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SUPER-RESOLUTION OF TIME-SPLITTING METHODS FOR THE DIRAC EQUATION IN THE NONRELATIVISTIC REGIME

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ABSTRACT. We establish error bounds of the Lie-Trotter splitting (S_1) and Strang splitting (S_2) for the Dirac equation in the nonrelativistic regime in the absence of external magnetic potentials, with a small parameter $0 < \varepsilon \leq 1$ inversely proportional to the speed of light. In this regime, the solution propagates waves with $O(\varepsilon^2)$ wavelength in time. Surprisingly, we find out that the splitting methods exhibit super-resolution, i.e., the methods can capture the solutions accurately even if the time step size τ is independent of ε, while the wavelength in time is at $O(\varepsilon^2)$. S_1 shows $1/2$ order convergence uniformly with respect to ε, by establishing that there are two independent error bounds $\tau + \varepsilon$ and $\tau + \tau/\varepsilon$. Moreover, if τ is nonresonant, i.e., τ is away from a certain region determined by ε, S_1 would yield an improved uniform first order $O(\tau)$ error bound. In addition, we show S_2 is uniformly convergent with $1/2$ order rate for general time step size τ and uniformly convergent with $3/2$ order rate for nonresonant time step size. Finally, numerical examples are reported to validate our findings.

1. INTRODUCTION

The splitting technique introduced by Trotter in 1959 [48] has been widely applied in analysis and numerical simulation [2, 9, 10, 20, 21], especially in computational quantum physics. In the Hamiltonian system and general ordinary differential equations (ODEs), the splitting approach has been shown to preserve the structural/geometric properties [33, 49] and is superior in many applications. Developments of splitting-type methods in solving partial differential equations (PDEs) include utilization in Schrödinger/nonlinear Schrödinger equations [2, 9, 10, 20, 21, 40, 47], Dirac/nonlinear Dirac equations [7, 8, 14, 39], the Maxwell-Dirac system [11, 34], the Zakharov system [12, 13, 30, 37, 38], Stokes equation [19], and Enrenfest dynamics [27], etc.

When dealing with oscillatory problems, the splitting method usually performs much better than traditional numerical methods [9, 33]. For instance, in order

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to obtain "correct" observables of the Schrödinger equation in the semiclassical regime, the time-splitting spectral method requires much weaker constraints on time step size and mesh size than the finite difference methods [9]. Similar properties have been observed for the nonlinear Schrödinger equation (NLSE)/Gross-Pitaevskii equation (GPE) in the semiclassical regime [2] and the Enrenfest dynamics [27]. However, in general, splitting methods still suffer from the mesh size/time step constraints related to the high frequencies in the aforementioned problems [5, 24, 36], i.e., in order to resolve a wave one needs to use a few grid points per wavelength. In this paper, we report a surprising finding that the splitting methods are uniformly accurate (w.r.t. the rapid oscillations), when applied to the Dirac equation in the nonrelativistic regime without external magnetic field. This fact reveals that there is no mesh size/time step restriction for splitting methods in this situation, e.g., the splitting methods have **super-resolution** independent of the wavelength, which is highly nontrivial. In the rest of the paper, we will discuss the oscillatory Dirac equation in the nonrelativistic regime, with conventional time-splitting numerical approach and its super-resolution properties.

Proposed by British physicist Paul Dirac in 1928 [25], the Dirac equation has now been extensively applied in the study of the structures and/or dynamical properties of graphene, graphite, and other two-dimensional (2D) materials [1, 28, 42, 43], as well as the relativistic effects of molecules in super intense lasers, e.g., attosecond lasers [16, 29]. Mathematically, the d-dimensional ($d = 1, 2, 3$) Dirac equation with external electro-magnetic potentials [7, 14] for the complex spinor vector field $\Psi := \Psi(t, \mathbf{x}) = (\psi_1(t, \mathbf{x}), \psi_2(t, \mathbf{x}), \psi_3(t, \mathbf{x}), \psi_4(t, \mathbf{x}))^T \in \mathbb{C}^4$ can be written as

$$i\partial_t \Psi = \left(-\frac{i}{\varepsilon} \sum_{j=1}^{d} \alpha_j \partial_j + \frac{1}{\varepsilon^2} \beta \right) \Psi + \left(V(t, \mathbf{x}) I_4 - \sum_{j=1}^{d} A_j(t, \mathbf{x}) \alpha_j \right) \Psi, \tag{1.1}$$

for $\mathbf{x} \in \mathbb{R}^d$, $t > 0$, with initial value

$$\Psi(t = 0, \mathbf{x}) = \Psi_0(\mathbf{x}), \qquad \mathbf{x} \in \mathbb{R}^d, \tag{1.2}$$

where $i = \sqrt{-1}$, t is time, $\mathbf{x} = (x_1, \ldots, x_d)^T \in \mathbb{R}^d$ is the spatial coordinate vector, $\partial_j = \frac{\partial}{\partial x_j}$ ($j = 1, \ldots, d$), $V := V(t, \mathbf{x})$ and $A_j := A_j(t, \mathbf{x})$ ($j = 1, \ldots, d$) are the given real-valued electric and magnetic potentials, respectively, $\varepsilon \in (0, 1]$ is a dimensionless parameter inversely proportional to the speed of light. There are two important regimes for the Dirac equation (1.1): the relativistic case $\varepsilon = O(1)$ (wave speed is comparable to the speed of light) and the nonrelativistic case $\varepsilon \ll 1$ (wave speed is much less than the speed of light). I_n is the $n \times n$ identity matrix for $n \in \mathbb{N}^*$, and the 4×4 matrices α_1, α_2, α_3, and β are

$$\begin{aligned} \alpha_1 &= \begin{pmatrix} \mathbf{0} & \sigma_1 \\ \sigma_1 & \mathbf{0} \end{pmatrix}, \qquad \alpha_2 = \begin{pmatrix} \mathbf{0} & \sigma_2 \\ \sigma_2 & \mathbf{0} \end{pmatrix}, \\ \alpha_3 &= \begin{pmatrix} \mathbf{0} & \sigma_3 \\ \sigma_3 & \mathbf{0} \end{pmatrix}, \qquad \beta = \begin{pmatrix} I_2 & \mathbf{0} \\ \mathbf{0} & -I_2 \end{pmatrix}, \end{aligned} \tag{1.3}$$

where σ_1, σ_2, σ_3 are the Pauli matrices

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \qquad \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \qquad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \tag{1.4}$$

In the relativistic regime $\varepsilon = O(1)$, extensive analytical and numerical studies have been carried out for the Dirac equation (1.1) in the literature. In the analytical aspect, for the existence and multiplicity of bound states and/or standing wave solutions, we refer to [22,23,26,31,32,45] and the references therein. In the numerical aspect, many accurate and efficient numerical methods have been proposed and analyzed [3,41], such as the finite difference time domain (FDTD) methods [4,44], the time-splitting Fourier pseudospectral (TSFP) method [7,34], the exponential wave integrator Fourier pseudospectral (EWI-FP) method [7], and the Gaussian beam method [50], etc.

In the nonrelativistic regime, as $\varepsilon \to 0^+$, the Dirac equation (1.1) converges to the Pauli equation [15,35] or the Schrödinger equation [5,15], and the solution propagates waves with wavelength $\mathrm{O}(\varepsilon^2)$ in time and $\mathrm{O}(1)$ in space, respectively. The highly oscillatory nature of the solution in time brings severe difficulties in numerical computation in the nonrelativistic regime, i.e., when $0 < \varepsilon \ll 1$. In fact, it would cause the time step size τ to be strictly dependent on ε in order to capture the solution accurately. Rigorous error estimates were established for the finite difference time domain method (FDTD), the exponential wave integrator Fourier pseudospectral method (EWI-FP), and the time-splitting Fourier pseudospectral method (TSFP) in this parameter regime [7]. The error bounds suggested $\tau = O(\varepsilon^3)$ for FDTD and $\tau = O(\varepsilon^2)$ for EWI-FP and TSFP. A new fourth order compact time-splitting method ($S_{4\mathrm{c}}$) was recently put forward to improve the efficiency and accuracy [14]. Moreover, a uniformly accurate multiscale time integrator pseudospectral method was proposed and analyzed for the Dirac equation in the nonrelativistic regime, where the errors are uniform with respect to $\varepsilon \in (0,1]$ [6], allowing for ε-independent time step τ.

From the analysis in [7], the error bounds for second order Strang splitting TSFP (also called S_2 later in this paper) depends on the small parameter ε as τ^2/ε^4. Surprisingly, through our extensive numerical experiments, we find out that if the magnetic potentials $A_j \equiv 0$ for $j = 1, \dots, d$ in (1.1), the errors of TSFP are then independent of ε and uniform w.r.t. ε, i.e., S_2 for Dirac equation (1.1) without magnetic potentials A_j has super-resolution w.r.t. ε. In such case, (1.1) reduces to ($d = 1,2,3$)

$$i\partial_t \Psi(t,\mathbf{x}) = \left(-\frac{i}{\varepsilon}\sum_{j=1}^{d} \alpha_j \partial_j + \frac{1}{\varepsilon^2}\beta + V(t,\mathbf{x}) I_4 \right) \Psi(t,\mathbf{x}), \quad \mathbf{x} \in \mathbb{R}^d,\ t > 0, \tag{1.5}$$

with the initial value given in (1.2). In lower dimensions ($d = 1,2$), the four component Dirac equation (1.5) can be reduced to the following two-component form for $\Phi(t,\mathbf{x}) = (\phi_1(t,\mathbf{x}), \phi_2(t,\mathbf{x}))^T \in \mathbb{C}^2$ ($d = 1,2$) [7]:

$$i\partial_t \Phi(t,\mathbf{x}) = \left(-\frac{i}{\varepsilon}\sum_{j=1}^{d} \sigma_j \partial_j + \frac{1}{\varepsilon^2}\sigma_3 + V(t,\mathbf{x}) I_2 \right) \Phi(t,\mathbf{x}), \quad \mathbf{x} \in \mathbb{R}^d,\ t > 0, \tag{1.6}$$

with initial value

$$\Phi(t = 0,\mathbf{x}) = \Phi_0(\mathbf{x}), \qquad \mathbf{x} \in \mathbb{R}^d. \tag{1.7}$$

The two-component form (1.6) is widely used in lower dimensions $d = 1,2$ due to its simplicity compared to the four-component form (1.5).

Our extensive numerical studies and theoretical analysis show that for first order, second order, and even higher order time-splitting Fourier pseudospectral methods, there are always uniform error bounds w.r.t. $\varepsilon \in (0,1]$. In other words, the splitting methods can capture the solutions accurately even if the time step size τ is independent of ε, i.e., they exhibit ε-independent **super-resolution**. As the **super-resolution** here suggests independence of the oscillation wavelength, it is even stronger than the "super-resolution" in [24] for the Schrödinger equation in the semiclassical regime, where the restriction on the time steps is still related to the wavelength, but not so strict as the resolution of the oscillation by a fixed number of points per wavelength. This super-resolution property of the splitting methods makes them more efficient and reliable for solving the Dirac equation without magnetic potentials in the nonrelativisitc regime, compared to other numerical approaches in the literature. In what follows, we will study rigorously the super-resolution phenomenon for first order (S_1) and second order (S_2) time-splitting methods, and present numerical results to validate the conclusions.

The rest of the paper is organized as follows. In section 2, we review the first and second order time-splitting methods for the Dirac equation in the nonrelativistic regime without magnetic potential, and state the main results. In sections 3 and 4, respectively, detailed proofs for the uniform error bounds and improved uniform error bounds are presented. Section 5 is devoted to numerical tests, and finally, some concluding remarks are drawn in section 6. Throughout the paper, we adopt the standard Sobolev spaces and the corresponding norms. Meanwhile, $A \lesssim B$ is used with the meaning that there exists a generic constant $C > 0$ independent of ε and τ, such that $|A| \le C\,B$. $A \lesssim_\delta B$ has a similar meaning that there exists a constant $C_\delta > 0$ dependent on δ but independent of ε and τ, such that $|A| \le C_\delta\, B$.

2. Time-splitting methods and main results

In this section, we recall the first and second order time-splitting methods applied to the Dirac equation and state the main results of this paper. For the simplicity of presentation, we only carry out the splitting methods and corresponding analysis for (1.6) in 1D ($d = 1$). Generalization to (1.5) and/or higher dimensions is straightforward and results remain valid without modifications (see the appendix).

2.1. Time-splitting methods.

Denote the Hermitian operator

$$\mathcal{T}^\varepsilon = -i\varepsilon\sigma_1\partial_x + \sigma_3, \quad x \in \mathbb{R}, \tag{2.1}$$

and the Dirac equation (1.6) in 1D can be written as

$$i\partial_t\Phi(t,x) = \frac{1}{\varepsilon^2}\mathcal{T}^\varepsilon\Phi(t,x) + V(t,x)\Phi(t,x), \quad x \in \mathbb{R}, \tag{2.2}$$

with initial value

$$\Phi(0,x) = \Phi_0(x), \quad x \in \mathbb{R}. \tag{2.3}$$

Choose $\tau > 0$ to be the time step size and $t_n = n\tau$ for $n = 0, 1, \ldots$ as the time steps. Denote $\Phi^n(x)$ as the numerical approximation of $\Phi(t_n, x)$, where $\Phi(t,x)$ is the exact solution to (2.2) with (2.3); then the first order and second order time-splitting methods can be expressed as follows.

