligned} e^{\tau(\mathbf{T}+\varepsilon\mathbf{V})} \approx\ & e^{a_1\tau\mathbf{T}} e^{b_1\varepsilon\tau\mathbf{V}} e^{a_2\tau\mathbf{T}} e^{b_2\varepsilon\tau\mathbf{V}} e^{a_3\tau\mathbf{T}} e^{b_3\varepsilon\tau\mathbf{V}} e^{a_4\tau\mathbf{T}} \\ & \times e^{b_3\varepsilon\tau\mathbf{V}} e^{a_3\tau\mathbf{T}} e^{b_2\varepsilon\tau\mathbf{V}} e^{a_2\tau\mathbf{T}} e^{b_1\varepsilon\tau\mathbf{V}} e^{a_1\tau\mathbf{T}}, \end{aligned}$$

where

$$\begin{aligned} & a_1 = 0.0792036964311957, \quad a_2 = 0.353172906049774, \\ & a_3 = -0.0420650803577195, \quad a_4 = 1 - 2(a_1 + a_2 + a_3), \\ & b_1 = 0.209515106613362, \quad b_2 = -0.143851773179818, \quad b_3 = \frac{1}{2} - (b_1 + b_2). \end{aligned}$$

2.2. The full-discretization. By noticing the definition of $\mathbf{V}$ in (2.3), it is easy to derive that

$$e^{\varepsilon\tau\mathbf{V}}\Phi(t,x) = e^{-i\varepsilon\tau(V(x)I_2 - A_1(x)\sigma_1)}\Phi(t,x), \quad x \in \overline{\Omega}, \quad t > 0. \tag{2.8}$$

On the other hand, to get $e^{\tau\mathbf{T}}\Phi(t,x)$, we can discretize (2.4) in space by the Fourier spectral method, and then it is possible to integrate the operator analytically in the phase space. We take $M+1$ uniformly sampled grid points in $\overline{\Omega}$ with M a positive even integer,

$$x_j = a + jh, \quad h = \frac{b-a}{M}, \quad j = 0, 1, \ldots, M, \tag{2.9}$$

and we denote the sets X_M, Y_M, Z_M as

$$\begin{aligned} & X_M = \left\{U = (U_0, U_1, \ldots, U_M)^T \,\check{}\,|\,\check{}\, U_j \in \mathbb{C}^2,\ j = 0, 1, \ldots, M,\ U_0 = U_M\right\}, \\ & Y_M = Z_M \times Z_M, \quad Z_M = \mathrm{span}\{\phi_l(x) = e^{i\mu_l(x-a)},\ l \in \mathcal{T}_M\}, \end{aligned}$$

where the index set $\mathcal{T}_M = \{l\,\check{}\,|\,\check{}\, l = -M/2, -M/2+1, \ldots, M/2-1\}$, and $\mu_l = 2\pi l/(b-a)$ for $l \in \mathcal{T}_M$. The projection operator $P_M : \left(L^2(\Omega)\right)^2 \to Y_M$ is defined as

$$\left(P_M U\right)(x) := \sum_{l\in\mathcal{T}_M} \widehat{U}_l e^{i\mu_l(x-a)}, \quad U(x) \in \left(L^2(\Omega)\right)^2,$$

where

$$\widehat{U}_l = \frac{1}{b-a}\int_a^b U(x) e^{-i\mu_l(x-a)}dx, \quad l \in \mathcal{T}_M, \tag{2.10}$$

and by taking $\left(C_{\mathrm{per}}(\overline{\Omega})\right)^2 = \left\{U \in \left(C(\overline{\Omega})\right)^{2\,\check{}}\,|\,\check{}\, U(a) = U(b)\right\}$, the interpolation operator $I_M : \left(C_{\mathrm{per}}(\overline{\Omega})\right)^2 \to Y_M$ or $I_M : X_M \to Y_M$ is defined as

$$\left(I_M U\right)(x) := \sum_{l\in\mathcal{T}_M} \widetilde{U}_l e^{i\mu_l(x-a)}, \qquad U(x) \in \left(C_{\mathrm{per}}(\overline{\Omega})\right)^2 \quad \text{or} \quad U \in X_M,$$

where

$$\widetilde{U}_l = \frac{1}{M}\sum_{j=0}^{M-1} U_j e^{-2ijl\pi/M}, \quad l \in \mathcal{T}_M. \tag{2.11}$$

Here we take $U_j = U(x_j)$ if U is a function.

Denote $\Phi^n = (\Phi_0^n, \Phi_1^n, \ldots, \Phi_M^n)^T \in X_M$ as the solution vector at $t = t_n$ with Φ_j^n the numerical approximation of $\Phi(t_n, x_j)$. Take the initial value $\Phi_j^0 = \Phi_0(x_j)$ for $j = 0, \ldots, M$; then the time-splitting Fourier pseudospectral (TSFP) method for discretizing the Dirac equation (2.1) is given as

$$
\begin{aligned}
\Phi_j^{(1)} &= \sum_{l\in\mathcal{T}_M} e^{-i\frac{\tau\Gamma_l}{2}}\widetilde{(\Phi^n)}_l\, e^{i\mu_l(x_j-a)} = \sum_{l\in\mathcal{T}_M} Q_l\, e^{-i\frac{\tau D_l}{2}}(Q_l)^T\widetilde{(\Phi^n)}_l\, e^{\frac{2ijl\pi}{M}},\\
\Phi_j^{(2)} &= e^{-i\varepsilon\tau G(x_j)}\Phi_j^{(1)} = Pe^{-i\varepsilon\Lambda_j}P^T\Phi_j^{(1)},\\
\Phi_j^{n+1} &= \sum_{l\in\mathcal{T}_M} e^{-i\frac{\tau\Gamma_l}{2}}\widetilde{(\Phi^{(2)})}_l\, e^{i\mu_l(x_j-a)} = \sum_{l\in\mathcal{T}_M} Q_l\, e^{-i\frac{\tau D_l}{2}}(Q_l)^T\widetilde{(\Phi^{(2)})}_l\, e^{\frac{2ijl\pi}{M}},
\end{aligned}
\tag{2.12}
$$

for $n = 0, 1, \ldots$, where $\Gamma_l = \mu_l\sigma_1 + \sigma_3 = Q_lD_l(Q_l)^T$ with $\delta_l = \sqrt{1+\mu_l^2}$, $(Q_l)^T$ is the transpose of Q_l, and

$$
\Gamma_l = \begin{pmatrix} 1 & \mu_l \\ \mu_l & -1 \end{pmatrix}, \quad Q_l = \begin{pmatrix} \frac{1+\delta_l}{\sqrt{2\delta_l(1+\delta_l)}} & -\frac{\mu_l}{\sqrt{2\delta_l(1+\delta_l)}} \\ \frac{\mu_l}{\sqrt{2\delta_l(1+\delta_l)}} & \frac{1+\delta_l}{\sqrt{2\delta_l(1+\delta_l)}} \end{pmatrix}, \quad D_l = \begin{pmatrix} \delta_l & 0 \\ 0 & -\delta_l \end{pmatrix},
\tag{2.13}
$$

and $G(x_j) = V(x_j)I_2 - A_1(x_j)\sigma_1 = P\Lambda_jP^T$ with $\Lambda_j = \mathrm{diag}(\Lambda_{j,+}, \Lambda_{j,-})$ and $\Lambda_{j,\pm} = V(x_j) \pm A_1(x_j)$, $P = I_2$ if $A_1(x_j) = 0$, and otherwise

$$
P = \begin{pmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ -\frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \end{pmatrix}.
$$

3. Uniform error bounds. In this section, we prove the uniform error bounds for the second-order time-splitting method in propagating the Dirac equation with small potentials in the long-time regime up to $T_\varepsilon = T/\varepsilon$ for any given $T > 0$. We will start with the results for the semidiscretized scheme, and then extend it to the full-discretization.

3.1. For semidiscretization. Suppose there exists a positive integer $m \geq 2$, such that for the potentials and the initial data Φ_0 in (2.2), we have

$$
V(x) \in W^{m^-,\infty}_{\mathrm{per}}(\Omega), \quad A_1(x) \in W^{m^-,\infty}_{\mathrm{per}}(\Omega), \quad \Phi_0 \in (H^m_{\mathrm{per}}(\Omega))^2,
\tag{A}
$$

where $m^- := \max\{2, m-1\}$, $W^{m,\infty}_{\mathrm{per}}(\Omega) := \{u | u \in W^{m,\infty}(\Omega), \partial_x^l u(a) = \partial_x^l u(b), l = 0, \ldots, m-1\}$, and $H^m_{\mathrm{per}}(\Omega) := \{u | u \in H^m(\Omega), \partial_x^l u(a) = \partial_x^l u(b), l = 0, \ldots, m-1\}$. Based on the above assumption (A), it is easy to obtain that the exact solution $\Phi := \Phi(t, x)$ of the Dirac equation (2.1) up to the long time $T_\varepsilon = T/\varepsilon$ satisfies

$$
\|\Phi\|_{L^\infty([0,T_\varepsilon];(H^m_{\mathrm{per}}(\Omega))^2)} \lesssim 1, \qquad \|\partial_t\Phi\|_{L^\infty([0,T_\varepsilon];(H^{m-1}_{\mathrm{per}}(\Omega))^2)} \lesssim 1,
\tag{3.1}
$$

where the equivalent H^m-norm on $H^m_{\mathrm{per}}(\Omega)$ is given as

$$
\|\phi\|_{H^m} = \left(\sum_{l\in\mathbb{Z}} (1+\mu_l^2)^m |\widehat{\phi}_l|^2\right)^{1/2}.
\tag{3.2}
$$

By taking the semidiscretized second-order time-splitting given by (2.7) for the Dirac equation (2.4) with the operators $\mathbf{T}$ and $\mathbf{V}$ defined as in (2.3), we have the following error estimate.