First order splitting (Lie-Trotter splitting). The discrete-in-time first order splitting (S_1) is written as [48]

$$\Phi^{n+1}(x) = e^{-\frac{i\tau}{\varepsilon^2}\mathcal{T}^\varepsilon} e^{-i\int_{t_n}^{t_{n+1}} V(s,x)\,ds}\Phi^n(x), \quad x \in \mathbb{R}, \tag{2.4}$$

with $\Phi^0(x) = \Phi_0(x)$.

Second order splitting (Strang splitting). The discrete-in-time second order splitting (S_2) is written as [46]

$$\Phi^{n+1}(x) = e^{-\frac{i\tau}{2\varepsilon^2}\mathcal{T}^\varepsilon} e^{-i\int_{t_n}^{t_{n+1}} V(s,x)\,ds} e^{-\frac{i\tau}{2\varepsilon^2}\mathcal{T}^\varepsilon}\Phi^n(x), \quad x \in \mathbb{R}, \tag{2.5}$$

with $\Phi^0(x) = \Phi_0(x)$.

Then the main results of this paper can be summarized below.

2.2. **Uniform error bounds.** For any $T > 0$, we are going to consider smooth enough solutions, i.e., we assume the electric potential satisfies

$$V(t,x) \in W^{m,\infty}([0,T]; L^\infty(\mathbb{R})) \cap L^\infty([0,T]; W^{2m+m_*,\infty}(\mathbb{R})), \tag{A}$$

with $m \in \mathbb{N}^*$, $m_* \in \{0,1\}$. In addition, we assume the exact solution $\Phi(t,x)$ satisfies

$$\Phi(t,x) \in L^\infty([0,T], (H^{2m+m_*}(\mathbb{R}))^2), \quad m \in \mathbb{N}^*, \quad m_* \in \{0,1\}. \tag{B}$$

We remark here that if the initial value $\Phi_0(\mathbf{x}) \in (H^{2m+m_*}(\mathbb{R}))^2$, then condition (B) is implied by condition (A).

For the numerical approximation $\Phi^n(x)$ obtained from S_1 (2.4) or S_2 (2.5), we introduce the error function

$$\mathbf{e}^n(x) = \Phi(t_n,x) - \Phi^n(x), \quad 0 \le n \le \frac{T}{\tau}; \tag{2.6}$$

then the following error estimates hold.

Theorem 2.1. *Let $\Phi^n(x)$ be the numerical approximation obtained from S_1* (2.4)*. Then under the assumptions* (A) *and* (B) *with $m = 1$ and $m_* = 0$, we have the following error estimates:*

$$\|\mathbf{e}^n(x)\|_{L^2} \lesssim \tau + \varepsilon, \quad \|\mathbf{e}^n(x)\|_{L^2} \lesssim \tau + \tau/\varepsilon, \quad 0 \le n \le \frac{T}{\tau}. \tag{2.7}$$

As a result, there is a uniform error bound for S_1

$$\|\mathbf{e}^n(x)\|_{L^2} \lesssim \tau + \max_{0<\varepsilon\le 1}\min\{\varepsilon, \tau/\varepsilon\} \lesssim \sqrt{\tau}, \quad 0 \le n \le \frac{T}{\tau}. \tag{2.8}$$

Theorem 2.2. *Let $\Phi^n(x)$ be the numerical approximation obtained from S_2* (2.5)*. Then under the assumptions* (A) *and* (B) *with $m = 2$ and $m_* = 0$, we have the following error estimates:*

$$\|\mathbf{e}^n(x)\|_{L^2} \lesssim \tau^2 + \varepsilon, \quad \|\mathbf{e}^n(x)\|_{L^2} \lesssim \tau^2 + \tau^2/\varepsilon^3, \quad 0 \le n \le \frac{T}{\tau}. \tag{2.9}$$

As a result, there is a uniform error bound for S_2

$$\|\mathbf{e}^n(x)\|_{L^2} \lesssim \tau^2 + \max_{0<\varepsilon\le 1}\min\{\varepsilon, \tau^2/\varepsilon^3\} \lesssim \sqrt{\tau}, \quad 0 \le n \le \frac{T}{\tau}. \tag{2.10}$$

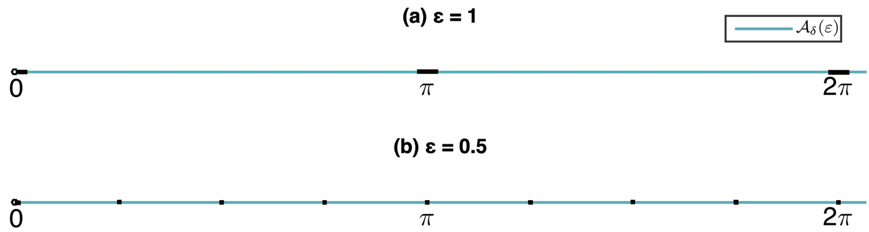

FIGURE 2.1. Illustration of nonresonant time steps $\mathcal{A}_\delta(\varepsilon)$ with $\delta = 0.15$ for (a) $\varepsilon = 1$ and (b) $\varepsilon = 0.5$.

Remark 2.3. The error bounds in Theorem 2.1 can be expressed as

$$\|\mathbf{e}^n(x)\|_{L^2} \le (C_1 + C_2 T) \max_{t\in[0,T]} \|\Phi(t,x)\|_{H^2} \left(\tau + \max_{0<\varepsilon\le 1} \min\{\varepsilon, \tau/\varepsilon\}\right), \tag{2.11}$$

and the error estimates in Theorem 2.2 can be restated as

$$\|\mathbf{e}^n(x)\|_{L^2} \le (C_3 + C_4 T) \max_{t\in[0,T]} \|\Phi(t,x)\|_{H^4} \left(\tau^2 + \max_{0<\varepsilon\le 1} \min\{\varepsilon, \tau^2/\varepsilon^3\}\right), \tag{2.12}$$

for $0 \le n \le \frac{T}{\tau}$, where C_1, C_2, C_3, and C_4 are constants depending only on $V(t,x)$. We notice here that the error constants are linear in T.

We note that higher order time-splitting methods also share the super-resolution property, but for simplicity, we only focus on S_1 and S_2 here. Remark 2.3 could be easily derived by examining the proofs of Theorems 2.1 and 2.2, and the details will be skipped.

2.3. **Improved uniform error bounds for nonresonant time steps.** In the Dirac equation (1.6) or (1.5), the leading term is $\frac{1}{\varepsilon^2}\sigma_3\Phi$ or $\frac{1}{\varepsilon^2}\beta\Psi$, which suggests the solution exhibits almost periodicity in time with periods $2k\pi\varepsilon^2$ ($k \in \mathbb{N}^*$, the periods of $e^{-it\sigma_3/\varepsilon^2}$ and $e^{-it\beta/\varepsilon^2}$). From numerical results, we observe the errors behave much better compared to the results in Theorems 2.1 and 2.2, when 2τ is away from the leading temporal oscillation periods $2k\pi\varepsilon^2$. In fact, for given $0 < \delta \le 1$, define

$$\mathcal{A}_\delta(\varepsilon) := \bigcup_{k=0}^{\infty} \left[\varepsilon^2 k\pi + \varepsilon^2 \arcsin\delta, \varepsilon^2(k+1)\pi - \varepsilon^2 \arcsin\delta\right], \quad 0 < \varepsilon \le 1, \tag{2.13}$$

and the errors of S_1 and S_2 can be improved compared to the previous subsection when $\tau \in \mathcal{A}_\delta(\varepsilon)$. To illustrate $\mathcal{A}_\delta(\varepsilon)$, we show in Figure 2.1 for $\varepsilon = 1$ and $\varepsilon = 0.5$ with fixed $\delta = 0.15$.

For $\tau \in \mathcal{A}_\delta(\varepsilon)$, we can derive improved uniform error bounds for the two splitting methods as shown in the following two theorems.

Theorem 2.4. *Let $\Phi^n(x)$ be the numerical approximation obtained from S_1* (2.4)*. If the time step size τ is nonresonant, i.e., there exists $0 < \delta \le 1$, such that $\tau \in \mathcal{A}_\delta(\varepsilon)$, under the assumptions* (A) *and* (B) *with $m = 1$ and $m_* = 1$, we have an improved uniform error bound*

$$\|\mathbf{e}^n(x)\|_{L^2} \lesssim_\delta \tau, \quad 0 \le n \le \frac{T}{\tau}. \tag{2.14}$$

Theorem 2.5. *Let $\Phi^n(x)$ be the numerical approximation obtained from S_2* (2.5)*. If the time step size τ is nonresonant, i.e., there exists $0 < \delta \le 1$, such that $\tau \in \mathcal{A}_\delta(\varepsilon)$, under the assumptions* (A) *and* (B) *with $m = 2$ and $m_* = 1$, we assume an extra regularity $V(t, x) \in W^{1,\infty}([0, T]; H^3(\mathbb{R}))$ and then the following two error estimates hold:*

$$\|\mathbf{e}^n(x)\|_{L^2} \lesssim_\delta \tau^2 + \tau\varepsilon, \quad \|\mathbf{e}^n(x)\|_{L^2} \lesssim_\delta \tau^2 + \tau^2/\varepsilon, \quad 0 \le n \le \frac{T}{\tau}. \tag{2.15}$$

As a result, there is an improved uniform error bound for S_2

$$\|\mathbf{e}^n(x)\|_{L^2} \lesssim_\delta \tau^2 + \max_{0<\varepsilon\le 1} \min\{\tau\varepsilon, \tau^2/\varepsilon\} \lesssim_\delta \tau^{3/2}, \quad 0 \le n \le \frac{T}{\tau}. \tag{2.16}$$

Remark 2.6. In Theorems 2.4 and 2.5, the constants in the error estimates depend on δ and the proof in the paper suggests that the constants are bounded from above by $\frac{T}{\tau}C$ and $\frac{2}{\delta}C$ with some common factor C independent of δ and τ. The optimality of the uniform error bounds in Theorems 2.4 and 2.5 will be verified by numerical examples presented in section 5.

Remark 2.7. The results in Theorems 2.1, 2.2, 2.4 and 2.5 can be generalized to higher dimensions ($d = 2, 3$) for Dirac equation (1.5)/(1.6) by similar arguments. We will sketch a proof in the appendix.

3. Proof of Theorems 2.1 and 2.2

In this section, we prove the uniform error bounds for the splitting methods S_1 and S_2. As $\mathcal{T}^\varepsilon$ is diagonalizable in the phase space (Fourier domain), it can be decomposed as [6, 7, 15]

$$\mathcal{T}^\varepsilon = \sqrt{\mathrm{Id} - \varepsilon^2\Delta}\, \Pi_+^\varepsilon - \sqrt{\mathrm{Id} - \varepsilon^2\Delta}\, \Pi_-^\varepsilon, \tag{3.1}$$

where $\Delta = \partial_{xx}$ is the Laplace operator in 1D and Id is the identity operator. Π_+^ε and Π_-^ε are projectors defined as

$$\Pi_+^\varepsilon = \frac{1}{2}\left[I_2 + \left(\mathrm{Id} - \varepsilon^2\Delta\right)^{-1/2}\mathcal{T}^\varepsilon\right], \quad \Pi_-^\varepsilon = \frac{1}{2}\left[I_2 - \left(\mathrm{Id} - \varepsilon^2\Delta\right)^{-1/2}\mathcal{T}^\varepsilon\right]. \tag{3.2}$$

It is straightforward to see that $\Pi_+^\varepsilon + \Pi_-^\varepsilon = I_2$, and $\Pi_+^\varepsilon\Pi_-^\varepsilon = \Pi_-^\varepsilon\Pi_+^\varepsilon = \mathbf{0}$, $(\Pi_\pm^\varepsilon)^2 = \Pi_\pm^\varepsilon$. Furthermore, through Taylor expansion, we have [15]

$$\Pi_+^\varepsilon = \Pi_+^0 + \varepsilon\mathcal{R}_1 = \Pi_+^0 - i\frac{\varepsilon}{2}\sigma_1\partial_x + \varepsilon^2\mathcal{R}_2, \quad \Pi_+^0 = \mathrm{diag}(1, 0), \tag{3.3}$$

$$\Pi_-^\varepsilon = \Pi_-^0 - \varepsilon\mathcal{R}_1 = \Pi_-^0 + i\frac{\varepsilon}{2}\sigma_1\partial_x - \varepsilon^2\mathcal{R}_2, \quad \Pi_-^0 = \mathrm{diag}(0, 1), \tag{3.4}$$

where $\mathcal{R}_1 : (H^m(\mathbb{R}))^2 \to (H^{m-1}(\mathbb{R}))^2$ for $m \ge 1$, $m \in \mathbb{N}^*$, and $\mathcal{R}_2 : (H^m(\mathbb{R}))^2 \to (H^{m-2}(\mathbb{R}))^2$ for $m \ge 2$, $m \in \mathbb{N}^*$ are uniformly bounded operators with respect to ε.

To help capture the features of solutions, denote

$$\mathcal{D}^\varepsilon = \frac{1}{\varepsilon^2}(\sqrt{\mathrm{Id} - \varepsilon^2\Delta} - \mathrm{Id}) = -(\sqrt{\mathrm{Id} - \varepsilon^2\Delta} + \mathrm{Id})^{-1}\Delta, \tag{3.5}$$

where $\mathcal{D}^\varepsilon$ is a uniformly bounded operator with respect to ε from $(H^m(\mathbb{R}))^2$ to $(H^{m-2}(\mathbb{R}))^2$ for $m \ge 2$. Then we have the decomposition for the unitary evolution operator $e^{it\mathcal{T}^\varepsilon/\varepsilon^2}$ as [6, 18]

$$e^{\frac{it}{\varepsilon^2}\mathcal{T}^\varepsilon} = e^{\frac{it}{\varepsilon^2}(\sqrt{\mathrm{Id}-\varepsilon^2\Delta}\,\Pi_+^\varepsilon - \sqrt{\mathrm{Id}-\varepsilon^2\Delta}\,\Pi_-^\varepsilon)} = e^{it/\varepsilon^2}e^{it\mathcal{D}^\varepsilon}\,\Pi_+^\varepsilon + e^{-it/\varepsilon^2}e^{-it\mathcal{D}^\varepsilon}\,\Pi_-^\varepsilon. \tag{3.6}$$

For the ease of the proof, we first introduce the following two lemmas for the Lie-Trotter splitting S_1 (2.4) and the Strang splitting S_2 (2.5), respectively. For simplicity, we denote $V(t) := V(t,x)$, and $\Phi(t) := \Phi(t,x)$ for short.

Lemma 3.1. *Let $\Phi^n(x)$ be the numerical approximation obtained from the Lie-Trotter splitting S_1 (2.4). Then under the assumptions (A) and (B) with $m=1$ and $m_*=0$, we have*

$$\mathbf{e}^{n+1}(x) = e^{-\frac{i\tau}{\varepsilon^2}\mathcal{T}^\varepsilon} e^{-i\int_{t_n}^{t_{n+1}} V(s,x)ds}\mathbf{e}^n(x) + \eta_1^n(x) + \eta_2^n(x), \quad 0 \le n \le \frac{T}{\tau} - 1, \tag{3.7}$$

with $\|\eta_1^n(x)\|_{L^2} \lesssim \tau^2$, $\eta_2^n(x) = -ie^{-\frac{i\tau}{\varepsilon^2}\mathcal{T}^\varepsilon}\left(\int_0^\tau f_2^n(s)ds - \tau f_2^n(0)\right)$, where

$$\begin{aligned} f_2^n(s) =& e^{i2s/\varepsilon^2} e^{is\mathcal{D}^\varepsilon}\Pi_+^\varepsilon \left(V(t_n)\Pi_-^\varepsilon e^{is\mathcal{D}^\varepsilon}\Phi(t_n)\right) \\ &+ e^{-i2s/\varepsilon^2} e^{-is\mathcal{D}^\varepsilon}\Pi_-^\varepsilon \left(V(t_n)\Pi_+^\varepsilon e^{-is\mathcal{D}^\varepsilon}\Phi(t_n)\right). \end{aligned} \tag{3.8}$$

Proof. From the definition of $\mathbf{e}^n(x)$, noticing the Lie-Trotter splitting formula (2.4), we have

$$\mathbf{e}^{n+1}(x) = e^{-\frac{i\tau}{\varepsilon^2}\mathcal{T}^\varepsilon} e^{-i\int_{t_n}^{t_{n+1}} V(s,x)\,ds}\mathbf{e}^n(x) + \eta^n(x), \quad 0 \le n \le \frac{T}{\tau} - 1, \quad x \in \mathbb{R}, \tag{3.9}$$

where $\eta^n(x)$ is the local truncation error defined as

$$\eta^n(x) = \Phi(t_{n+1},x) - e^{-\frac{i\tau}{\varepsilon^2}\mathcal{T}^\varepsilon} e^{-i\int_{t_n}^{t_{n+1}} V(s,x)\,ds}\Phi(t_n,x), \quad x \in \mathbb{R}. \tag{3.10}$$

Noticing (2.2), and applying Duhamel's principle, we derive

$$\Phi(t_{n+1},x) = e^{-\frac{i\tau}{\varepsilon^2}\mathcal{T}^\varepsilon}\Phi(t_n,x) - i\int_0^\tau e^{-\frac{i(\tau-s)}{\varepsilon^2}\mathcal{T}^\varepsilon} V(t_n+s,x)\Phi(t_n+s,x)ds, \tag{3.11}$$

while Taylor expansion gives

$$\begin{aligned} &e^{-\frac{i\tau}{\varepsilon^2}\mathcal{T}^\varepsilon} e^{-i\int_{t_n}^{t_{n+1}} V(s,x)\,ds}\Phi(t_n,x) \\ &= e^{-\frac{i\tau}{\varepsilon^2}\mathcal{T}^\varepsilon}\left(1 - i\int_{t_n}^{t_{n+1}} V(s,x)\,ds + O(\tau^2)\right)\Phi(t_n,x). \end{aligned} \tag{3.12}$$

Combining (3.11), (3.12), and (3.10), we get

$$\begin{aligned} \eta^n(x) =& \tau i e^{-\frac{i\tau}{\varepsilon^2}\mathcal{T}^\varepsilon} V(t_n)\Phi(t_n) - i\int_0^\tau e^{-\frac{i(\tau-s)}{\varepsilon^2}\mathcal{T}^\varepsilon}\left(V(t_n)e^{-\frac{is}{\varepsilon^2}\mathcal{T}^\varepsilon}\Phi(t_n)\right) ds \\ &+ \sum_{j=1}^2 R_j^n(x), \end{aligned} \tag{3.13}$$

where

$$\begin{aligned} R_1^n(x) &= e^{-\frac{i\tau}{\varepsilon^2}\mathcal{T}^\varepsilon}\left(\lambda_1^n(x) + \lambda_2^n(x)\right)\Phi(t_n,x), \\ R_2^n(x) &= -i\int_0^\tau e^{-\frac{i(\tau-s)}{\varepsilon^2}\mathcal{T}^\varepsilon}\left(V(t_n)\lambda_4^n(s,x) + \lambda_3^n(s,x)\Phi(t_n+s,x)\right) ds, \end{aligned}$$

with

$$\lambda_1^n(x) = e^{-i\int_{t_n}^{t_{n+1}} V(s,x)ds} - \left(1 - i\int_{t_n}^{t_{n+1}} V(s,x)ds\right), \tag{3.14}$$

$$\lambda_2^n(x) = -i\int_{t_n}^{t_{n+1}} V(u,x)\,du + i\tau V(t_n,x), \tag{3.15}$$

$$\lambda_3^n(s,x) = V(t_n+s,x) - V(t_n,x), \quad 0 \le s \le \tau, \tag{3.16}$$

$$\lambda_4^n(s,x) = -i\int_0^s e^{-\frac{i(s-w)}{\varepsilon^2}\mathcal{T}^\varepsilon}\left(V(t_n+w,x)\Phi(t_n+w,x)\right)dw, \quad 0 \le s \le \tau. \tag{3.17}$$

It is easy to see that for $0 \le n \le \frac{T}{\tau} - 1$,

$$\begin{aligned}
&\|\lambda_1^n(x)\|_{L^\infty} \lesssim \tau^2 \|V(t,x)\|^2_{L^\infty(L^\infty)}, \quad \|\lambda_2^n(x)\|_{L^\infty} \lesssim \tau^2 \|\partial_t V(t,x)\|_{L^\infty(L^\infty)},\\
&\|\lambda_3^n(s,x)\|_{L^\infty([0,\tau];L^\infty)} \lesssim \tau \|\partial_t V(t,x)\|_{L^\infty(L^\infty)},\\
&\|\lambda_4^n(s,x)\|_{L^\infty([0,\tau];(L^2)^2)} \lesssim \tau \|V(t,x)\|_{L^\infty(L^\infty)} \|\Phi(t,x)\|_{L^\infty((L^2)^2)}.
\end{aligned}$$

As a consequence, we obtain the following bounds for $0 \le n \le \frac{T}{\tau} - 1$:

$$\|R_1^n(x)\|_{L^2} \lesssim \left(\|\lambda_1^n(x)\|_{L^\infty} + \|\lambda_2^n(x)\|_{L^\infty}\right)\|\Phi(t_n)\|_{L^2} \lesssim \tau^2, \tag{3.18}$$

$$\begin{aligned}
\|R_2^n(x)\|_{L^2} \lesssim \tau \Big(&\|V(t_n)\|_{L^\infty} \|\lambda_4^n(s,x)\|_{L^\infty([0,\tau];(L^2)^2)}\\
&+ \|\lambda_3^n(s,x)\|_{L^\infty([0,\tau];L^\infty)} \|\Phi\|_{L^\infty((L^2)^2)} \Big) \lesssim \tau^2.
\end{aligned} \tag{3.19}$$

Recalling $\eta_2^n(x)$ given in Lemma 3.1, we introduce for $0 \le s \le \tau$

$$f^n(s) := f^n(s,x) = e^{\frac{is}{\varepsilon^2}\mathcal{T}^\varepsilon}\left(V(t_n,x) e^{-\frac{is}{\varepsilon^2}\mathcal{T}^\varepsilon}\Phi(t_n,x)\right) = f_1^n(s) + f_2^n(s), \tag{3.20}$$

with f_2^n given in (3.8) and f_1^n from the decomposition (3.6) as

$$f_1^n(s) = e^{is\mathcal{D}^\varepsilon}\,\Pi_+^\varepsilon\left(V(t_n)e^{-is\mathcal{D}^\varepsilon}\Pi_+^\varepsilon\Phi(t_n)\right) + e^{-is\mathcal{D}^\varepsilon}\,\Pi_-^\varepsilon\left(V(t_n)e^{is\mathcal{D}^\varepsilon}\Pi_-^\varepsilon\Phi(t_n)\right),$$

and then $\eta^n(x)$ (3.13) can be written as

$$\begin{aligned}
\eta^n(x) = &- ie^{-\frac{i\tau}{\varepsilon^2}\mathcal{T}^\varepsilon}\left(\int_0^\tau (f_1^n(s) + f_2^n(s))ds - \tau(f_1^n(0) + f_2^n(0))\right)\\
&+ R_1^n(x) + R_2^n(x).
\end{aligned} \tag{3.21}$$

Now, it is easy to verify that $\eta^n(x) = \eta_1^n(x) + \eta_2^n(x)$ with $\eta_2^n(x)$ given in Lemma 3.1 if we let

$$\eta_1^n(x) = -ie^{-\frac{i\tau}{\varepsilon^2}\mathcal{T}^\varepsilon}\left(\int_0^\tau f_1^n(s)ds - \tau f_1^n(0)\right) + R_1^n(x) + R_2^n(x). \tag{3.22}$$

Noticing that

$$\begin{aligned}
&\left\| e^{-\frac{i\tau}{\varepsilon^2}\mathcal{T}^\varepsilon}\left(\int_0^\tau f_1^n(s)ds - \tau f_1^n(0)\right)\right\|_{L^2}\\
&\lesssim \tau^2 \|\partial_s f_1^n(\cdot)\|_{L^\infty([0,\tau];(L^2)^2)} \lesssim \tau^2 \|V(t_n)\|_{W^{2,\infty}} \|\Phi(t_n)\|_{H^2},
\end{aligned}$$

recalling the regularity assumptions (A) and (B), and combining (3.18) and (3.19), we can get

$$\begin{aligned}\|\eta_1^n(x)\|_{L^2} &\leq \|R_1^n(x)\|_{L^2} + \|R_2^n(x)\|_{L^2} + \left\| e^{-\frac{i\tau}{\varepsilon^2}\mathcal{T}^\varepsilon} \left(\int_0^\tau f_1^n(s)ds - \tau f_1^n(0) \right) \right\|_{L^2} \\ &\lesssim \tau^2,\end{aligned}$$

which completes the proof of Lemma 3.1. ☐

Lemma 3.2. *Let $\Phi^n(x)$ be the numerical approximation obtained from the Strang splitting S_2 (2.5). Then under the assumptions* (A) *and* (B) *with $m = 2$ and $m_* = 0$, we have for $0 \leq n \leq \frac{T}{\tau} - 1$,*

$$\mathbf{e}^{n+1}(x) = e^{-\frac{i\tau}{2\varepsilon^2}\mathcal{T}^\varepsilon} e^{-i\int_{t_n}^{t_{n+1}} V(s,x)ds} e^{-\frac{i\tau}{2\varepsilon^2}\mathcal{T}^\varepsilon} \mathbf{e}^n(x) + \eta_1^n(x) + \eta_2^n(x) + \eta_3^n(x), \tag{3.23}$$

with

$$\|\eta_1^n(x)\|_{L^2} \lesssim \tau^3, \quad \eta_2^n(x) = -ie^{-\frac{i\tau}{\varepsilon^2}\mathcal{T}^\varepsilon} \left(\int_0^\tau f_2^n(s)ds - \tau f_2^n(\tau/2) \right), \tag{3.24}$$

$$\eta_3^n(x) = -e^{-\frac{i\tau}{\varepsilon^2}\mathcal{T}^\varepsilon} \left(\int_0^\tau \int_0^s \sum_{j=2}^4 g_j^n(s,w)dwds - \frac{\tau^2}{2} \sum_{j=2}^4 g_j^n(\tau/2, \tau/2) \right), \tag{3.25}$$