THEOREM 3.1. *Let $\Phi^{[n]}(x)$ be the numerical approximation obtained from the semidiscretized second-order time-splitting* (2.7) *for the Dirac equation* (2.4)*; then under the assumption (A), for any $0 < \varepsilon \leq 1$, we have the uniform error estimate*

$$\left\|\Phi(t_n, x) - \Phi^{[n]}(x)\right\|_{L^2} \leq C_1 \varepsilon t_n \tau^2 \leq C_1 T \tau^2, \quad 0 \leq n \leq \frac{T/\varepsilon}{\tau}, \tag{3.3}$$

where C_1 is a positive constant independent of τ, n, and ε.

Proof. We notice that $\mathbf{T}$ generates a unitary group in $(H^k_{\rm per}(\Omega))^2$ $(k \geq 0)$. We denote the exact solution flow $\Phi(t_n) \to \Phi(t_{n+1})$ as

$$\Phi(t_{n+1}) = \mathcal{S}_{e,\tau}(\Phi(t_n)), \quad 0 \leq n \leq \frac{T/\varepsilon}{\tau}, \tag{3.4}$$

where we take $\Phi(t_n) := \Phi(t_n, x)$ for simplicity.

In order to prove the convergence, we adopt the approach via formal Lie calculus introduced in [32] and split the proof into the following two steps.

Step 1 (bounds for local truncation error). We begin with the local truncation error, i.e., to estimate the error generated by one time step computed via (2.7). By using Taylor expansion for $e^{\varepsilon\tau\mathbf{V}}$, we have

$$\mathcal{S}_\tau(\Phi_0) = e^{\tau\mathbf{T}}\Phi_0 + \varepsilon\tau e^{\frac{\tau\mathbf{T}}{2}}\mathbf{V}e^{\frac{\tau\mathbf{T}}{2}}\Phi_0 + \varepsilon^2\tau^2\int_0^1 (1-\theta)e^{\frac{\tau\mathbf{T}}{2}}e^{\varepsilon\theta\tau\mathbf{V}}\mathbf{V}^2 e^{\frac{\tau\mathbf{T}}{2}}\Phi_0 d\theta.$$

By Duhamel's principle, we can write

$$\begin{aligned}\mathcal{S}_{e,\tau}(\Phi_0) = e^{\tau\mathbf{T}}\Phi_0 &+ \varepsilon\int_0^\tau e^{(\tau-s)\mathbf{T}}\mathbf{V}e^{s\mathbf{T}}\Phi_0 ds \\ &+ \varepsilon^2\int_0^\tau\int_0^s e^{(\tau-s)\mathbf{T}}\mathbf{V}e^{(s-w)\mathbf{T}}\mathbf{V}\Phi(w)dwds.\end{aligned}$$

Denote

$$Y(s) = e^{(\tau-s)\mathbf{T}}\mathbf{V}e^{s\mathbf{T}}\Phi_0, \quad B(s,w) = e^{(\tau-s)\mathbf{T}}\mathbf{V}e^{(s-w)\mathbf{T}}\mathbf{V}e^{w\mathbf{T}}\Phi_0; \tag{3.5}$$

then the local truncation error can be written as

$$\begin{aligned}\mathcal{S}_\tau(\Phi_0) - \mathcal{S}_{e,\tau}(\Phi_0) = \varepsilon\tau Y\left(\frac{\tau}{2}\right) - \varepsilon\int_0^\tau Y(s)ds + \frac{\varepsilon^2\tau^2}{2}B\left(\frac{\tau}{2},\frac{\tau}{2}\right) \\ - \varepsilon^2\int_0^\tau\int_0^s B(s,w)dsdw + \varepsilon^2 R_1 + \varepsilon^2 R_2,\end{aligned}$$

with

$$\begin{aligned}R_1 &= \tau^2\int_0^1 (1-\theta)e^{\frac{\tau\mathbf{T}}{2}}e^{\varepsilon\theta\tau\mathbf{V}}\mathbf{V}^2 e^{\frac{\tau\mathbf{T}}{2}}\Phi_0 d\theta - \frac{\tau^2}{2}B\left(\frac{\tau}{2},\frac{\tau}{2}\right), \\ R_2 &= -\int_0^\tau\int_0^s e^{(\tau-s)\mathbf{T}}\mathbf{V}e^{(s-w)\mathbf{T}}\mathbf{V}\Phi(w) - B(s,w)dwds.\end{aligned}$$

It is easy to check that

$$\begin{aligned}\|R_1\|_{L^2} &\lesssim \tau^2 \max_{\theta\in(0,1)}\{\|\partial_{\theta\theta}((1-\theta)e^{\frac{\tau\mathbf{T}}{2}}e^{\varepsilon\theta\tau\mathbf{V}}\mathbf{V}^2 e^{\frac{\tau\mathbf{T}}{2}}\Phi_0)\|_{L^2}\} \\ &\lesssim \varepsilon\tau^3\left(\|\mathbf{V}^3\Phi_0\|_{L^2} + \varepsilon\tau\|\mathbf{V}^4\Phi_0\|_{L^2}\right) \lesssim \varepsilon\tau^3.\end{aligned}$$

In view of the properties of $\mathbf{T}$ and $B(s,w)$, the quadrature rule implies

$$\begin{aligned}\|R_2\|_{L^2} &\lesssim \tau^3 \max_{s,w\in(0,\tau)} \{\|e^{(\tau-s)\mathbf{T}}\mathbf{V}e^{(s-w)\mathbf{T}}\mathbf{V}\partial_w\Phi(w)\|_{L^2}\}\\ &\lesssim \tau^3\|\partial_s\Phi(\cdot)\|_{L^\infty([0,\tau];(L^2)^2)} \lesssim \tau^3,\end{aligned}$$

and

$$\left\|\frac{\tau^2}{2}B\left(\frac{\tau}{2},\frac{\tau}{2}\right)-\int_0^\tau\int_0^s B(s,w)dwds\right\|_{L^2} \lesssim \tau^3 \max_{0\le w\le s\le\tau}(\|\partial_s B\|_{L^2}+\|\partial_w B\|_{L^2}) \lesssim \tau^3.$$

Finally, we estimate the last term, which contains the major part of the local error

$$\mathcal{F}(\Phi_0) := \varepsilon\tau Y\left(\frac{\tau}{2}\right)-\varepsilon\int_0^\tau Y(s)ds = \varepsilon\tau^3\int_0^1 \ker(\theta)Y''(\theta\tau)d\theta, \tag{3.6}$$

where $\ker(\theta)$ is the Peano kernel for midpoint rule. In addition, we have

$$Y''(s) = e^{(\tau-s)\mathbf{T}}[\mathbf{T},[\mathbf{T},\mathbf{V}]]e^{s\mathbf{T}}\Phi_0.$$

For the double commutator $[\mathbf{T},[\mathbf{T},\mathbf{V}]]$, we have

$$\|[\mathbf{T},[\mathbf{T},\mathbf{V}]]\Psi\|_{L^2} \lesssim \left(\|V(\cdot)\|_{W^{2,\infty}}+\|A_1(\cdot)\|_{W^{2,\infty}}\right)\|\Psi\|_{H^1}.$$

By combining all the results above, we find the one step local error as

$$\mathcal{S}_\tau(\Phi_0)-\mathcal{S}_{e,\tau}(\Phi_0) = \mathcal{F}(\Phi_0)+\mathcal{R}^0, \tag{3.7}$$

where $\|\mathcal{R}^0\|_{L^2}\lesssim\varepsilon^2\tau^3$ and

$$\mathcal{F}(\Phi_0) = \varepsilon\tau^3\int_0^1 \ker(\theta)\mathrm{e}^{\tau(1-\theta)\mathbf{T}}[\mathbf{T},[\mathbf{T},\mathbf{V}]]\mathrm{e}^{\tau\theta\mathbf{T}}\Phi_0\mathrm{d}\theta. \tag{3.8}$$

Define the local truncation error at t_n for $0\le n\le\frac{T/\varepsilon}{\tau}-1$ as

$$\mathcal{E}^n(x) = \mathcal{S}_\tau(\Phi(t_n,x))-\mathcal{S}_{e,\tau}(\Phi(t_n,x)),\quad a\le x\le b; \tag{3.9}$$

then from the above computation, we can get

$$\mathcal{E}^n(x) = \mathcal{F}(\Phi(t_n))+\mathcal{R}^n,\quad a\le x\le b,\quad 0\le n\le\frac{T/\varepsilon}{\tau}-1, \tag{3.10}$$

where for $0\le n\le\frac{T/\varepsilon}{\tau}-1$,

$$\|\mathcal{F}(\Phi(t_n))\|_{L^2}\lesssim\varepsilon\tau^3\|\Phi(t_n)\|_{H^1},\quad \|\mathcal{R}^n\|_{L^2}\lesssim\varepsilon^2\tau^3. \tag{3.11}$$

Step 2 (bounds for the global error). We are going to prove the error bound (3.3). Denote $\mathbf{e}^{[n]}(x) = \Phi^{[n]}-\Phi(t_n)$; then $\|\mathbf{e}^{[0]}(x)\|_{L^2}=0$ by definition. For $0\le n\le\frac{T/\varepsilon}{\tau}-1$, we have

$$\mathbf{e}^{[n+1]} = \mathcal{S}_\tau(\Phi^{[n]})-\mathcal{S}_\tau(\Phi(t_n))+\mathcal{S}_\tau(\Phi(t_n))-\mathcal{S}_{e,\tau}(\Phi(t_n)). \tag{3.12}$$