where

$$\begin{aligned} f_2^n(s) =& e^{\frac{i2s}{\varepsilon^2}} e^{is\mathcal{D}^\varepsilon}\, \Pi_+^\varepsilon (V(t_n+s) e^{is\mathcal{D}^\varepsilon} \Pi_-^\varepsilon \Phi(t_n)) \\ &+ e^{\frac{-i2s}{\varepsilon^2}} e^{-is\mathcal{D}^\varepsilon}\, \Pi_-^\varepsilon (V(t_n+s) e^{-is\mathcal{D}^\varepsilon} \Pi_+^\varepsilon \Phi(t_n)), \end{aligned} \tag{3.26}$$

$$\begin{aligned} g_2^n(s,w) =& e^{i2w/\varepsilon^2} e^{is\mathcal{D}^\varepsilon} \Pi_+^\varepsilon \left(V(t_n) e^{-i(s-w)\mathcal{D}^\varepsilon} \Pi_+^\varepsilon \left(V(t_n) e^{iw\mathcal{D}^\varepsilon} \Pi_-^\varepsilon \Phi(t_n) \right) \right) \\ &+ e^{-i2w/\varepsilon^2} e^{-is\mathcal{D}^\varepsilon} \Pi_-^\varepsilon \left(V(t_n) e^{i(s-w)\mathcal{D}^\varepsilon} \Pi_-^\varepsilon \left(V(t_n) e^{-iw\mathcal{D}^\varepsilon} \Pi_+^\varepsilon \Phi(t_n) \right) \right), \end{aligned} \tag{3.27}$$

$$\begin{aligned} g_3^n(s,w) =& e^{\frac{i2(s-w)}{\varepsilon^2}} e^{is\mathcal{D}^\varepsilon} \Pi_+^\varepsilon \left(V(t_n) e^{i(s-w)\mathcal{D}^\varepsilon} \Pi_-^\varepsilon \left(V(t_n) e^{-iw\mathcal{D}^\varepsilon} \Pi_+^\varepsilon \Phi(t_n) \right) \right) \\ &+ e^{-\frac{i2(s-w)}{\varepsilon^2}} e^{-is\mathcal{D}^\varepsilon} \Pi_-^\varepsilon \left(V(t_n) e^{-i(s-w)\mathcal{D}^\varepsilon} \Pi_+^\varepsilon \left(V(t_n) e^{iw\mathcal{D}^\varepsilon} \Pi_-^\varepsilon \Phi(t_n) \right) \right), \end{aligned} \tag{3.28}$$

$$\begin{aligned} g_4^n(s,w) =& e^{i2s/\varepsilon^2} e^{is\mathcal{D}^\varepsilon} \Pi_+^\varepsilon \left(V(t_n) e^{i(s-w)\mathcal{D}^\varepsilon} \Pi_-^\varepsilon \left(V(t_n) e^{iw\mathcal{D}^\varepsilon} \Pi_-^\varepsilon \Phi(t_n) \right) \right) \\ &+ e^{-i2s/\varepsilon^2} e^{-is\mathcal{D}^\varepsilon} \Pi_-^\varepsilon \left(V(t_n) e^{-i(s-w)\mathcal{D}^\varepsilon} \Pi_+^\varepsilon \left(V(t_n) e^{-iw\mathcal{D}^\varepsilon} \Pi_+^\varepsilon \Phi(t_n) \right) \right). \end{aligned} \tag{3.29}$$

Proof. From the definition of $\mathbf{e}^n(x)$, noticing the Strang splitting formula (2.5), we have

$$\mathbf{e}^{n+1}(x) = e^{-\frac{i\tau}{2\varepsilon^2}\mathcal{T}^\varepsilon} e^{-i\int_{t_n}^{t_{n+1}} V(s,x)\,ds} e^{-\frac{i\tau}{2\varepsilon^2}\mathcal{T}^\varepsilon} \mathbf{e}^n(x) + \eta^n(x), \quad x \in \mathbb{R}, \tag{3.30}$$

where $\eta^n(x)$ is the local truncation error defined as

$$\eta^n(x) = \Phi(t_{n+1}, x) - e^{-\frac{i\tau}{2\varepsilon^2}\mathcal{T}^\varepsilon} e^{-i\int_{t_n}^{t_{n+1}} V(s,x)\,ds} e^{-\frac{i\tau}{2\varepsilon^2}\mathcal{T}^\varepsilon} \Phi(t_n, x), \quad x \in \mathbb{R}. \tag{3.31}$$

Similar to the S_1 case, repeatedly using Duhamel's principle and Taylor expansion, we can obtain

$$\begin{aligned}&\Phi(t_{n+1})\\&=e^{-\frac{i\tau}{\varepsilon^2}\mathcal{T}^\varepsilon}\Phi(t_n)-i\int_0^\tau e^{-\frac{i(\tau-s)}{\varepsilon^2}\mathcal{T}^\varepsilon}\left(V(t_n+s)e^{-\frac{is}{\varepsilon^2}\mathcal{T}^\varepsilon}\Phi(t_n)\right)ds\\&\quad-\int_0^\tau\int_0^s e^{-\frac{i(\tau-s)}{\varepsilon^2}\mathcal{T}^\varepsilon}\left(V(t_n)e^{-\frac{i(s-w)}{\varepsilon^2}\mathcal{T}^\varepsilon}\left(V(t_n+w)\Phi(t_n+w)\right)\right)dw\,ds,\end{aligned}\tag{3.32}$$

$$\begin{aligned}&e^{-\frac{i\tau}{2\varepsilon^2}\mathcal{T}^\varepsilon}e^{-i\int_{t_n}^{t_{n+1}}V(s)\,ds}e^{-\frac{i\tau}{2\varepsilon^2}\mathcal{T}^\varepsilon}\Phi(t_n)\\&=e^{-\frac{i\tau}{2\varepsilon^2}\mathcal{T}^\varepsilon}\left(1-i\int_0^\tau V(t_n+s)\,ds-\frac{1}{2}(\int_0^\tau V(t_n+s)\,ds)^2\right)e^{-\frac{i\tau}{2\varepsilon^2}\mathcal{T}^\varepsilon}\Phi(t_n)\\&\quad+e^{-\frac{i\tau}{2\varepsilon^2}\mathcal{T}^\varepsilon}\left(O(\tau^3)\right)e^{-\frac{i\tau}{2\varepsilon^2}\mathcal{T}^\varepsilon}\Phi(t_n).\end{aligned}\tag{3.33}$$

Denoting

$$f^n(s)=e^{\frac{is}{\varepsilon^2}\mathcal{T}^\varepsilon}\left(V(t_n+s,x)e^{-\frac{is}{\varepsilon^2}\mathcal{T}^\varepsilon}\Phi(t_n,x)\right),\tag{3.34}$$

for $0\le s\le\tau$, and

$$g^n(s,w)=e^{\frac{is}{\varepsilon^2}\mathcal{T}^\varepsilon}\left(V(t_n,x)e^{-\frac{i(s-w)}{\varepsilon^2}\mathcal{T}^\varepsilon}\left(V(t_n,x)e^{-\frac{iw}{\varepsilon^2}\mathcal{T}^\varepsilon}\Phi(t_n,x)\right)\right),\tag{3.35}$$

for $0\le s,w\le\tau$, in view of (3.32) and (3.33), $\eta^n(x)$ (3.31) can be written as

$$\begin{aligned}\eta^n(x)=&-e^{-\frac{i\tau}{\varepsilon^2}\mathcal{T}^\varepsilon}\left[i\int_0^\tau f^n(s)\,ds-i\tau f^n\left(\frac{\tau}{2}\right)+\int_0^\tau\int_0^s g^n(s,w)\,dwds\right.\\&\left.-\frac{\tau^2}{2}g^n\left(\frac{\tau}{2},\frac{\tau}{2}\right)\right]+\sum_{j=1}^2R_j^n(x),\end{aligned}\tag{3.36}$$

where

$$\begin{aligned}&R_1^n(x)=-e^{-\frac{i\tau}{2\varepsilon^2}\mathcal{T}^\varepsilon}(\lambda_1^n(x)+\lambda_2^n(x))e^{-\frac{i\tau}{2\varepsilon^2}\mathcal{T}^\varepsilon}\Phi(t_n,x),\\&R_2^n(x)\\&=-\int_0^\tau\int_0^s e^{-\frac{i(\tau-s)}{\varepsilon^2}\mathcal{T}^\varepsilon}\left(V(t_n+s,x)e^{-\frac{i(s-w)}{\varepsilon^2}\mathcal{T}^\varepsilon}\left(V(t_n+w,x)\lambda_3^n(w,x)\right)\right)dw\,ds,\end{aligned}$$

with

$$\begin{aligned}\lambda_1^n(x)&=-i\left(\int_0^\tau V(t_n+s,x)\,ds-\tau V(t_n+\frac{\tau}{2},x)\right)-\frac{1}{2}\left(\int_0^\tau V(t_n+s,x)ds\right)^2\\&\qquad+\frac{1}{2}\tau^2V^2(t_n,x),\\\lambda_2^n(x)&=e^{-i\int_0^\tau V(t_n+s,x)ds}-1+i\int_0^\tau V(t_n+s,x)ds+\frac{1}{2}\left(\int_0^\tau V(t_n+s,x)ds\right)^2,\\\lambda_3^n(w,x)&=-i\int_0^w e^{-\frac{i(w-u)}{\varepsilon^2}\mathcal{T}^\varepsilon}\left(V(t_n+u,x)\Phi(t_n+u,x)\right)du.\end{aligned}$$

It is easy to check that $\|\lambda_2^n(x)\|_{L^\infty}\lesssim\tau^3\|V(t,x)\|^3_{L^\infty(L^\infty)}$ and

$$\begin{aligned}&\|\lambda_1^n(x)\|_{L^\infty}\lesssim\tau^3\|\partial_{tt}V(t,x)\|_{L^\infty(L^\infty)}+\tau^3\|\partial_tV(t,x)\|_{L^\infty(L^\infty)}\|V(t,x)\|_{L^\infty(L^\infty)},\\&\|\lambda_3^n(w,x)\|_{L^\infty([0,\tau];(L^2)^2)}\lesssim\tau\|V(t,x)\|_{L^\infty(L^\infty)}\|\Phi\|_{L^\infty((L^2)^2)},\end{aligned}$$

which immediately implies that

$$\|R_1^n(x)\|_{L^2} \lesssim (\|\lambda_1^n(x)\|_{L^\infty} + \|\lambda_2^n(x)\|_{L^\infty})\,\|\Phi(t_n)\|_{L^2} \lesssim \tau^3, \tag{3.37}$$

$$\|R_2^n(x)\|_{L^2} \lesssim \tau^2 \|V(t,x)\|^2_{L^\infty(L^\infty)} \|\lambda_3^n(w,x)\|_{L^\infty([0,\tau];L^2)} \lesssim \tau^3. \tag{3.38}$$

In view of (3.6), recalling the definitions of $f_2^n(s)$ and $g_j^n(s,w)$ ($j = 2,3,4$) given in Lemma 3.2, we introduce $f_1^n(s)$ and $g_1^n(s,w)$ such that

$$f^n(s) = f_1^n(s) + f_2^n(s), \quad g^n(s,w) = \sum_{j=1}^{4} g_j^n(s,w), \tag{3.39}$$

where

$$\begin{aligned} f_1^n(s) &= e^{is\mathcal{D}^\varepsilon}\, \Pi_+^\varepsilon \left(V(t_n+s)e^{-is\mathcal{D}^\varepsilon}\Pi_+^\varepsilon \Phi(t_n)\right) \\ &\quad + e^{-is\mathcal{D}^\varepsilon}\, \Pi_-^\varepsilon \left(V(t_n+s)e^{is\mathcal{D}^\varepsilon}\Pi_-^\varepsilon \Phi(t_n)\right), \\ g_1^n(s,w) &= e^{is\mathcal{D}^\varepsilon}\Pi_+^\varepsilon \left(V(t_n)e^{-i(s-w)\mathcal{D}^\varepsilon}\Pi_+^\varepsilon \left(V(t_n)e^{-iw\mathcal{D}^\varepsilon}\Pi_+^\varepsilon \Phi(t_n)\right)\right) \\ &\quad + e^{-is\mathcal{D}^\varepsilon}\Pi_-^\varepsilon \left(V(t_n)e^{i(s-w)\mathcal{D}^\varepsilon}\Pi_-^\varepsilon \left(V(t_n)e^{iw\mathcal{D}^\varepsilon}\Pi_-^\varepsilon \Phi(t_n)\right)\right). \end{aligned}$$