By the error bound (3.11) for the local truncation error, we obtain for $0\le n\le\frac{T/\varepsilon}{\tau}-1$,

$$\left\|\mathbf{e}^{[n+1]}\right\|_{L^2}\le\left\|\mathbf{e}^{[n]}\right\|_{L^2}+C_1\varepsilon\tau^3, \tag{3.13}$$

where $C_1 > 0$ is a constant and independent of h, n, τ, and ε. Then it is straightforward to derive

$$\left\|\mathbf{e}^{[n+1]}\right\|_{L^2} \le \left\|\mathbf{e}^{[0]}\right\|_{L^2} + C_1(n+1)\varepsilon\tau^3 \le C_1\varepsilon t_{n+1}\tau^2, \tag{3.14}$$

which completes the proof of Theorem 3.1. ∎

Remark 3.2. In Theorem 3.1, the constant C_1 depends on $\|\Phi\|_{L^\infty([0,T_\varepsilon];(H^m_{\rm per}(\Omega))^2)}$. When the Sobolev norm is uniformly bounded for all $t \ge 0$, the uniform error bound on the time-splitting method for the Dirac equation grows linearly with respect to t. In fact, given an accuracy bound $\delta_0 > 0$, the time (for simplicity, assume $\varepsilon = 1$ here) for the second-order splitting method to violate the accuracy requirement δ_0 is $O(\delta_0/\tau^2)$. The results can be extended to other time-splitting methods. For the first-order Lie–Trotter splitting and fourth-order compact splitting or partitioned Runge–Kutta splitting (PRK4), the times are at $O(\delta_0/\tau)$ and $O(\delta_0/\tau^4)$, respectively. In other words, higher order splitting methods perform much better in the long-time simulation not only regarding the higher accuracy but also longer simulation time to produce accurate solutions. In addition, extensions to 2D/3D are straightforward.

3.2. For full-discretization. For the full-discretization given in (2.12) by the second-order time-splitting method for the Dirac equation (2.4), we can further derive the following uniform error estimate.

THEOREM 3.3. *Let Φ^n be the approximation obtained from the TSFP* (2.12) *for the Dirac equation* (2.4). *Under the assumption (A), for any $0 < \varepsilon \le 1$, we have*

$$\|\Phi(t_n, x) - I_M\Phi^n\|_{L^2} \le C(t_n)\left(h^m + \tau^2\right), \qquad 0 \le n \le \frac{T/\varepsilon}{\tau}, \tag{3.15}$$

where $C(t) = C_0 + C_1\varepsilon t \le C_0 + C_1 T$, with C_0 and C_1 two positive constants independent of h, τ, n, and ε.

Proof. Noticing that

$$I_M\Phi^n - \Phi(t_n) = I_M\Phi^n - P_M\Phi(t_n) + P_M\Phi(t_n) - \Phi(t_n), \tag{3.16}$$

under the assumption (B), we get from the standard Fourier projection properties [36]

$$\|I_M\Phi^n - \Phi(t_n)\|_{L^2} \le \|I_M\Phi^n - P_M\Phi(t_n)\|_{L^2} + C_2h^m, \quad 0 \le n \le \frac{T/\varepsilon}{\tau}. \tag{3.17}$$

Thus, it suffices to consider the error function $\mathbf{e}^n \in Y_M$ at t_n as

$$\mathbf{e}^n := \mathbf{e}^n(x) = I_M\Phi^n - P_M\Phi(t_n), \quad 0 \le n \le \frac{T/\varepsilon}{\tau}. \tag{3.18}$$

Since $\Phi_j^0 = \Phi_0(x_j)$, it is obvious from (B) that $\|\mathbf{e}^0\|_{L^2} \le C_3h^m$. From the local truncation error (3.9), we have the error equation for $\mathbf{e}^n$ $(0 \le n \le \frac{T/\varepsilon}{\tau} - 1)$,

$$\mathbf{e}^{n+1} = I_M\Phi^{n+1} - P_M\mathcal{S}_\tau(\Phi(t_n)) + P_M(\mathcal{E}^n). \tag{3.19}$$

By recalling the semidiscretization (2.7) and the full-discretization (2.12), we have

$$I_M\Phi^{n+1} = e^{\frac{\tau\mathbf{T}}{2}}(I_M\Phi^{(2)}),\ I_M\Phi^{(2)} = I_M\left(e^{\varepsilon\tau\mathbf{V}}\Phi^{(1)}\right),\ I_M\Phi^{(1)} = e^{\frac{\tau\mathbf{T}}{2}}(I_M\Phi^n),$$
$$P_M(\mathcal{S}_\tau(\Phi(t_n))) = e^{\frac{\tau\mathbf{T}}{2}}(P_M\Phi^{\langle 2\rangle}),\ \Phi^{\langle 2\rangle} := e^{\varepsilon\tau\mathbf{V}}\Phi^{\langle 1\rangle},\ \Phi^{\langle 1\rangle} := e^{\frac{\tau\mathbf{T}}{2}}\Phi(t_n).$$

In view of the facts that I_M and P_M are identical on Y_M and that $e^{\tau\mathbf{T}/2}$ preserves the H^k-norm ($k \geq 0$), using the Taylor expansion $e^{\varepsilon\tau\mathbf{V}} = 1 + \varepsilon\tau\mathbf{V}\int_0^1 e^{\varepsilon\tau\theta\mathbf{V}}d\theta$ and assumptions (A) and (B), we have

$$\left\|I_M\Phi^{n+1} - P_M(\mathcal{S}_\tau(\Phi(t_n)))\right\|_{L^2} = \left\|I_M\Phi^{\langle 2\rangle} - P_M\Phi^{\langle 2\rangle}\right\|_{L^2}, \tag{3.20}$$

$$\left\|P_M\Phi^{\langle 2\rangle} - I_M\Phi^{\langle 2\rangle}\right\|_{L^2} \leq C_4\varepsilon\tau h^m. \tag{3.21}$$

In addition, noticing $\mathbf{V} = -i(V(x)I_2 - A_1(x)\sigma_1)$, by direct computation and Parseval's identity, we have

$$\begin{aligned}\left\|I_M\Phi^{(2)} - I_M\Phi^{\langle 2\rangle}\right\|_{L^2} &= \sqrt{h\sum_{j=0}^{M-1}\left|\Phi_j^{(2)} - \Phi^{\langle 2\rangle}(x_j)\right|^2} = \sqrt{h\sum_{j=0}^{M-1}\left|\Phi_j^{(1)} - \Phi^{\langle 1\rangle}(x_j)\right|^2}\\ &= \left\|I_M\Phi^{(1)} - I_M\Phi^{\langle 1\rangle}\right\|_{L^2} = \left\|I_M\Phi^n - P_M\Phi(t_n)\right\|_{L^2}\\ &= \left\|\mathbf{e}^n\right\|_{L^2}. \end{aligned} \tag{3.22}$$

From (3.10), (3.11), and the assumption (A), it is clear that there exists $C_5 > 0$ such that $\|\mathcal{E}^n\|_{L^2} \leq C_5\varepsilon\tau^3$ for $0 \leq n \leq \frac{T/\varepsilon}{\tau} - 1$. Taking the L^2-norm on both sides of (3.19) and combining the above estimates, we obtain for $0 \leq n \leq \frac{T/\varepsilon}{\tau} - 1$,

$$\begin{aligned}\left\|\mathbf{e}^{n+1}\right\|_{L^2} &\leq \left\|I_M\Phi^{(2)} - P_M\Phi^{\langle 2\rangle}\right\|_{L^2} + \left\|\mathcal{E}^n\right\|_{L^2}\\ &\leq \left\|I_M\Phi^{(2)} - I_M\Phi^{\langle 2\rangle}\right\|_{L^2} + \left\|P_M\Phi^{\langle 2\rangle} - I_M\Phi^{\langle 2\rangle}\right\|_{L^2} + \left\|\mathcal{E}^n\right\|_{L^2}\\ &\leq \left\|\mathbf{e}^n\right\|_{L^2} + C_6\left(\varepsilon\tau h^m + \varepsilon\tau^3\right), \end{aligned} \tag{3.23}$$

where $C_6 = \max\{C_4, C_5\}$. Thus, we arrive at

$$\left\|\mathbf{e}^{n+1}\right\|_{L^2} \leq C_6\varepsilon t_{n+1}\left(h^m + \tau^2\right) + C_3h^m, \quad 0 \leq n \leq \frac{T/\varepsilon}{\tau} - 1, \tag{3.24}$$

which completes the proof of Theorem 3.3 by taking $C_0 = C_2 + C_3$ and $C_1 = C_6$. ∎

4. Improved uniform error bounds. In this section, we establish the improved uniform error bounds for the time-splitting methods applied to the Dirac equation (2.1) up to the long-time T_ε under the assumption (A).

4.1. For semidiscretization. THEOREM 4.1. *Let $\Phi^{[n]}(x)$ be the numerical approximation obtained from the semidiscretized second-order time-splitting* (2.7) *for the Dirac equation* (2.4). *Under the assumption (A), for $0 < \tau_0 < 1$ sufficiently small and independent of ε, when $0 < \tau < \alpha\frac{\pi(b-a)\tau_0}{\sqrt{\tau_0^2(b-a)^2 + 4\pi^2(1+\tau_0)^2}}$ for a fixed constant $\alpha \in (0,1)$, we have the following improved uniform error bound for any $\varepsilon \in (0,1]$:*

$$\left\|\Phi(t_n,x) - \Phi^{[n]}\right\|_{L^2} \lesssim \varepsilon\tau^2 + \tau_0^m, \quad 0 \leq n \leq \frac{T/\varepsilon}{\tau}. \tag{4.1}$$

In particular, if the exact solution is smooth, e.g., $\Phi(t,x) \in L^\infty([0,T_\varepsilon];(H^\infty_{\rm per}(\Omega))^2)$, the last term τ_0^m decays exponentially fast and can be ignored practically for a sufficiently small τ_0, where the improved uniform error bound for $\tau < \tau_0$ will be

$$\left\|\Phi(t_n,x) - \Phi^{[n]}\right\|_{L^2} \lesssim \varepsilon\tau^2, \quad 0 \leq n \leq \frac{T/\varepsilon}{\tau}. \tag{4.2}$$

Proof. From the local truncation error (3.9) and the error equation (3.12), we have

$$\mathbf{e}^{[n+1]} = \mathcal{S}_\tau(\Phi^{[n]}) - \mathcal{S}_\tau(\Phi(t_n)) + \mathcal{E}^n = e^{\tau\mathbf{T}}\mathbf{e}^{[n]} + W^n + \mathcal{E}^n, \quad n \geq 0, \tag{4.3}$$

where $W^n := W^n(x)$ $(n = 0, 1, \ldots)$ is given by

$$W^n(x) = \varepsilon\tau e^{\frac{\tau\mathbf{T}}{2}}\mathbf{V}\int_0^1 e^{\varepsilon\tau\theta\mathbf{V}}d\theta\, e^{\frac{\tau\mathbf{T}}{2}}\mathbf{e}^{[n]}. \tag{4.4}$$

Under the assumption (A), we have the estimate

$$\|W^n(x)\|_{L^2} \lesssim \varepsilon\tau \left\|\mathbf{e}^{[n]}\right\|_{L^2}. \tag{4.5}$$

Based on (4.3), we arrive at

$$\mathbf{e}^{[n+1]} = e^{(n+1)\tau\mathbf{T}}\mathbf{e}^{[0]} + \sum_{k=0}^{n} e^{(n-k)\tau\mathbf{T}}\left(W^k + \mathcal{E}^k\right), \quad 0 \leq n \leq \frac{T/\varepsilon}{\tau} - 1. \tag{4.6}$$

Combining (3.10), (3.11), and (4.5), noticing $\mathbf{e}^{[0]} = \mathbf{0}$, we have the following estimates for $0 \leq n \leq \frac{T/\varepsilon}{\tau} - 1$:

$$\left\|\mathbf{e}^{[n+1]}\right\|_{L^2} \lesssim \varepsilon\tau^2 + \varepsilon\tau\sum_{k=0}^{n}\left\|\mathbf{e}^{[k]}\right\|_{L^2} + \left\|\sum_{k=0}^{n} e^{(n-k)\tau\mathbf{T}}\mathcal{F}(\Phi(t_k))\right\|_{L^2}. \tag{4.7}$$

In order to obtain the improved uniform error bounds, we shall employ the *regularity compensation oscillation* (RCO) technique [2, 3] to deal with the last term on the right-hand side of the inequality (4.7).

The key idea is a summation-by-parts procedure combined with spectrum cut-off and phase cancellation. First, we employ the spectral projection on $\Phi(t_k)$ such that only finite Fourier modes of $\Phi(t_k)$ need to be considered and the projection error could be controlled by the regularity of $\Phi(t_k)$. Then we apply the summation-by-parts formula to the low Fourier modes such that the phase could be canceled for small τ (the terms of type $\sum_{k=0}^{n} e^{(n-k)\tau\mathbf{T}}$) and an extra order of ε could be gained from the terms like $\mathcal{F}(\Phi(t_k)) - \mathcal{F}(\Phi(t_{k+1}))$.

From the Dirac equation (2.4) and the assumption (A), we notice that $\partial_t\Phi(t,x) - \mathbf{T}\Phi(t,x) = O(\varepsilon)$. In order to gain an extra order of ε, it is natural to introduce the "twisted variable" as

$$\Psi(t,x) = e^{-t\mathbf{T}}\Phi(t,x), \quad t \geq 0, \tag{4.8}$$

which satisfies the equation

$$\partial_t\Psi(t,x) = \varepsilon e^{-t\mathbf{T}}\left(\mathbf{V}e^{t\mathbf{T}}\Psi(t,x)\right), \quad t \geq 0. \tag{4.9}$$

Noticing $\mathbf{T} = -\sigma_1\partial_x - i\sigma_3$, under the assumptions (A) and (B), we can prove that

$$\|\Psi\|_{L^\infty([0,T_\varepsilon];(H^m_{\rm per}(\Omega))^2)} \lesssim 1, \quad \|\partial_t\Psi\|_{L^\infty([0,T_\varepsilon];(H^m_{\rm per}(\Omega))^2)} \lesssim \varepsilon \tag{4.10}$$

and

$$\|\Psi(t_{n+1}) - \Psi(t_n)\|_{H^m} \lesssim \varepsilon\tau, \quad 0 \leq n \leq \frac{T/\varepsilon}{\tau} - 1. \tag{4.11}$$

The RCO technique will be used to force $\partial_t \Psi$ to appear with the gain of order ε for the summation-by-parts procedure in the last term $\sum_{k=0}^{n} e^{(n-k)\tau \mathbf{T}} \mathcal{F}(\Phi(t_k))$, where the small τ is required to control the accumulation of the frequency of type $e^{(n-k)\tau \mathbf{T}}$.

Step 1. As introduced in [2], we choose the cut-off parameter $\tau_0 \in (0,1)$ and $M_0 = 2\lceil 1/\tau_0 \rceil \in \mathbb{Z}^+$ ($\lceil \cdot \rceil$ is the ceiling function) with $1/\tau_0 \le M_0/2 < 1 + 1/\tau_0$. Under the assumptions (A) and (B), we have the estimate

$$\left\| P_{M_0} \mathcal{F}(P_{M_0} \Phi(t_n)) - \mathcal{F}(\Phi(t_n)) \right\|_{L^2} \lesssim \varepsilon \tau \tau_0^m. \tag{4.12}$$

Based on the above estimates, (4.7) would imply for $0 \le n \le T_\varepsilon/\tau - 1$,

$$\left\| \mathbf{e}^{[n+1]} \right\|_{L^2} \lesssim \tau_0^m + \varepsilon \tau^2 + \varepsilon \tau \sum_{k=0}^{n} \left\| \mathbf{e}^{[k]} \right\|_{L^2} + \left\| \mathcal{L}^n \right\|_{L^2}, \tag{4.13}$$

where

$$\mathcal{L}^n = \sum_{k=0}^{n} e^{-(k+1)\tau \mathbf{T}} P_{M_0} \mathcal{F}\left(e^{t_k \mathbf{T}} (P_{M_0} \Psi(t_k)) \right). \tag{4.14}$$

Step 2. Now, we concentrate on $\mathcal{L}^n$, which represents the summation of low Fourier modes. For $l \in \mathcal{T}_{M_0}$, define the index set $\mathcal{I}_l^{M_0}$ associated to l as

$$\mathcal{I}_l^{M_0} = \{ (l_1, l_2) \mid l_1 + l_2 = l,\ l_1 \in \mathbb{Z},\ l_2 \in \mathcal{T}_{M_0} \}. \tag{4.15}$$

Following the notation in (2.13), we denote

$$\Pi_l^+ = Q_l \operatorname{diag}(1,0)(Q_l)^T, \quad \Pi_l^- = Q_l \operatorname{diag}(0,1)(Q_l)^T, \tag{4.16}$$

where $\Pi_l^\pm$ are the projectors onto the eigenspaces of Γ_l corresponding to the eigenvalues $\pm\delta_l$, respectively. Moreover, we have $(\Pi_l^\pm)^T = \Pi_l^\pm$, $\Pi_l^+ + \Pi_l^- = I_2$, $(\Pi_l^\pm)^2 = \Pi_l^\pm$, $\Pi_l^\pm \Pi_l^\mp = \mathbf{0}$. By direct computation, we have

$$e^{t\mathbf{T}} P_{M_0} \Psi(t_k) = \sum_{l \in \mathcal{T}_{M_0}} \left(e^{-it\delta_l} \Pi_l^+ + e^{it\delta_l} \Pi_l^- \right) \widehat{\Psi}_l(t_k) e^{i\mu_l (x-a)}. \tag{4.17}$$