Denote

$$\begin{aligned} \zeta_1^n(x) &= -ie^{-\frac{i\tau}{\varepsilon^2}\mathcal{T}^\varepsilon}\left(\int_0^\tau f_1^n(s)\,ds - \tau f_1^n(\tau/2)\right), \\ \zeta_2^n(x) &= -e^{-\frac{i\tau}{\varepsilon^2}\mathcal{T}^\varepsilon}\left(\int_0^\tau \int_0^s g_1^n(s,w)\,dwds - \frac{\tau^2}{2} g_1^n(\tau/2,\tau/2)\right); \end{aligned}$$

then it is easy to show that for $J = [0,\tau]^2$,

$$\|\zeta_1^n(x)\|_{L^2} \lesssim \tau^3 \|\partial_{ss} f_1(s)\|_{L^\infty([0,\tau];(L^2)^2)} \lesssim \tau^3, \tag{3.40}$$

$$\|\zeta_2^n(x)\|_{L^2} \lesssim \tau^3 (\|\partial_s g_1(s,w)\|_{L^\infty(J;(L^2)^2)} + \|\partial_w g_1(s,w)\|_{L^\infty(J;(L^2)^2)}) \lesssim \tau^3, \tag{3.41}$$

by noticing that $V \in L^\infty(W^{2m,\infty})$ and $\Phi(t,x) \in L^\infty((H^{2m})^2)$ with $m = 2$ as well as the fact that $\mathcal{D}^\varepsilon : (H^l)^2 \to (H^{l-2})^2$ ($l \geq 2$) is uniformly bounded w.r.t. ε. Recalling (3.34), (3.35), (3.36), (3.39), and η_j^n ($j = 2,3$) (3.24)-(3.25) given in Lemma 3.2, we have

$$\eta^n(x) = \eta_1^n(x) + \eta_2^n(x) + \eta_3^n(x), \tag{3.42}$$

where $\eta_2^n(x)$ and $\eta_3^n(x)$ are given in Lemma 3.2, and

$$\eta_1^n(x) = R_1^n(x) + R_2^n(x) + \zeta_1^n(x) + \zeta_2^n(x).$$

Combining (3.37), (3.38), (3.40), and (3.41), we can get

$$\|\eta_1^n(x)\|_{L^2} \leq \|R_1^n(x)\|_{L^2} + \|R_2^n(x)\|_{L^2} + \|\zeta_1^n(x)\|_{L^2} + \|\zeta_2^n(x)\|_{L^2} \lesssim \tau^3, \tag{3.43}$$

which completes the proof. □

Utilizing these lemmas, we now proceed to prove Theorems 2.1 and 2.2.

Proof of Theorem 2.1.

Proof. From Lemma 3.1, it is straightforward that

$$\|\mathbf{e}^{n+1}(x)\|_{L^2} \leq \|\mathbf{e}^n(x)\|_{L^2} + \|\eta_1^n(x)\|_{L^2} + \|\eta_2^n(x)\|_{L^2}, \quad 0 \leq n \leq \frac{T}{\tau} - 1, \tag{3.44}$$

with $\mathbf{e}^0(x) = 0$, $\|\eta_1^n(x)\|_{L^2} \lesssim \tau^2$, and $\eta_2^n(x) = -ie^{-i\tau\mathcal{T}^\varepsilon/\varepsilon^2}\left(\int_0^\tau f_2^n(s)ds - \tau f_2^n(0)\right)$, where $f_2^n(s)$ is defined in (3.8).

To analyze $f_2^n(s)$, using (3.3) and (3.4), we expand $\Pi_+^\varepsilon V(t_n)\Pi_-^\varepsilon$ and $\Pi_-^\varepsilon V(t_n)\Pi_+^\varepsilon$ to get

$$\begin{aligned}\Pi_+^\varepsilon V(t_n)\Pi_-^\varepsilon =& -\varepsilon\Pi_+^0 V(t_n)\mathcal{R}_1 + \varepsilon\mathcal{R}_1 V(t_n)\Pi_-^\varepsilon,\\ \Pi_-^\varepsilon V(t_n)\Pi_+^\varepsilon =& \varepsilon\Pi_-^0 V(t_n)\mathcal{R}_1 - \varepsilon\mathcal{R}_1 V(t_n)\Pi_+^\varepsilon.\end{aligned}$$

As $\mathcal{R}_1 : (H^m)^2 \to (H^{m-1})^2$ is uniformly bounded with respect to $\varepsilon \in (0,1]$, we have

$$\left\|\Pi_+^\varepsilon\left(V(t_n)\Pi_-^\varepsilon e^{is\mathcal{D}^\varepsilon}\Phi(t_n)\right)\right\|_{L^2} \lesssim \varepsilon\|V(t_n)\|_{W^{1,\infty}}\|\Phi(t_n)\|_{H^1}, \tag{3.45}$$

$$\left\|\Pi_-^\varepsilon\left(V(t_n)\Pi_+^\varepsilon e^{is\mathcal{D}^\varepsilon}\Phi(t_n)\right)\right\|_{L^2} \lesssim \varepsilon\|V(t_n)\|_{W^{1,\infty}}\|\Phi(t_n)\|_{H^1}. \tag{3.46}$$

Noting the assumptions (A) and (B) with $m = 1$ and $m_* = 0$, we obtain from (3.8) $(0 \le s \le \tau)$

$$\|f_2^n(s)\|_{L^\infty([0,\tau];(L^2)^2)} \lesssim \varepsilon, \quad \|\partial_s(f_2^n)(\cdot)\|_{L^\infty([0,\tau];(L^2)^2)} \lesssim \varepsilon/\varepsilon^2 = 1/\varepsilon. \tag{3.47}$$

As a result, from the first inequality, we get

$$\left\|\int_0^\tau f_2^n(s)\,ds - \tau f_2^n(0)\right\|_{L^2} \lesssim \tau\varepsilon. \tag{3.48}$$

On the other hand, noticing Taylor expansion and the second inequality in (3.47), we have

$$\left\|\int_0^\tau f_2^n(s)\,ds - \tau f_2^n(0)\right\|_{L^2} \le \frac{\tau^2}{2}\|\partial_s f_2^n(\cdot)\|_{L^\infty([0,\tau];(L^2)^2)} \lesssim \tau^2/\varepsilon. \tag{3.49}$$

Combining (3.48) and (3.49), we arrive at

$$\|\eta_2^n(x)\|_{L^2} \lesssim \min\{\tau\varepsilon, \tau^2/\varepsilon\}. \tag{3.50}$$

Then from (3.44) and $\mathbf{e}^0 = 0$, we get

$$\begin{aligned}\|\mathbf{e}^{n+1}(x)\|_{L^2} \le& \|\mathbf{e}^0(x)\|_{L^2} + \sum_{k=0}^n \|\eta_1^k(x)\|_{L^2} + \sum_{k=0}^n \|\eta_2^k(x)\|_{L^2}\\ \lesssim& n\tau^2 + n\min\{\tau\varepsilon, \tau^2/\varepsilon\} \lesssim \tau + \min\{\varepsilon, \tau/\varepsilon\}, \quad 0 \le n \le \frac{T}{\tau} - 1,\end{aligned}$$

which gives the desired results. $\square$

Proof of Theorem 2.2.

Proof. From Lemma 3.2, it is easy to get that

$$\|\mathbf{e}^{n+1}(x)\|_{L^2} \le \|\mathbf{e}^n(x)\|_{L^2} + \|\eta_1^n(x)\|_{L^2} + \|\eta_2^n(x)\|_{L^2} + \|\eta_3^n(x)\|_{L^2}, \tag{3.51}$$

with $\mathbf{e}^0(x) = 0$ and $\|\eta_1^n(x)\|_{L^2} \lesssim \tau^3$.

Through similar computations in the S_1 case, under the hypothesis of Theorem 2.2, we can show that for $0 \le s, w, \le \tau$,

$$\begin{aligned}&\|f_2^n(s)\|_{L^2} \lesssim \varepsilon, \quad \|\partial_s f_2^n(s)\|_{L^2} \lesssim \varepsilon/\varepsilon^2 = 1/\varepsilon, \quad \|\partial_{ss} f_2^n(s)\|_{L^2} \lesssim 1/\varepsilon^3;\\ &\|g_j^n(s,w)\|_{L^2} \lesssim \varepsilon, \quad \|\partial_s g_j^n(s,w)\|_{L^2} \lesssim 1/\varepsilon, \quad \|\partial_w g_j^n(s,w)\|_{L^2} \lesssim 1/\varepsilon, \quad j = 2,3,4.\end{aligned}$$

As a result, for $j = 2, 3, 4$, we have

$$\left\|\int_0^\tau f_2^n(s)\,ds - \tau f_2^n(\frac{\tau}{2})\right\|_{L^2} \lesssim \tau\varepsilon, \quad \left\|\int_0^\tau \int_0^s g_j^n(s,w)\,dwds - \frac{\tau^2}{2} g_j^n(\frac{\tau}{2}, \frac{\tau}{2})\right\|_{L^2} \lesssim \tau^2\varepsilon.$$

On the other hand, for $j = 2, 3, 4$, Taylor expansion will lead to

$$\left\|\int_0^\tau f_2^n(s)\,ds - \tau f_2^n(\frac{\tau}{2})\right\|_{L^2} \lesssim \frac{\tau^3}{\varepsilon^3}, \quad \left\|\int_0^\tau \int_0^s g_j^n(s,w)\,dwds - \frac{\tau^2}{2} g_j^n(\frac{\tau}{2}, \frac{\tau}{2})\right\|_{L^2} \lesssim \frac{\tau^3}{\varepsilon}.$$

The two estimates above together with (3.24) and (3.25) imply

$$\|\eta_2^n(x)\|_{L^2} + \|\eta_3^n(x)\|_{L^2} \lesssim \min\{\tau\varepsilon, \tau^3/\varepsilon^3\}. \tag{3.52}$$

Recalling (3.51), we can get

$$\begin{aligned}
\|\mathbf{e}^{n+1}(x)\|_{L^2} \leq & \|\mathbf{e}^0(x)\|_{L^2} + \sum_{k=0}^n \|\eta_1^k(x)\|_{L^2} + \sum_{k=0}^n \|\eta_2^k(x)\|_{L^2} + \sum_{k=0}^n \|\eta_3^k(x)\|_{L^2} \\
\lesssim & n\tau^3 + n\min\{\tau\varepsilon, \tau^3/\varepsilon^3\} \lesssim \tau^2 + \min\{\varepsilon, \tau^2/\varepsilon^3\}, \quad 0 \leq n \leq \frac{T}{\tau} - 1,
\end{aligned}$$

which gives the desired results. □

4. Proof of Theorems 2.4 and 2.5

If the time step size τ is away from the resonance, i.e., for given ε, there is a $\delta > 0$, such that $\tau \in \mathcal{A}_\delta(\varepsilon)$, we can show improved uniform error bounds for the splitting methods given in Theorems 2.4 and 2.5 from Lemmas 3.1 and 3.2, as observed in our extensive numerical tests.

Proof of Theorem 2.4.

Proof. We divide the proof into three steps.

Step 1 (Explicit representation of the error). From Lemma 3.1, we have

$$\mathbf{e}^{n+1}(x) = e^{-\frac{i\tau}{\varepsilon^2}\mathcal{T}^\varepsilon} e^{-i\int_{t_n}^{t_{n+1}} V(s)ds} \mathbf{e}^n(x) + \eta_1^n(x) + \eta_2^n(x), \quad 0 \leq n \leq \frac{T}{\tau} - 1, \tag{4.1}$$

with $\|\eta_1^n(x)\|_{L^2} \lesssim \tau^2$, $\mathbf{e}^0 = 0$, $\eta_2^n(x) = -ie^{-\frac{i\tau}{\varepsilon^2}\mathcal{T}^\varepsilon}\left(\int_0^\tau f_2^n(s)ds - \tau f_2^n(0)\right)$, and f_2^n is given in Lemma 3.1 (3.8).