According to the definition of $\mathcal{F}$ in (3.6), the expansion below follows

$$\begin{aligned} &e^{-(k+1)\tau \mathbf{T}} P_{M_0} \left(e^{(\tau - s)\mathbf{T}} \mathbf{V} e^{(t_k + s)\mathbf{T}} P_{M_0} \Psi(t_k) \right) \\ &= \sum_{l \in \mathcal{T}_{M_0}} \sum_{(l_1, l_2) \in \mathcal{I}_l^{M_0}} \sum_{\nu_j = \pm, j = 1,2} \mathcal{G}_{k,l,l_1,l_2}^{\nu_1,\nu_2}(s) e^{i\mu_l (x-a)}, \end{aligned} \tag{4.18}$$

where $\mathcal{G}_{k,l,l_1,l_2}^{\nu_1,\nu_2}(s)$ is a function of s defined as

$$\mathcal{G}_{k,l,l_1,l_2}^{\nu_1,\nu_2}(s) = e^{i(t_k+s)\delta_{l,l_2}^{\nu_1,\nu_2}} \Pi_l^{\nu_1} \widehat{\mathbf{V}}_{l_1} \Pi_{l_2}^{\nu_2} \widehat{\Psi}_{l_2}(t_k), \tag{4.19}$$

with $\delta_{l,l_2}^{\nu_1,\nu_2} = \nu_1 \delta_l - \nu_2 \delta_{l_2}$. Then the remainder term $\mathcal{L}^n$ in (4.13) reads

$$\mathcal{L}^n = \varepsilon \sum_{k=0}^{n} \sum_{l \in \mathcal{T}_{M_0}} \sum_{(l_1, l_2) \in \mathcal{I}_l^{M_0}} \sum_{\nu_j = \pm, j = 1,2} \lambda_{k,l,l_1,l_2}^{\nu_1,\nu_2} e^{i\mu_l (x-a)}, \tag{4.20}$$

where the coefficients $\lambda^{\nu_1,\nu_2}_{k,l,l_1,l_2}$ are given by

$$\begin{aligned}\lambda^{\nu_1,\nu_2}_{k,l,l_1,l_2} &= \tau \mathcal{G}^{\nu_1,\nu_2}_{k,l,l_1,l_2}(\tau/2) - \int_0^\tau \mathcal{G}^{\nu_1,\nu_2}_{k,l,l_1,l_2}(s)\,ds \\ &= r^{\nu_1,\nu_2}_{l,l_2} e^{it_k \delta^{\nu_1,\nu_2}_{l,l_2}} c^{\nu_1,\nu_2}_{k,l,l_1,l_2} \end{aligned} \tag{4.21}$$

and

$$c^{\nu_1,\nu_2}_{k,l,l_1,l_2} = \Pi^{\nu_1}_{l} \widehat{\mathbf{V}}_{l_1} \Pi^{\nu_2}_{l_2} \widehat{\Psi}_{l_2}(t_k), \tag{4.22}$$

$$r^{\nu_1,\nu_2}_{l,l_2} = \tau e^{i\tau \delta^{\nu_1,\nu_2}_{l,l_2}/2} - \int_0^\tau e^{is\delta^{\nu_1,\nu_2}_{l,l_2}}\, ds = O(\tau^3 (\delta^{\nu_1,\nu_2}_{l,l_2})^2). \tag{4.23}$$

We only need to consider the case $\delta^{\nu_1,\nu_2}_{l,l_2} \neq 0$ as $r^{\nu_1,\nu_2}_{l,l_2} = 0$ if $\delta^{\nu_1,\nu_2}_{l,l_2} = 0$. For $l \in \mathcal{T}_{M_0}$ and $(l_1, l_2) \in \mathcal{I}^{M_0}_l$, we have

$$|\delta^{\nu_1,\nu_2}_{l,l_2}| \leq 2\delta_{M_0/2} = 2\sqrt{1+\mu^2_{M_0/2}} < 2\sqrt{1+\frac{4\pi^2(1+\tau_0)^2}{\tau_0^2(b-a)^2}}, \tag{4.24}$$

which implies for $0 < \tau \leq \alpha \frac{\pi(b-a)\tau_0}{\sqrt{\tau_0^2(b-a)^2+4\pi^2(1+\tau_0)^2}}$ with $0 < \alpha, \tau_0 < 1$ that $\frac{\tau}{2}|\delta^{\nu_1,\nu_2}_{l,l_2}| \leq \alpha\pi$ holds. Denoting $S^{\nu_1,\nu_2}_{n,l,l_2} = \sum_{k=0}^{n} e^{it_k \delta^{\nu_1,\nu_2}_{l,l_2}}$, for $0 < \tau \leq \alpha \frac{\pi(b-a)\tau_0}{\sqrt{\tau_0^2(b-a)^2+4\pi^2(1+\tau_0)^2}}$, we obtain

$$|S^{\nu_1,\nu_2}_{n,l,l_2}| \leq \frac{1}{|\sin(\tau\delta^{\nu_1,\nu_2}_{l,l_2}/2)|} \leq \frac{C}{\tau|\delta^{\nu_1,\nu_2}_{l,l_2}|}, \quad C = \frac{2\alpha\pi}{\sin(\alpha\pi)}, \quad \forall n \geq 0. \tag{4.25}$$

Using summation-by-parts formula, we find that

$$\sum_{k=0}^{n} \lambda^{\nu_1,\nu_2}_{k,l,l_1,l_2} = r^{\nu_1,\nu_2}_{l,l_2} \left[\sum_{k=0}^{n-1} S^{\nu_1,\nu_2}_{k,l,l_2} (c^{\nu_1,\nu_2}_{k,l,l_1,l_2} - c^{\nu_1,\nu_2}_{k+1,l,l_1,l_2}) + S^{\nu_1,\nu_2}_{n,l,l_2} c^{\nu_1,\nu_2}_{n,l,l_1,l_2} \right], \tag{4.26}$$

with

$$c^{\nu_1,\nu_2}_{k,l,l_1,l_2} - c^{\nu_1,\nu_2}_{k+1,l,l_1,l_2} = \Pi^{\nu_1}_{l} \widehat{\mathbf{V}}_{l_1} \Pi^{\nu_2}_{l_2} \left(\widehat{\Psi}_{l_2}(t_k) - \widehat{\Psi}_{l_2}(t_{k+1}) \right). \tag{4.27}$$

Combining (4.23), (4.25), (4.26), and (4.27), we have

$$\left| \sum_{k=0}^{n} \lambda^{\nu_1,\nu_2}_{k,l,l_1,l_2} \right| \lesssim \tau^2 |\delta^{\nu_1,\nu_2}_{l,l_2}| \left| \widehat{\mathbf{V}}_{l_1} \right| \left[\sum_{k=0}^{n-1} \left| \widehat{\Psi}_{l_2}(t_k) - \widehat{\Psi}_{l_2}(t_{k+1}) \right| + \left| \widehat{\Psi}_{l_2}(t_n) \right| \right]. \tag{4.28}$$

Step 3. Now, we are ready to give the improved estimates. For $l \in \mathcal{T}_{M_0}$ and $(l_1, l_2) \in \mathcal{I}^{M_0}_l$, simple calculations show ($l = l_1 + l_2$)

$$|\delta^{\nu_1,\nu_2}_{l,l_2}| \lesssim \prod_{j=1}^{2} (1+\mu^2_{l_j})^{1/2}. \tag{4.29}$$

Based on (4.20), (4.28), and (4.29), using the Cauchy inequality, we have

(4.30)

$$\begin{aligned}
&\|\mathcal{L}^n\|_{L^2}^2 \\
&= \varepsilon^2 \sum_{l\in\mathcal{T}_{N_0}} \Big| \sum_{(l_1,l_2)\in\mathcal{I}_l^{N_0}} \sum_{\nu_j=\pm, j=1,2} \sum_{k=0}^{n} \lambda_{k,l,l_1,l_2}^{\nu_1,\nu_2} \Big|^2 \\
&\lesssim \varepsilon^2\tau^4 \Big\{ \sum_{l\in\mathcal{T}_{M_0}} \Big(\sum_{(l_1,l_2)\in\mathcal{I}_l^{N_0}} \Big|\widehat{\mathbf{V}}_{l_1}\Big| \Big|\widehat{\Psi}_{l_2}(t_n)\Big| \prod_{j=1}^{2} (1+\mu_{l_j}^2)^{1/2} \Big)^2 \\
&\quad + n\sum_{k=0}^{n-1} \Big[\sum_{l\in\mathcal{T}_{M_0}} \Big(\sum_{(l_1,l_2)\in\mathcal{I}_l^{N_0}} \Big|\widehat{\mathbf{V}}_{l_1}\Big| \Big|\widehat{\Psi}_{l_2}(t_k) - \widehat{\Psi}_{l_2}(t_{k+1})\Big| \prod_{j=1}^{2} (1+\mu_{l_j}^2)^{1/2} \Big)^2 \Big] \Big\}.
\end{aligned}$$

In order to estimate each term in the above inequality, we use the auxiliary function $\Theta(x) = \sum_{l\in\mathbb{Z}} (1+\mu_l^2)^{1/2} \Big|\widehat{\Psi}_l(t_n)\Big| e^{i\mu_l(x-a)}$, where $\Theta(x) \in \big(H_{\rm per}^{m-1}(\Omega)\big)^2$, which can be verified from the assumption (B), and we can prove $\|\Theta(x)\|_{H^s} \lesssim \|\Psi(t_n)\|_{H^{s+1}}$ $(s \le m-1)$. Similarly, introduce the function $\mathbf{U}(x) = \sum_{l\in\mathbb{Z}} (1+\mu_l^2)^{1/2} \Big|\widehat{\mathbf{V}}_l\Big| e^{i\mu_l(x-a)}$, where $\mathbf{U}(x) \in W_{\rm per}^{m-1,\infty}(\Omega)$, as can be derived from the assumption (A). We can prove directly that $\|\mathbf{U}(x)\|_{W^{0,\infty}} \lesssim \|\mathbf{V}(x)\|_{W^{2,\infty}}$. By expanding

$$\mathbf{U}(x)\Theta(x) = \sum_{l\in\mathbb{Z}} \sum_{l_1+l_2=l} \prod_{j=1}^{2} (1+\mu_{l_j}^2)^{1/2} \Big|\widehat{\mathbf{V}}_{l_1}\Big| \Big|\widehat{\Psi}_{l_2}(t_n)\Big| e^{i\mu_l(x-a)},$$

we can obtain

$$\begin{aligned}
&\sum_{l\in\mathcal{T}_{M_0}} \Big(\sum_{(l_1,l_2)\in\mathcal{I}_l^{M_0}} \Big|\widehat{\mathbf{V}}_{l_1}\Big| \Big|\widehat{\Psi}_{l_2}(t_n)\Big| \prod_{j=1}^{2} (1+\mu_{l_j}^2)^{1/2} \Big)^2 \\
&\le \|\mathbf{U}(x)\Theta(x)\|_{L^2}^2 \lesssim \|\mathbf{V}(x)\|_{W^{2,\infty}}^2 \|\Psi(t_n)\|_{H^1}^2,
\end{aligned} \tag{4.31}$$

which together with the assumption (A), (4.10) and (4.11) gives

$$\begin{aligned}
\|\mathcal{L}^n\|_{L^2}^2 &\lesssim \varepsilon^2\tau^4 \|\mathbf{V}(x)\|_{W^{2,\infty}}^2 \Big(\|\Psi(t_n)\|_{H^1}^2 + n\sum_{k=0}^{n-1} \|\Psi(t_k) - \Psi(t_{k+1})\|_{H^1}^2 \Big) \\
&\lesssim \varepsilon^2\tau^4 + n^2\varepsilon^4\tau^6 \lesssim \varepsilon^2\tau^4
\end{aligned} \tag{4.32}$$

for $0 \le n \le \frac{T/\varepsilon}{\tau} - 1$, where the same trick is applied to the rest terms. By combining (4.13) and (4.32), we have

$$\|\mathbf{e}^{n+1}\|_{L^2} \lesssim \tau_0^m + \varepsilon\tau^2 + \varepsilon\tau \sum_{k=0}^{n} \|\mathbf{e}^k\|_{L^2}, \quad 0 \le n \le \frac{T/\varepsilon}{\tau} - 1. \tag{4.33}$$