Denote the numerical solution propagator $S_{n,\tau} := e^{-\frac{i\tau}{\varepsilon^2}\mathcal{T}^\varepsilon} e^{-i\int_{t_n}^{t_{n+1}} V(s,x)ds}$ for $n \geq 0$. Then for all $\widetilde{\Phi} \in \mathbb{C}^2$, for $m \geq 1$,

$$\left\|S_{n,\tau}\widetilde{\Phi}\right\|_{L^2} = \left\|\widetilde{\Phi}\right\|_{L^2}, \quad \left\|S_{n,\tau}\widetilde{\Phi}\right\|_{H^m} \leq e^{C\tau\|V(t,x)\|_{L^\infty([0,T];W^{m,\infty})}}\|\widetilde{\Phi}\|_{H^m}, \tag{4.2}$$

with some generic constant $C > 0$ and

$$\begin{aligned}
\mathbf{e}^{n+1}(x) &= S_{n,\tau}\mathbf{e}^n(x) + (\eta_1^n(x) + \eta_2^n(x)) \\
&= S_{n,\tau}(S_{n-1,\tau}\mathbf{e}^{n-1}(x)) + S_{n,\tau}\left(\eta_1^{n-1}(x) + \eta_2^{n-1}(x)\right) + (\eta_1^n(x) + \eta_2^n(x)) \\
&= ... \\
&= S_{n,\tau}S_{n-1,\tau}...S_{0,\tau}\mathbf{e}^0(x) + \sum_{k=0}^n S_{n,\tau}...S_{k+2,\tau}S_{k+1,\tau}\left(\eta_1^k(x) + \eta_2^k(x)\right), \qquad (4.3)
\end{aligned}$$

where for $k = n$, we take $S_{n,\tau}...S_{k+2,\tau}S_{k+1,\tau} = \mathrm{Id}$. Since $S_{n,\tau}$ preserves the L^2 norm, noting $\|\eta_1^k(x)\|_{L^2} \lesssim \tau^2$, $k = 0, 1, ..., n$, we have

$$\left\|\sum_{k=0}^{n} S_{n,\tau}...S_{k+1,\tau}\eta_1^k(x)\right\|_{L^2} \lesssim \sum_{k=0}^{n} \tau^2 \lesssim \tau,$$

which leads to

$$\|\mathbf{e}^{n+1}(x)\|_{L^2} \lesssim \tau + \left\|\sum_{k=0}^{n} S_{n,\tau}...S_{k+1,\tau}\eta_2^k(x)\right\|_{L^2}. \tag{4.4}$$

The improved estimates rely on the refined analysis of the terms involving η_2^k in (4.4). To this aim, we introduce the following approximation of η_2^k to focus on the most relevant terms:

$$\tilde{\eta}_2^k(x) = \int_0^\tau \tilde{f}_2^k(s)ds - \tau\tilde{f}_2^k(0), \quad k = 0, 1, \ldots, n, \tag{4.5}$$

with

$$\tilde{f}_2^k(s) = -ie^{i(2s-\tau)/\varepsilon^2}\Pi_+^\varepsilon\left(V(t_k)\Pi_-^\varepsilon\Phi(t_k)\right) - ie^{i(\tau-2s)/\varepsilon^2}\Pi_-^\varepsilon\left(V(t_k)\Pi_+^\varepsilon\Phi(t_k)\right). \tag{4.6}$$

Then it is easy to verify that (using Taylor expansion $e^{i\tau\mathcal{D}^\varepsilon} = \mathrm{Id} + O(\tau\mathcal{D}^\varepsilon)$)

$$\|\eta_2^k(x) - \tilde{\eta}_2^k(x)\|_{L^2} \lesssim \tau^2\|V(t_k)\|_{H^2}\|\Phi(t_k)\|_{H^2} \lesssim \tau^2. \tag{4.7}$$

As a result, from (4.4), we have

$$\begin{aligned}\|\mathbf{e}^{n+1}(x)\|_{L^2} &\lesssim \tau + \left\|\sum_{k=0}^{n} S_{n,\tau}...S_{k+1,\tau}(\eta_2^k(x) - \tilde{\eta}_2^k(x))\right\|_{L^2} \\ &\quad + \left\|\sum_{k=0}^{n} S_{n,\tau}...S_{k+1,\tau}\tilde{\eta}_2^k(x)\right\|_{L^2} \\ &\le \tau + \sum_{k=0}^{n}\|\eta_2^k(x) - \tilde{\eta}_2^k(x)\|_{L^2} + \left\|\sum_{k=0}^{n} S_{n,\tau}...S_{k+1,\tau}\tilde{\eta}_2^k(x)\right\|_{L^2} \\ &\lesssim \tau + \left\|\sum_{k=0}^{n} S_{n,\tau}...S_{k+1,\tau}\tilde{\eta}_2^k(x)\right\|_{L^2}.\end{aligned}$$

Step 2 (Representation of the error using the exact solution flow). Denote $S_e(t;t_k)$ ($k = 0, 1, \ldots, n$) to be the exact solution operator of the Dirac equation, acting on some $\tilde{\Phi}(x) = (\tilde{\phi}_1(x), \tilde{\phi}_2(x))^T \in \mathbb{C}^2$ so that $S_e(t;t_k)\tilde{\Phi}(x)$ is the exact solution $\Psi(t,x)$ at time t of

$$\begin{cases} i\partial_t\Psi(t,x) = \dfrac{\mathcal{T}^\varepsilon}{\varepsilon^2}\Psi(t,x) + V(t,x)\Psi(t,x), \\ \Psi(t_k,x) = \tilde{\Phi}(x), \end{cases} \tag{4.8}$$

and the following properties hold true for $t \ge t_k$, $m \ge 1$ and some generic constant $C > 0$:
(4.9)

$$\left\|S_e(t;t_k)\widetilde{\Phi}\right\|_{L^2} = \left\|\widetilde{\Phi}\right\|_{L^2}, \ \left\|S_e(t;t_k)\widetilde{\Phi}\right\|_{H^m} \le e^{C(t-t_k)\|V(t,x)\|_{L^\infty([0,T];W^{m,\infty})}}\|\widetilde{\Phi}\|_{H^m}.$$

It is convenient to write $\tilde{\eta}_2^k(x)$ (4.5) as

$$\tilde{\eta}_2^k(x) = p_+(\tau)\Pi_+^\varepsilon\left(V(t_k)\Pi_-^\varepsilon\Phi(t_k)\right) + p_-(\tau)\Pi_-^\varepsilon\left(V(t_k)\Pi_+^\varepsilon\Phi(t_k)\right), \tag{4.10}$$

with

$$p_\pm(\tau) = -ie^{\mp i\tau/\varepsilon^2}\left(\int_0^\tau e^{\pm i2s/\varepsilon^2}ds - \tau\right)$$

and by the inequality

$$\left|\int_0^\tau e^{i2s/\varepsilon^2}ds - \tau\right| + \left|\int_0^\tau e^{-i2s/\varepsilon^2}ds - \tau\right| \leq 4\tau$$

and similar computations in (3.45)-(3.46), it follows that

$$\|\tilde{\eta}_2^k\|_{H^2} \lesssim \tau\varepsilon\|V(t_k)\|_{W^{3,\infty}}\|\Phi(t_k)\|_{H^3} \lesssim \varepsilon\tau. \tag{4.11}$$

Recalling the error bounds in Theorem 2.1 and Remark 2.3, we have

$$\|(S_{n,\tau}...S_{k+1,\tau} - S_e(t_{n+1};t_{k+1}))\tilde{\eta}_2^k(x)\|_{L^2} \lesssim \left(\tau + \frac{\tau}{\varepsilon}\right)\|\tilde{\eta}_2^k\|_{H^2} \lesssim \tau^2,$$

and

$$\begin{aligned}\|\mathbf{e}^{n+1}(x)\|_{L^2} &\lesssim \tau + \sum_{k=0}^n \left\|(S_{n,\tau}...S_{k+1,\tau} - S_e(t_{n+1};t_{k+1}))\tilde{\eta}_2^k(x)\right\|_{L^2} \\ &\quad + \left\|\sum_{k=0}^n S_e(t_{n+1};t_{k+1})\tilde{\eta}_2^k(x)\right\|_{L^2} \\ &\lesssim \tau + \left\|\sum_{k=0}^n S_e(t_{n+1};t_{k+1})\tilde{\eta}_2^k(x)\right\|_{L^2}. \end{aligned} \tag{4.12}$$

Noting (4.10), we have

$$\begin{aligned} S_e(t_{n+1};t_{k+1})\tilde{\eta}_2^k(x) = p_+(\tau)S_e(t_{n+1};t_{k+1})\Pi_+^\varepsilon V(t_k)\Pi_-^\varepsilon S_e(t_k;t_0)\Phi(0) \\ + p_-(\tau)S_e(t_{n+1};t_{k+1})\Pi_-^\varepsilon V(t_k)\Pi_+^\varepsilon S_e(t_k;t_0)\Phi(0), \end{aligned} \tag{4.13}$$

and it remains to estimate the S_e part in (4.12).

Step 3 (Improved error bounds for nonresonant time steps). From [6], we know that the exact solution of the Dirac equation is structured as follows:

$$S_e(t_n;t_k)\tilde{\Phi}(x) = e^{-i(t_n-t_k)/\varepsilon^2}\Psi_+(t,x) + e^{i(t_n-t_k)/\varepsilon^2}\Psi_-(t,x) + R_k^n\tilde{\Phi}(x), \tag{4.14}$$

where $R_k^n : (H^2)^2 \to (L^2)^2$ is the residue operator and $\|R_k^n\tilde{\Phi}(x)\|_{L^2} \lesssim \varepsilon^2\|\tilde{\Phi}(x)\|_{H^2}$ $(0 \leq k \leq n)$, and

$$\begin{cases} i\partial_t\Psi_\pm(t,x) = \pm\mathcal{D}^\varepsilon\Psi_\pm(t,x) + \Pi_\pm^\varepsilon(V(t)\Psi_\pm(t,x)), \\ \Psi_\pm(t_k,x) = \Pi_\pm^\varepsilon\tilde{\Phi}(x). \end{cases} \tag{4.15}$$

Denote $S_e^+(t;t_k)\tilde{\Phi}(x) = \Psi_+(t,x)$, $S_e^-(t;t_k)\tilde{\Phi}(x) = \Psi_-(t,x)$ to be the solution propagator of the above equation for $\Psi_+(t,x)$, $\Psi_-(t,x)$, respectively, and $S_e^\pm$ share the same properties in (4.9). Plugging (4.14) into (4.13), we derive

$$
\begin{aligned}
&\sum_{k=0}^{n} S_e(t_{n+1};t_{k+1})\tilde{\eta}_2^k(x)\\
=&\sum_{k=0}^{n}\sum_{\sigma=\pm}\left(e^{-i\frac{t_{n+1}-t_{k+1}}{\varepsilon^2}}S_e^{+}(t_{n+1};t_{k+1})+e^{i\frac{t_{n+1}-t_{k+1}}{\varepsilon^2}}S_e^{-}(t_{n+1};t_{k+1})+R_{k+1}^{n+1}\right)\\
&\quad\Pi_\sigma^\varepsilon V(t_k)\Pi_{\sigma^*}^\varepsilon\left(e^{-i\frac{t_k-t_0}{\varepsilon^2}}S_e^{+}(t_k;t_0)+e^{i\frac{t_k-t_0}{\varepsilon^2}}S_e^{-}(t_k;t_0)+R_0^k\right)\Phi(0)p_\sigma(\tau)\\
=&\underbrace{\sum_{k=0}^{n}\sum_{\sigma=\pm}e^{-i\sigma\frac{t_{n+1}-t_{k+1}}{\varepsilon^2}}S_e^{\sigma}(t_{n+1};t_{k+1})\Pi_\sigma^\varepsilon V(t_k)\Pi_{\sigma^*}^\varepsilon e^{i\sigma\frac{t_k-t_0}{\varepsilon^2}}S_e^{\sigma^*}(t_k;t_0)\Phi(0)p_\sigma(\tau)}_{I_1^n(x)}\\
&+\underbrace{\sum_{k=0}^{n}\sum_{\sigma=\pm}\left(R_{k+1}^{n+1}\Pi_\sigma^\varepsilon V(t_k)\Pi_{\sigma^*}^\varepsilon\Phi(t_k)+S_e(t_{n+1};t_{k+1})\Pi_\sigma^\varepsilon V(t_k)\Pi_{\sigma^*}^\varepsilon R_0^k\Phi(0)\right)p_\sigma(\tau)}_{I_2^n(x)}\\
=&I_1^n(x)+I_2^n(x),
\end{aligned}
$$

where $\sigma^*=+$ if $\sigma=-$ and $\sigma^*=-$ if $\sigma=+$. As $|p_\pm(\tau)|=\left|\int_0^\tau e^{\pm 2is/\varepsilon^2}ds-\tau\right|\lesssim\tau^2/\varepsilon^2$ by Taylor expansion, we have

$$
\|I_2^n(x)\|_{L^2}\lesssim\frac{\tau^2}{\varepsilon^2}\sum_{k=0}^{n}\left(\varepsilon^2\|V(t_k)\|_{W^{2,\infty}}\|\Phi(t_k)\|_{H^2}+\varepsilon^2\|V(t_k)\|_{L^\infty}\|\Phi(t_0)\|_{H^2}\right)\lesssim\tau.
$$

We can rewrite $I_1^n(x)$ as

$$
\begin{aligned}
I_1^n(x)=&\sum_{k=0}^{n}\sum_{\sigma=\pm}e^{-i\sigma\frac{t_{n+1}-2t_k-\tau}{\varepsilon^2}}S_e^{\sigma}(t_{n+1};t_{k+1})\Pi_\sigma^\varepsilon V(t_k)\Pi_{\sigma^*}^\varepsilon S_e^{\sigma^*}(t_k;t_0)\Phi(0)p_\sigma(\tau)\\
=&p_+(\tau)\sum_{k=0}^{n}(\theta_k-\theta_{k-1})S_e^{+}(t_{n+1};t_{k+1})\Pi_+^\varepsilon V(t_k)\Pi_-^\varepsilon S_e^{-}(t_k;t_0)\Phi(0)\\
&+p_-(\tau)\sum_{k=0}^{n}\overline{(\theta_k-\theta_{k-1})}S_e^{-}(t_{n+1};t_{k+1})\Pi_-^\varepsilon V(t_k)\Pi_+^\varepsilon S_e^{+}(t_k;t_0)\Phi(0)\\
=&\gamma_1^n(x)+\gamma_2^n(x),
\end{aligned}
$$

where $\bar{\theta}$ is the complex conjugate of θ and for $0\le k\le n$,

$$
\theta_k=\sum_{l=0}^{k}e^{-i(t_{n+1}-2t_l-\tau)/\varepsilon^2}=\frac{e^{-in\tau/\varepsilon^2}-e^{-i(n-2k-2)\tau/\varepsilon^2}}{1-e^{2i\tau/\varepsilon^2}},\quad \theta_{-1}=0, \tag{4.16}
$$

$$
\gamma_1^n(x)=p_+(\tau)\sum_{k=0}^{n}(\theta_k-\theta_{k-1})S_e^{+}(t_{n+1};t_{k+1})\Pi_+^\varepsilon V(t_k)\Pi_-^\varepsilon S_e^{-}(t_k;t_0)\Phi(0), \tag{4.17}
$$

$$
\gamma_2^n(x)=p_-(\tau)\sum_{k=0}^{n}\overline{(\theta_k-\theta_{k-1})}S_e^{-}(t_{n+1};t_{k+1})\Pi_-^\varepsilon V(t_k)\Pi_+^\varepsilon S_e^{+}(t_k;t_0)\Phi(0). \tag{4.18}
$$