The discrete Grönwall's inequality would yields $\|\mathbf{e}^{n+1}\|_{L^2} \lesssim \varepsilon\tau^2 + \tau_0^m$ $(0 \le n \le \frac{T/\varepsilon}{\tau} - 1)$, and the proof for the improved uniform error bound (4.1) in Theorem 4.1 is complete. ∎

Remark 4.2. $\tau_0 \in (0,1)$ is a parameter introduced in analysis, and the requirement on τ (essentially $\tau \lesssim \tau_0$) enables the improved estimates on the low Fourier

modes $|l| \le 1/\tau_0$, where the error constant depends on α. τ_0 can be arbitrary as long as the assumed relation between τ and τ_0 holds, i.e., τ_0 could be either fixed, or dependent on τ, e.g., $\tau_0 = \frac{\sqrt{16\pi^2+(b-a)^2}}{\alpha(b-a)\pi}\tau$.

Remark 4.3. The improved uniform error bounds are established for the second-order (Strang) splitting method. Under appropriate assumptions of the exact solution, the improved uniform error bounds can be extended to the first-order (Lie–Trotter) splitting and the fourth-order PRK splitting (PRK4) method with improved uniform error bounds at $\varepsilon\tau$ and $\varepsilon\tau^4$, respectively.

Remark 4.4. By introducing a rescale in time,

$$t = \frac{s}{\varepsilon} \Leftrightarrow s = \varepsilon t, \quad \Upsilon(s,x) = \Phi(t,x), \tag{4.34}$$

we can reformulate the Dirac equation (2.1) into the following oscillatory Dirac equation:

$$i\partial_s \Upsilon = (-\frac{i}{\varepsilon}\sigma_1\partial_x + \frac{1}{\varepsilon}\sigma_3)\Upsilon + (V(x)I_2 - A_1(x)\sigma_1)\Upsilon, \qquad x \in \Omega, \quad s > 0, \tag{4.35}$$

$$\Upsilon(s,a) = \Upsilon(s,b), \quad s \ge 0; \qquad \Upsilon(0,x) = \Phi_0(x), \quad x \in \overline{\Omega}, \tag{4.36}$$

where $\Upsilon := \Upsilon(s,x)$.

The long-time dynamics of the Dirac equation (2.1) up to the time $t = T/\varepsilon$ is equivalent to the oscillatory Dirac equation (4.35) up to the time $s = T$. The solution of the oscillatory Dirac equation (4.35) propagates waves with wavelength in space and time at $O(1)$ and $O(\varepsilon)$, respectively, and the wave velocity is at $O(1/\varepsilon)$. These properties of the wave are quite different from those of the Dirac equation in the nonrelativistic limit regime [4, 5], whose solutions propagate waves with wavelength in space and time at $O(1)$ and $O(\varepsilon^2)$, respectively, and the wave velocity is at $O(1)$!

According to Theorem 4.1, by taking the time step $\kappa = \varepsilon\tau$, the improved error bounds on the time-splitting method for the long-time problem can be extended to the oscillatory Dirac equation (4.35) up to the fixed time T. Let $\Upsilon^{[n]}(x)$ be the numerical approximation obtained from the semidiscretized second-order time-splitting for the Dirac equation (4.35). Under the assumption of the regularity of the exact solution(A), for $0 < \kappa_0 < 1$ sufficiently small and independent of ε, when $0 < \kappa < \alpha\varepsilon\kappa_0$ for a fixed constant $\alpha > 0$, we have the following improved error bound:

$$\left\|\Upsilon(s_n,x) - \Upsilon^{[n]}\right\|_{L^2} \lesssim \frac{\kappa^2}{\varepsilon} + \kappa_0^m, \quad 0 \le n \le \frac{T}{\kappa}. \tag{4.37}$$

In particular, if the exact solution is smooth, e.g., $\Upsilon(s,x) \in L^\infty([0,T];(H^\infty_{\rm per}(\Omega))^2)$, the improved error bound for sufficiently small κ will be

$$\left\|\Upsilon(s_n,x) - \Upsilon^{[n]}\right\|_{L^2} \lesssim \frac{\kappa^2}{\varepsilon}, \quad 0 \le n \le \frac{T}{\kappa}. \tag{4.38}$$

4.2. For full-discretization. For the TSFP method (2.12), we can establish the following improved uniform error bounds.

THEOREM 4.5. *Let Φ^n be the approximation obtained from the TSFP* (2.12) *for the Dirac equation* (2.4). *Under the assumption (A), for $0 < \tau_0 < 1$ sufficiently small and independent of ε, when $0 < \tau \le \alpha\frac{\pi(b-a)\tau_0}{\sqrt{\tau_0^2(b-a)^2+4\pi^2(1+\tau_0)^2}}$ for a fixed constant $\alpha \in (0,1)$, we have*

$$\|\Phi(t_n,x) - I_M\Phi^n\|_{L^2} \lesssim h^m + \varepsilon\tau^2 + \tau_0^m, \quad 0 \le n \le \frac{T/\varepsilon}{\tau}, \tag{4.39}$$

for any $0 < \varepsilon \le 1$. *In particular, if the exact solution is smooth, e.g.,* $\Phi(t,x) \in L^\infty([0,T_\varepsilon];(H^\infty_{\rm per}(\Omega))^2)$, *the improved uniform error bounds for sufficiently small* τ *will be*

$$\|\Phi(t_n,x) - I_M\Phi^n\|_{H^1} \lesssim h^m + \varepsilon\tau^2, \quad 0 \le n \le \frac{T/\varepsilon}{\tau}. \tag{4.40}$$

Proof. From the error estimates in previous sections, we have for $0 \le n \le \frac{T/\varepsilon}{\tau}$,

$$\left\|\Phi(t_n,x) - \Phi^{[n]}\right\|_{L^2} \lesssim \varepsilon\tau^2 + \tau_0^m, \quad \left\|\Phi^{[n]} - P_M\Phi^{[n]}\right\|_{L^2} \lesssim h^m. \tag{4.41}$$

Since $\Phi(t_n,x) - I_M\Phi^n = \Phi(t_n,x) - \Phi^{[n]} + \Phi^{[n]} - P_M\Phi^{[n]} + P_M\Phi^{[n]} - I_M\Phi^n$, we derive

$$\|\Phi(t_n,x) - I_M\Phi^n\|_{L^2} \le \left\|P_M\Phi^{[n]} - I_M\Phi^n\right\|_{L^2} + C_1\left(h^m + \varepsilon\tau^2 + \tau_0^m\right), \tag{4.42}$$

where C_1 is a constant independent of h, τ, n, ε, and τ_0. As a result, it remains to establish the estimates on the error function $\widetilde{\mathbf{e}}^n := \widetilde{\mathbf{e}}^n(x) \in Y_M$ given as

$$\widetilde{\mathbf{e}}^n(x) := P_M\Phi^{[n]} - I_M\Phi^n, \quad 0 \le n \le \frac{T/\varepsilon}{\tau}.$$

From (2.7) and (2.12), we get

$$I_M\Phi^{n+1} = e^{\frac{\tau\mathbf{T}}{2}}\left(I_M\left(e^{\varepsilon\tau\mathbf{V}}e^{\frac{\tau\mathbf{T}}{2}}(I_M\Phi^n)\right)\right),$$
$$P_M\Phi^{[n+1]} = e^{\frac{\tau\mathbf{T}}{2}}\left(P_M\left(e^{\varepsilon\tau\mathbf{V}}e^{\frac{\tau\mathbf{T}}{2}}(P_M\Phi^{[n]})\right)\right),$$

which lead to

$$\widetilde{\mathbf{e}}^{n+1} = e^{\tau\mathbf{T}}\widetilde{\mathbf{e}}^n + W^n(x), \tag{4.43}$$

where

$$W^n(x) = e^{\frac{\tau\mathbf{T}}{2}}\left[P_M\left((e^{\varepsilon\tau\mathbf{V}} - 1)e^{\frac{\tau\mathbf{T}}{2}}(P_M\Phi^{[n]})\right) - I_M\left((e^{\varepsilon\tau\mathbf{V}} - 1)e^{\frac{\tau\mathbf{T}}{2}}(I_M\Phi^n)\right)\right].$$

Similar to the error estimates in [5], we have the following error bounds:

$$\|W^n(x)\|_{L^2} \lesssim \varepsilon\tau\left(h^m + \|\widetilde{\mathbf{e}}^n\|_{L^2}\right). \tag{4.44}$$

Thus, we can obtain

$$\left\|\widetilde{\mathbf{e}}^{n+1}\right\|_{L^2} \le \|\widetilde{\mathbf{e}}^n\|_{L^2} + C_2\varepsilon\tau\left(h^m + \|\widetilde{\mathbf{e}}^n\|_{L^2}\right), \quad 0 \le n \le \frac{T/\varepsilon}{\tau} - 1, \tag{4.45}$$

where C_2 is a constant independent of h, τ, n, and ε. Since $\widetilde{\mathbf{e}}^0 = P_M\Phi_0 - I_M\Phi_0$, we have $\left\|\widetilde{\mathbf{e}}^0\right\|_{L^2} \lesssim h^m$, and the discrete Grönwall's inequality implies $\left\|\widetilde{\mathbf{e}}^{n+1}\right\|_{L^2} \lesssim h^m$ for $0 \le n \le \frac{T/\varepsilon}{\tau} - 1$. Combining the above estimates with (4.42), we derive

$$\|\Phi(t_n,x) - I_M\Phi^n\|_{L^2} \lesssim h^m + \varepsilon\tau^2 + \tau_0^m, \quad 0 \le n \le \frac{T/\varepsilon}{\tau},$$

which shows the improved uniform error bound (4.39), and the proof for Theorem 4.5 is complete. ∎

Remark 4.6. If the electromagnetic potential V and/or A_1 are time-dependent, the time-ordering technique [40] should be applied when we implement (2.7), as the operator $\mathbf{T} + \varepsilon\mathbf{V}$ is no longer commutable for different time coordinates $t_1 \ne t_2$.

Remark 4.7. The TSFP (2.12) conserves the mass in the discretized level as [4]

$$\|\Phi^n\|_{l^2}^2 := h\sum_{j=0}^{M-1}|\Phi_j^n|^2 \equiv h\sum_{j=0}^{M-1}|\Phi_j^0|^2 = \left\|\Phi^0\right\|_{l^2}^2 = h\sum_{j=0}^{M-1}|\Phi_0(x_j)|^2, \quad n \geq 0.$$

Introduce the discrete energy at $t = t_n$ as

$$E_h^n := h\sum_{j=0}^{M-1}\left[-i(\Phi_j^n)^*\sigma_1(\partial_x\Phi)_j^n + (\Phi_j^n)^*\sigma_3\Phi_j^n + \varepsilon V_j|\Phi_j^n|^2 - \varepsilon A_{1,j}(\Phi_j^n)^*\sigma_1\Phi_j^n\right],$$

where

$$(\partial_x\Phi)_j^n = i\sum_{l\in\mathcal{T}_M}\mu_l\widetilde{(\Phi^n)}_l e^{i\mu_l(x_j-a)}, \quad j = 0, 1, \ldots, M-1.$$

Then we have the following estimates for the discrete energy:

$$\left|E_h^n - E_h^0\right| \lesssim h^m + \varepsilon\tau^2 + \tau_0^m, \quad 0 \leq n \leq \frac{T/\varepsilon}{\tau}. \tag{4.46}$$

Furthermore, if the exact solution is smooth, e.g., $\Phi(t,x) \in L^\infty([0,T_\varepsilon];(H^\infty_{\rm per}(\Omega))^2)$, the estimate for the discrete energy for sufficiently small τ is

$$\left|E_h^n - E_h^0\right| \lesssim h^m + \varepsilon\tau^2, \quad 0 \leq n \leq \frac{T/\varepsilon}{\tau}. \tag{4.47}$$

5. Numerical results. In this section, we present numerical results of the TSFP method for the long-time dynamics of the Dirac equation with $O(\varepsilon)$-potentials up to the long time $T_\varepsilon = T/\varepsilon$.

5.1. For $\varepsilon = 1$ with $T \gg 1$ regime. First, we show an example to confirm that the uniform error bound grows linearly with respect to the time t. We take $\Omega = (0,1)$, the electromagnetic potentials

$$V(x) = x^2(x-1)^2 + 1, \quad A_1(x) = x^2(x-1)^2 + 1, \quad x \in \Omega, \tag{5.1}$$

and the $(H^2_{\rm per}(\Omega))^2$ initial data

$$\phi_1(x) = \phi_2(x) = \frac{1}{2}x^2(1-x)^2 + 3, \quad x \in \Omega. \tag{5.2}$$

The regularity is enough to ensure the uniform and improved error bounds. The "exact" solution $\Phi(t,x)$ is obtained numerically by the TSFP (2.12) with a very fine mesh size $h_e = 1/128$ and time step size $\tau_e = 10^{-4}$. To quantify the error, we introduce the following error functions:

$$e(t_n) = \left\|\Phi(t_n,x) - I_N\Phi^n\right\|_{L^2}, \quad e_{\max}(t_n) = \max_{0\leq q\leq n} e(t_q).$$

In the rest of the paper, the spatial mesh size is always chosen sufficiently small, and thus spatial errors can be ignored when considering the long-time error growth and/or the temporal errors.

Figure 1 depicts the long-time temporal errors of the TSFP method for the Dirac equation (2.1) with $\varepsilon = 1$ and different time step τ, which shows that the uniform errors grow linearly with respect to the time. In addition, for a given accuracy bound, the time to exceed the error bar is quadruple when the time step is half, which also confirms the linear growth. For comparisons, Figure 2 plots the long-time errors of the fourth-order partitioned Runge–Kutta splitting (PRK4) method, which indicates that higher order time-splitting methods get better accuracy with the same time step size as well as longer time simulations within a given accuracy bound.

5.2. For $\varepsilon \to 0$ with fixed T regime. Next, we report the convergence test for the TSFP method (2.12) for the Dirac equation (2.1) with the electromagnetic potentials (5.1) and the initial data (5.2).

Figure 3 plots the long-time errors of the TSFP method for the Dirac equation (2.1) with the fixed time step τ and different ε, which confirms the improved uniform error bound at $O(\varepsilon\tau^2)$ up to the long time at $O(1/\varepsilon)$. Figures 4 and 5 exhibit the

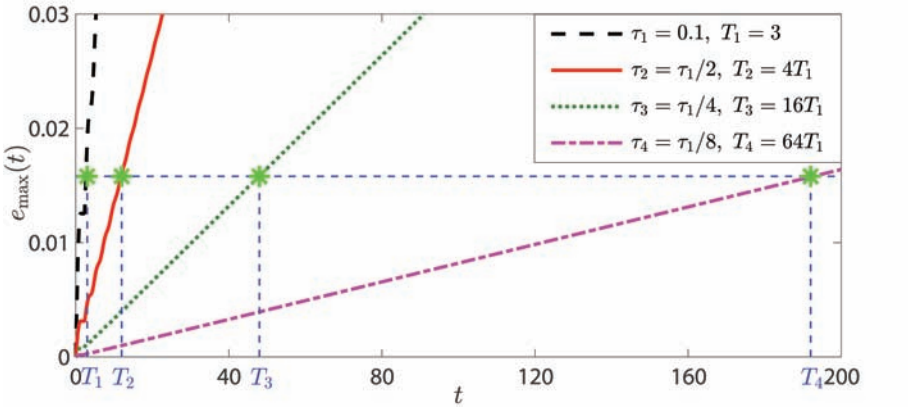

FIG. 1. *Long-time temporal errors of the TSFP* (2.12) *for the Dirac equation* (2.1) *with* $\varepsilon = 1$ *and different time step* τ.

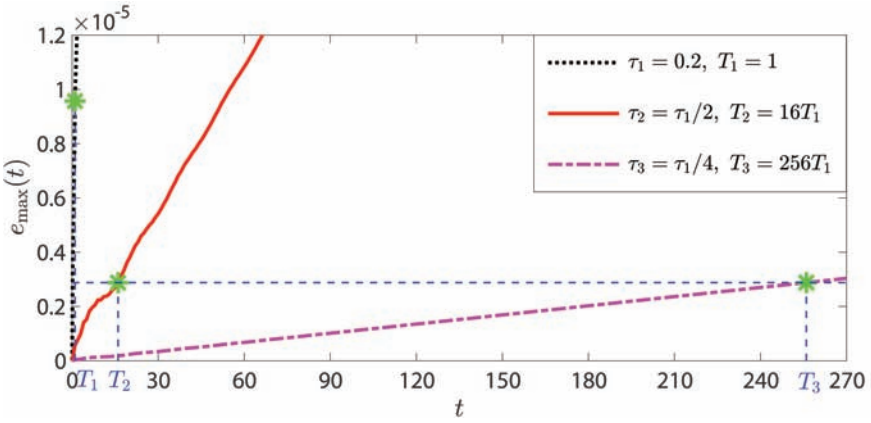

FIG. 2. *Long-time temporal errors of the PRK4 method for the Dirac equation* (2.1) *with* $\varepsilon = 1$ *and different time step* τ.