It is easy to check that if $\tau \in \mathcal{A}_\delta(\varepsilon)$, it satisfies $|1-e^{2i\tau/\varepsilon^2}| = 2|\sin(\tau/\varepsilon^2)| \geq 2\delta > 0$, then we have

$$|\theta_k| \leq \frac{1}{\delta}, \quad k = 0, 1, \ldots, n.$$

As a result, noticing $|p_\pm(\tau)| \leq 2\tau$, we can get

$$\begin{aligned}
&\|\gamma_1^n(x)\|_{L^2} \\
&\leq 2\tau \Bigg\| \sum_{k=0}^{n-1} \theta_k \big[S_e^+(t_{n+1};t_{k+1})\Pi_+^\varepsilon V(t_k)\Pi_-^\varepsilon S_e^-(t_k;t_0) - S_e^+(t_{n+1};t_{k+2})\Pi_+^\varepsilon V(t_{k+1}) \\
&\qquad \Pi_-^\varepsilon S_e^-(t_{k+1};t_0)\big]\Phi(0)\Bigg\|_{L^2} + \tau\|\theta_n S_e^+(t_{n+1};t_{n+1})\Pi_+^\varepsilon V(t_n)\Pi_-^\varepsilon S_e^-(t_n;t_0)\Phi(0)\|_{L^2} \\
&\lesssim \tau \sum_{k=0}^{n-1} \tau/\delta + \tau/\delta \lesssim_\delta \tau,
\end{aligned}$$

where we have used the triangle inequality and properties of the solution flows $S_e^\pm$ to deduce that (omitted for brevity as they are standard)

$$\begin{aligned}
&\Big\| \big[S_e^+(t_{n+1};t_{k+1})\Pi_+^\varepsilon V(t_k)\Pi_-^\varepsilon S_e^-(t_k;t_0) - S_e^+(t_{n+1};t_{k+2})\Pi_+^\varepsilon V(t_{k+1})\Pi_-^\varepsilon S_e^-(t_{k+1};t_0)\big]\Phi(0)\Big\|_{L^2} \\
&\leq \left\|S_e^+(t_{n+1};t_{k+1})\Pi_+^\varepsilon \left((V(t_k) - V(t_{k+1}))\Pi_-^\varepsilon S_e^-(t_k;t_0)\right)\Phi(0)\right\|_{L^2} \\
&\quad + \left\|S_e^+(t_{n+1};t_{k+1})\Pi_+^\varepsilon \left(V(t_{k+1})\Pi_-^\varepsilon (S_e^-(t_k;t_0) - S_e^-(t_{k+1};t_0))\right)\Phi(0)\right\|_{L^2} \\
&\quad + \left\|\left(S_e^+(t_{n+1};t_{k+1}) - S_e^+(t_{n+1};t_{k+2})\right)\Pi_+^\varepsilon V(t_{k+1})\Pi_-^\varepsilon S_e^-(t_{k+1};t_0)\Phi(0)\right\|_{L^2} \\
&\lesssim \tau\,\|\partial_t V\|_{L^\infty(L^\infty)}\,\|\Phi(0)\|_{L^2} + \tau\left\|\partial_t S_e^-(t;t_0)\Phi(0)\right\|_{L^\infty([0,T];(L^2)^2)} \\
&\qquad + \tau\left\|\partial_t\left(S_e^+(t_{n+1};t)\Pi_+^\varepsilon V(t_{k+1})\Pi_-^\varepsilon S_e^-(t_{k+1};t_0)\Phi(0)\right)\right\|_{L^\infty([t_{k+1},t_{n+1}];(L^2)^2)} \\
&\lesssim \tau + \tau\,\|\Phi(0)\|_{H^2} + \tau\|V(t_{k+1})\|_{W^{2,\infty}}\|\Phi(0)\|_{H^2} \lesssim \tau.
\end{aligned}$$

Similarly, we could get $\|\gamma_2^n(x)\|_{L^2} \lesssim_\delta \tau$ and hence $\|I_1^n(x)\|_{L^2} \lesssim_\delta \tau$. In summary, we have

$$\|\mathbf{e}^{n+1}(x)\|_{L^2} \lesssim \tau + \|I_1^n(x)\|_{L^2} + \|I_2^n(x)\|_{L^2} \lesssim_\delta \tau,$$

which gives the desired results. ☐

Proof of Theorem 2.5.

Proof. We divide the proof into two steps.

Step 1 (Representation of the error using the exact solution flow). From Lemma 3.2, we have for $0 \leq n \leq \frac{T}{\tau} - 1$,

$$\mathbf{e}^{n+1}(x) = e^{-\frac{i\tau}{2\varepsilon^2}\mathcal{T}^\varepsilon} e^{-i\int_{t_n}^{t_{n+1}} V(s,x)ds} e^{-\frac{i\tau}{2\varepsilon^2}\mathcal{T}^\varepsilon}\mathbf{e}^n(x) + \eta_1^n(x) + \eta_2^n(x) + \eta_3^n(x), \tag{4.19}$$

with η_j^n $(j = 1, 2, 3)$ stated in Lemma 3.2 as

$$\|\eta_1^n(x)\|_{L^2} \lesssim \tau^3, \quad \eta_2^n(x) = -ie^{-\frac{i\tau}{\varepsilon^2}\mathcal{T}^\varepsilon}\left(\int_0^\tau f_2^n(s)ds - \tau f_2^n(\tau/2)\right), \tag{4.20}$$

$$\eta_3^n(x) = -e^{-\frac{i\tau}{\varepsilon^2}\mathcal{T}^\varepsilon}\left(\int_0^\tau\int_0^s \sum_{j=2}^4 g_j^n(s,w)dwds - \frac{\tau^2}{2}\sum_{j=2}^4 g_j^n(\tau/2,\tau/2)\right), \tag{4.21}$$

where f_2^n and g_j^n $(j = 2, 3, 4)$ are given in (3.26)-(3.29).

Denote the second order splitting integrator $S_{n,\tau}=e^{-\frac{i\tau}{2\varepsilon^2}\mathcal{T}^\varepsilon}e^{-i\int_{t_n}^{t_{n+1}}V(s)ds}e^{-\frac{i\tau}{2\varepsilon^2}\mathcal{T}^\varepsilon}$ for $n\geq 0$, and $S_e(t;t_k)$ to be the exact solution flow (4.8) for the Dirac equation (2.2). Then $S_{n,\tau}$ enjoys the similar properties as those in the first order Lie-Trotter splitting case (4.2) and we can get

$$\begin{aligned}\mathbf{e}^{n+1}(x)=&S_e(t_{n+1};t_n)\mathbf{e}^n(x)+\eta_1^n(x)+\eta_2^n(x)+\eta_3^n(x)+\left(S_{n,\tau}-S_e(t_{n+1};t_n)\right)\mathbf{e}^n(x)\\ =&\ldots\\ =&S_e(t_{n+1};t_0)\mathbf{e}^0(x)+\sum_{k=0}^{n}S_e(t_{n+1};t_{k+1})(\eta_1^k(x)+\eta_2^k(x)+\eta_3^k(x))\\ &+\sum_{k=0}^{n}S_e(t_{n+1};t_{k+1})(S_{k,\tau}-S_e(t_{k+1};t_k))\mathbf{e}^k(x).\end{aligned}\tag{4.22}$$

By Duhamel's principle, it is straightforward to compute

$$\begin{aligned}\left(S_{k,\tau}-S_e(t_{k+1};t_k)\right)\tilde{\Phi}(x)=&\,e^{-\frac{i\tau}{2\varepsilon^2}\mathcal{T}^\varepsilon}(e^{-i\int_{t_k}^{t_{k+1}}V(s,x)ds}-1)e^{-\frac{i\tau}{2\varepsilon^2}\mathcal{T}^\varepsilon}\\ &-i\int_0^\tau e^{-\frac{i(\tau-s)\mathcal{T}^\varepsilon}{\varepsilon^2}}V(t_k+s,x)S_e(t_k+s;t_k)\tilde{\Phi}(x)\,ds.\end{aligned}\tag{4.23}$$

Recalling $\|e^{-i\int_{t_k}^{t_{k+1}}V(s,x)ds}-1\|_{L^\infty}\leq\tau\|V(t,x)\|_{L^\infty([t_k,t_{k+1}];L^\infty)}$ and the properties of $S_e(t;t_k)$ (4.9), we obtain from (4.23)

$$\begin{aligned}&\left\|\left(S_{k,\tau}-S_e(t_{k+1};t_k)\right)\tilde{\Phi}(x)\right\|_{L^2}\\ &\leq\tau\|V(t,x)\|_{L^\infty([t_k,t_{k+1}];L^\infty)}\|\tilde{\Phi}\|_{L^2}+\tau\|V(t,x)\|_{L^\infty([t_k,t_{k+1}];L^\infty)}\|\tilde{\Phi}\|_{L^2}\lesssim\tau\|\tilde{\Phi}\|_{L^2},\end{aligned}$$

and

$$\|S_e(t_{n+1};t_{k+1})(S_{k,\tau}-S_e(t_{k+1};t_k))\mathbf{e}^k(x)\|_{L^2}\lesssim\tau\|\mathbf{e}^k(x)\|_{L^2},\quad k=0,\ldots,n.\tag{4.24}$$

Noting $\|\mathbf{e}^0(x)\|_{L^2}=0$, combining (4.24) and (4.22), and recalling $\|\eta_1^n(x)\|_{L^2}\lesssim\tau^3$, we can control

$$\begin{aligned}&\|\mathbf{e}^{n+1}(x)\|_{L^2}\\ &\leq\sum_{k=0}^{n}\|S_e(t_{n+1};t_{k+1})(S_{k,\tau}-S_e(t_{k+1};t_k))\mathbf{e}^k\|_{L^2}+\sum_{j=1}^{3}\left\|\sum_{k=0}^{n}S_e(t_{n+1};t_{k+1})\eta_j^k(x)\right\|_{L^2}\\ &\lesssim\tau^2+\sum_{k=0}^{n}\tau\|\mathbf{e}^k(x)\|_{L^2}+\sum_{j=2}^{3}\left\|\sum_{k=0}^{n}S_e(t_{n+1};t_{k+1})\eta_j^k(x)\right\|_{L^2}.\end{aligned}\tag{4.25}$$

Similar to the Lie-Trotter splitting S_1, the key to establish the improved error bounds for nonresonant τ is to derive refined estimates for the terms involving η_j^k ($j=2,3$) in (4.25). To this purpose, we introduce the approximations $\tilde{\eta}_l^k(x)$ of $\eta_l^k(x)$ ($l=2,3$, $k=0,1,\ldots,n$) as

$$\tilde{\eta}_2^k(x)=\int_0^\tau\tilde{f}_2^k(s)ds-\tau\tilde{f}_2^k(\frac{\tau}{2}),\ \tilde{\eta}_3^k(x)=-\int_0^\tau\int_0^s\sum_{j=2}^{4}\tilde{g}_j^k(s,w)dwds+\frac{\tau^2}{2}\sum_{j=2}^{4}\tilde{g}_j^k(\frac{\tau}{2},\frac{\tau}{2}),$$

where we expand $V(t_k+s,x)=V(t_k,x)+s\partial_tV(t_k,x)+O(s^2)$ and $e^{is\mathcal{D}^\varepsilon}=\mathrm{Id}+is\mathcal{D}^\varepsilon+O(s^2)$ up to the linear term in $f_2^k(s)$ (3.26) and the zeroth order term in