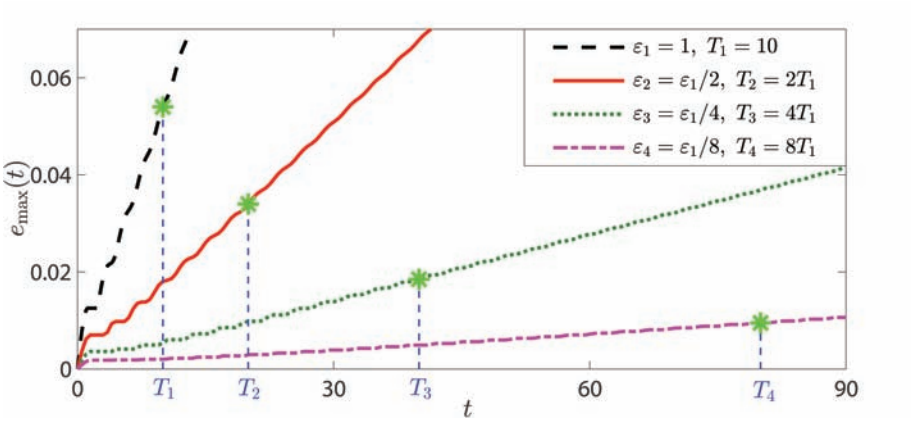

FIG. 3. *Long-time temporal errors of the TSFP* (2.12) *for the Dirac equation* (2.1) *with* $\tau = 0.1$ *and different* ε.

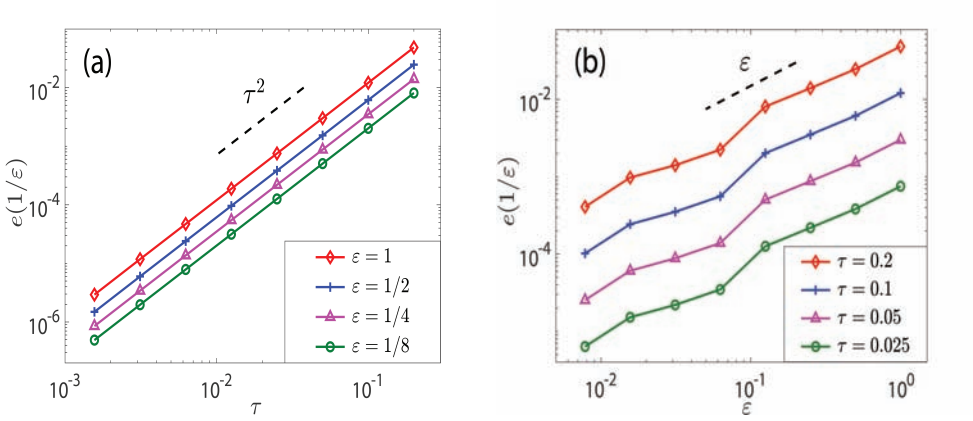

FIG. 4. *Temporal convergence rates of the TSFP* (2.12) *for the Dirac equation* (2.1) *over long-time dynamics at* $t = 1/\varepsilon$*; convergence rates in* τ (a)*, and convergence rates in* ε (b).

temporal and spatial errors of the TSFP (2.12) for the Dirac equation (2.1) at $t = 1/\varepsilon$. Figure 4(a) shows the second-order convergence of the TSFP method in time. Each line in Figure 4(b) gives the global errors with a fixed time step τ and verifies that the global error performs like $O(\varepsilon\tau^2)$ up to the long time at $O(1/\varepsilon)$. Each line in Figure 5(a) shows the spectral accuracy of the TSFP method in space, and Figure 5(b) verifies the spatial errors are independent of the small parameter ε in the long-time regime. Figure 6 plots the long-time errors for the discrete energy denoted as $e_{\text{Energy}}(t)$, which confirms the improved uniform error bounds (4.46) for the discrete energy.

5.3. Comparisons of different temporal discretizations. In this subsection, we compare the long-time temporal errors of the time-splitting methods with the finite difference method (FDM) and the exponential wave integrator (EWI) method [23, 24]. In order to compare the temporal errors, we adopt the Fourier pseudospectral

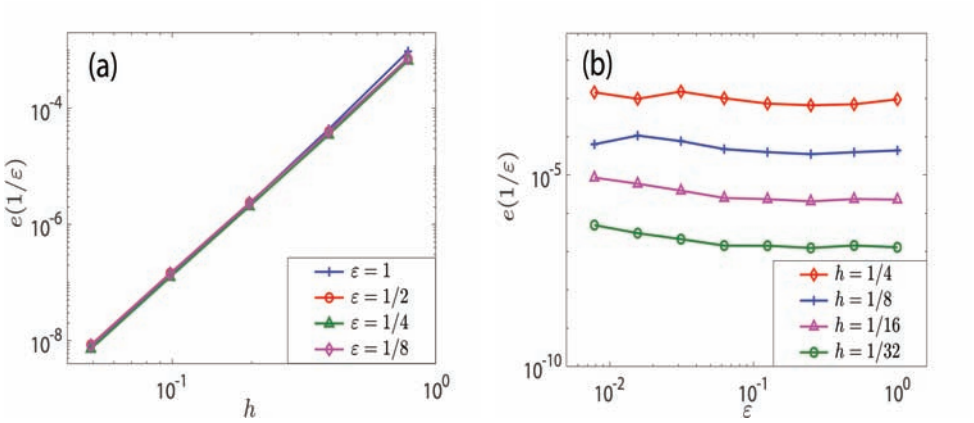

FIG. 5. *Spatial convergence rates of the TSFP* (2.12) *for the Dirac equation* (2.1) *over long-time dynamics at* $t = 1/\varepsilon$*; convergence rates in* h (a)*, and convergence rates in* ε (b).

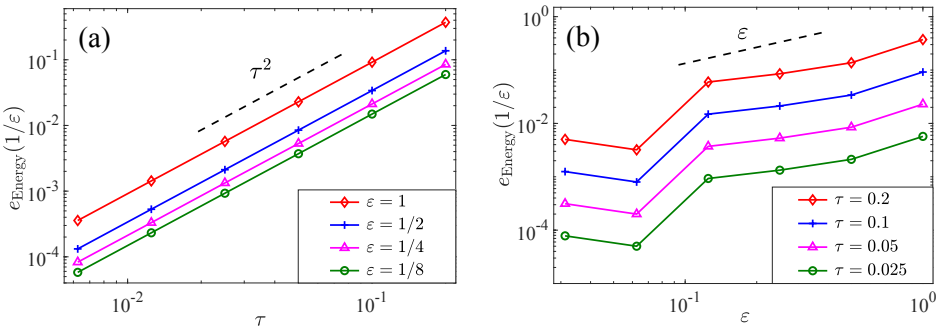

FIG. 6. *Convergences rates for the discrete energy of the TSFP* (2.12) *for the Dirac equation* (2.1) *over long-time dynamics at* $t = 1/\varepsilon$*; convergence rates in* τ (a)*, and convergence rates in* ε (b).

method in space combined with each temporal discretization and choose a fine mesh size such that the spatial errors are neglected.

Figure 7(a) displays the temporal errors for the fixed $\varepsilon = 1$ with different time step τ. For the three second-order schemes, the second-order (Strang) time-splitting method obtains smaller temporal errors than the other two methods with the same time step. The fourth-order time-splitting method (PRK4) not only has higher order convergent rate but also gives much smaller errors than the other three methods with the same time step. Figure 7(b) shows the long-time temporal errors of these methods for different ε with a fixed time step τ. The splitting methods have improved uniform error bounds like $O(\varepsilon\tau^2)$ up to the long time at $O(1/\varepsilon)$. The EWI method has uniform error bounds, while the long-time temporal errors of the finite difference method depend on the parameter ε and behave like $O(1/\varepsilon)$. As a result, time-splitting methods perform much better than FDM and EWI in the long-time simulations.

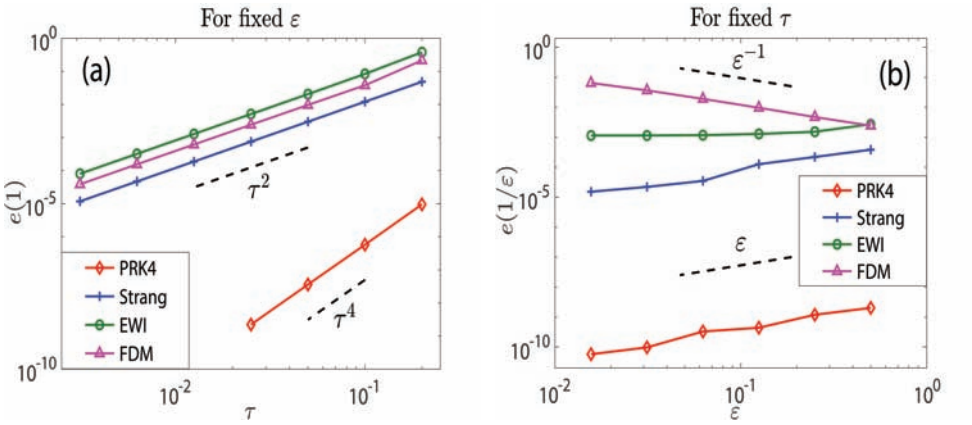

FIG. 7. *Temporal convergence rates of different temporal discretizations for the Dirac equation* (2.1) *over long-time dynamics at* $t = 1/\varepsilon$*; convergence rates in* τ (a)*, and convergence rates in* ε (b).

6. Conclusions. Improved uniform error bounds for the time-splitting methods for the long-time dynamics of the Dirac equation with small electromagnetic potentials were rigorously established. With the help of the unitary property of the solution flow in $L^2(\Omega)$, the linear growth of the uniform error bound for the time-splitting methods was strictly proven. By employing the regularity compensation oscillation (RCO) technique, the improved uniform error bounds were proved to be $O(\varepsilon\tau^2)$ and $O(h^m + \varepsilon\tau^2)$ up to the long time at $O(1/\varepsilon)$ for the semidiscretization and full-discretization, respectively. Numerical results were shown to validate our error bounds and to demonstrate that they are sharp. Finally, comparisons of different time discretizations were presented to illustrate the superior property of the time-splitting methods for the numerical simulation of the long-time dynamics of the Dirac equation.

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