$g_j^k(s,w)$ $(j=2,3,4)$ (3.27)-(3.29), respectively,

$$
\begin{aligned}
\tilde{f}_2^k(s) = {}& e^{\frac{i(2s-\tau)}{\varepsilon^2}} \left((s-\tau)\mathcal{D}^\varepsilon \Pi_+^\varepsilon(V(t_k)\Pi_-^\varepsilon\Phi(t_k)) + s\Pi_+^\varepsilon(V(t_k)\mathcal{D}^\varepsilon\Pi_-^\varepsilon\Phi(t_k))\right)\\
&- e^{\frac{i(\tau-2s)}{\varepsilon^2}} \left((s-\tau)\mathcal{D}^\varepsilon \Pi_-^\varepsilon(V(t_k)\Pi_+^\varepsilon\Phi(t_k)) + s\Pi_-^\varepsilon(V(t_k)\mathcal{D}^\varepsilon\Pi_+^\varepsilon\Phi(t_k))\right)\\
&- ise^{\frac{i(2s-\tau)}{\varepsilon^2}}\Pi_+^\varepsilon(\partial_t V(t_k)\Pi_-^\varepsilon\Phi(t_k)) - ise^{\frac{i(\tau-2s)}{\varepsilon^2}}\Pi_-^\varepsilon(\partial_t V(t_k)\Pi_+^\varepsilon\Phi(t_k))\\
&- ie^{\frac{i(2s-\tau)}{\varepsilon^2}}\Pi_+^\varepsilon(V(t_k)\Pi_-^\varepsilon\Phi(t_k)) - ie^{\frac{i(\tau-2s)}{\varepsilon^2}}\Pi_-^\varepsilon(V(t_k)\Pi_+^\varepsilon\Phi(t_k)),\\
\tilde{g}_2^k(s,w) = {}& ie^{\frac{i(2w-\tau)}{\varepsilon^2}}\Pi_+^\varepsilon\left(V(t_k)\Pi_+^\varepsilon\left(V(t_k)\Pi_-^\varepsilon\Phi(t_k)\right)\right)\\
&+ ie^{\frac{i(\tau-2w)}{\varepsilon^2}}\Pi_-^\varepsilon\left(V(t_k)\Pi_-^\varepsilon\left(V(t_k)\Pi_+^\varepsilon\Phi(t_k)\right)\right),\\
\tilde{g}_3^k(s,w) = {}& ie^{\frac{i(2(s-w)-\tau)}{\varepsilon^2}}\Pi_+^\varepsilon\left(V(t_k)\Pi_-^\varepsilon\left(V(t_k)\Pi_+^\varepsilon\Phi(t_k)\right)\right)\\
&+ ie^{\frac{i(\tau-2(s-w))}{\varepsilon^2}}\Pi_-^\varepsilon\left(V(t_k)\Pi_+^\varepsilon\left(V(t_k)\Pi_-^\varepsilon\Phi(t_k)\right)\right),\\
\tilde{g}_4^k(s,w) = {}& ie^{\frac{i(2s-\tau)}{\varepsilon^2}}\Pi_+^\varepsilon\left(V(t_k)\Pi_-^\varepsilon\left(V(t_k)\Pi_-^\varepsilon\Phi(t_k)\right)\right)\\
&+ ie^{\frac{i(\tau-2s)}{\varepsilon^2}}\Pi_-^\varepsilon\left(V(t_k)\Pi_+^\varepsilon\left(V(t_k)\Pi_+^\varepsilon\Phi(t_k)\right)\right).
\end{aligned}
$$

Using Taylor expansion in $f_2^k(s)$ (3.26) and $g_j^k(s,w)$ $(j=2,3,4)$ (3.27)-(3.29) as well as properties of $\mathcal{D}^\varepsilon$, it is not difficult to check that

$$
\begin{aligned}
&\|\eta_2^k(x) - \tilde{\eta}_2^k(x)\|_{L^2}\\
&\lesssim \tau^3\bigg(\|V(t,x)\|_{W^{2,\infty}([0,T];L^\infty)}\|\Phi(t_k)\|_{L^2} + \|\partial_t V(t,x)\|_{W^{1,\infty}([0,T];H^2)}\|\|\Phi(t_k)\|_{H^2}\\
&\qquad + \|V(t,x)\|_{L^\infty([0,T];H^4)}\|\Phi(t_k)\|_{H^4}\bigg) \lesssim \tau^3,\\
&\|\eta_3^k(x) - \tilde{\eta}_3^k(x)\|_{L^2} \lesssim \tau^3\|V(t_n,x)\|_{W^{2,\infty}}^2\|\Phi(t_k)\|_{H^2} \lesssim \tau^3,
\end{aligned}
$$

which would yield for $k \le n \le \frac{T}{\tau} - 1$,

$$
\left\|S_e(t_{n+1};t_{k+1})\eta_2^k(x) - S_e(t_{n+1};t_{k+1})\tilde{\eta}_2^k(x)\right\|_{L^2} \lesssim \|\eta_2^k(x) - \tilde{\eta}_2^k(x)\|_{L^2} \lesssim \tau^3, \tag{4.26}
$$
$$
\left\|S_e(t_{n+1};t_{k+1})\eta_3^k(x) - S_e(t_{n+1};t_{k+1})\tilde{\eta}_3^k(x)\right\|_{L^2} \lesssim \|\eta_3^k(x) - \tilde{\eta}_3^k(x)\|_{L^2} \lesssim \tau^3. \tag{4.27}
$$

Plugging the above inequalities (4.26)-(4.27) into (4.25), we derive

$$
\begin{aligned}
\|\mathbf{e}^{n+1}(x)\|_{L^2} &\lesssim \tau^2 + \sum_{k=0}^n \tau^3 + \sum_{j=2}^3 \left\|\sum_{k=0}^n S_e(t_{n+1};t_{k+1})\tilde{\eta}_j^k(x)\right\|_{L^2} + \sum_{k=0}^n \tau\|\mathbf{e}^k(x)\|_{L^2}\\
&\lesssim \tau^2 + \sum_{j=2}^3 \left\|\sum_{k=0}^n S_e(t_{n+1};t_{k+1})\tilde{\eta}_j^k(x)\right\|_{L^2} + \sum_{k=0}^n \tau\|\mathbf{e}^k(x)\|_{L^2}.
\end{aligned} \tag{4.28}
$$

Step 2 (Improved estimates for nonresonant time steps). It remains to show the estimates on the terms related to $\tilde{\eta}_2^k$ and $\tilde{\eta}_3^k$. The arguments will be similar to those in the proof of the Lie-Trotter splitting case Theorem 2.4, so we only sketch the proof below. Taking $\tilde{\eta}_2^k$ for example, we write

(4.29)

$$\tilde{\eta}_2^k(s) = \tilde{\eta}_{2+}^k(s) + \tilde{\eta}_{2-}^k(s), \quad \tilde{\eta}_{2\pm}^k(x) = \int_0^\tau \tilde{f}_{2\pm}^k(s)ds - \tau \tilde{f}_{2\pm}^k(\tau/2), \quad k = 0, 1, \ldots, n,$$

with

$$\begin{aligned}\tilde{f}_{2\pm}^k(s) =& e^{\pm i(2s-\tau)/\varepsilon^2}\left(\pm(s-\tau)\mathcal{D}^\varepsilon \Pi_\pm^\varepsilon(V(t_k)\Pi_\mp^\varepsilon \Phi(t_k)) \pm s\Pi_\pm^\varepsilon(V(t_k)\mathcal{D}^\varepsilon \Pi_\mp^\varepsilon \Phi(t_k))\right) \\ & - ise^{\pm i(2s-\tau)/\varepsilon^2}\ \Pi_\pm^\varepsilon(\partial_t V(t_k)\Pi_\mp^\varepsilon \Phi(t_k)) - ie^{\pm i(2s-\tau)/\varepsilon^2}\Pi_\pm^\varepsilon(V(t_k)\Pi_\mp^\varepsilon \Phi(t_k))\end{aligned}$$

and $\tilde{f}_2^k(s) = \tilde{f}_{2+}^k(s) + \tilde{f}_{2-}^k(s)$.

Recalling the structure of the exact solution to the Dirac equation in (4.14), we have for $0 \le k \le n$

$$S_e(t_n; t_k)\tilde{\Phi}(x) = e^{-i(t_n-t_k)/\varepsilon^2} S_e^+(t_n; t_k)\tilde{\Phi}(x) + e^{i(t_n-t_k)/\varepsilon^2} S_e^-(t_n; t_k)\tilde{\Phi}(x) + R_k^n \tilde{\Phi}(x),$$

where the propagators $S_e^\pm$ and the residue operator $R_k^n : (L^2)^2 \to (L^2)^2$ are defined in (4.14). Therefore, we can get

$$\sum_{k=0}^n S_e(t_{n+1}; t_{k+1})\tilde{\eta}_{2+}^k(x) = \sum_{j=1}^4 \tilde{I}_j^n(x),$$

with

$$\begin{aligned}\tilde{I}_1^n(x) &= \tilde{p}_1(\tau)\sum_{k=0}^n e^{-\frac{i(t_{n+1}-2t_k-\tau)}{\varepsilon^2}} S_e^+(t_{n+1}; t_{k+1})\Pi_+^\varepsilon V(t_k)\Pi_-^\varepsilon S_e^-(t_k; t_0)\Phi(0), \\ \tilde{I}_2^n(x) &= \tilde{p}_1(\tau)\sum_{k=0}^n (R_{k+1}^{n+1}\Pi_+^\varepsilon V(t_k)\Pi_-^\varepsilon \Phi(t_k) + S_e(t_{n+1}; t_{k+1})\Pi_+^\varepsilon V(t_k)\Pi_-^\varepsilon R_0^k \Phi(0)), \\ \tilde{I}_3^n(x) &= \sum_{k=0}^n e^{-\frac{i(t_{n+1}-2t_k-\tau)}{\varepsilon^2}} S_e^+(t_{n+1}; t_{k+1})\Big(\tilde{p}_2(\tau)\mathcal{D}^\varepsilon \Pi_+^\varepsilon V(t_k) \\ &\quad + \tilde{p}_3(\tau)\Pi_+^\varepsilon V(t_k)\mathcal{D}^\varepsilon - i\tilde{p}_3(\tau)\Pi_+^\varepsilon \partial_t V(t_k)\Big)\Pi_-^\varepsilon S_e^-(t_k; t_0)\Phi(0), \\ \tilde{I}_4^n(x) &= \sum_{k=0}^n \Bigg(R_{k+1}^{n+1}\left(\tilde{p}_2(\tau)\mathcal{D}^\varepsilon \Pi_+^\varepsilon V(t_k) + \tilde{p}_3(\tau)\left(\Pi_+^\varepsilon V(t_k)\mathcal{D}^\varepsilon - i\Pi_+^\varepsilon \partial_t V(t_k)\right)\right)\Pi_-^\varepsilon \Phi(t_k) \\ &\qquad + S_e(t_{n+1}; t_{k+1})\left(\tilde{p}_2(\tau)\mathcal{D}^\varepsilon \Pi_+^\varepsilon V(t_k) + \tilde{p}_3(\tau)\left(\Pi_+^\varepsilon V(t_k)\mathcal{D}^\varepsilon - i\Pi_+^\varepsilon \partial_t V(t_k)\right)\right) \\ &\quad \Pi_-^\varepsilon R_0^k \Phi(0)\Bigg),\end{aligned}$$

where

$$\tilde{p}_1(\tau) = -i\left(\int_0^\tau e^{i(2s-\tau)/\varepsilon^2}ds - \tau\right), \quad \tilde{p}_2(\tau) = \left(\int_0^\tau (s-\tau)e^{i(2s-\tau)/\varepsilon^2}ds + \frac{\tau^2}{2}\right),$$
$$\tilde{p}_3(\tau) = \left(\int_0^\tau se^{i(2s-\tau)/\varepsilon^2}ds - \frac{\tau^2}{2}\right).$$

The residue terms $\tilde{I}_2^n$ and $\tilde{I}_4^n$ will be estimated first. Using the properties of R_k^n and S_e, and noting (3.45)-(3.46), we have

$$
\begin{aligned}
&\|R_{k+1}^{n+1}\Pi_+^\varepsilon V(t_k)\Pi_-^\varepsilon \Phi(t_k) + S_e(t_{n+1};t_{k+1})\Pi_+^\varepsilon V(t_k)\Pi_-^\varepsilon R_0^k\Phi(0)\|_{L^2}\\
&\lesssim \varepsilon^3\|V(t_k)\|_{W^{3,\infty}}\left(\|\Phi(t_k)\|_{H^3}+\|\Phi(0)\|_{H^3}\right),\\
&\|R_{k+1}^{n+1}\mathcal{D}^\varepsilon\Pi_+^\varepsilon V(t_k)\Pi_-^\varepsilon\Phi(t_k)\|_{L^2} + \|R_{k+1}^{n+1}(\Pi_+^\varepsilon V(t_k)\mathcal{D}^\varepsilon - i\Pi_+^\varepsilon\partial_t V(t_k))\Pi_-^\varepsilon\Phi(t_k)\|_{L^2}\\
&\lesssim \varepsilon^3\|V(t,x)\|_{W^{1,\infty}([0,T];W^{5,\infty})}\|\Phi(t_k)\|_{H^5},\\
&\|S_e(t_{n+1};t_{k+1})\mathcal{D}^\varepsilon\Pi_+^\varepsilon V(t_k)\Pi_-^\varepsilon R_0^k\Phi(0)\|_{L^2} \lesssim \varepsilon^3\|V(t,x)\|_{W^{1,\infty}([0,T];W^{3,\infty})}\|\Phi(0)\|_{H^5},\\
&\|S_e(t_{n+1};t_{k+1})(\Pi_+^\varepsilon V(t_k)\mathcal{D}^\varepsilon - i\Pi_+^\varepsilon\partial_t V(t_k))\Pi_-^\varepsilon R_0^k\Phi(0)\|_{L^2}\\
&\lesssim \varepsilon^3\|V(t,x)\|_{W^{1,\infty}([0,T];W^{3,\infty})}\|\Phi(0)\|_{H^5},
\end{aligned}
$$

which will lead to the following conclusions in view of the fact that $|\tilde{p}_1(\tau)| = |\int_0^\tau e^{i(2s-\tau)/\varepsilon^2}ds - \tau| \lesssim \min\{\tau^2/\varepsilon^2, \tau^3/\varepsilon^4\}$ and $|\tilde{p}_2(\tau)|, |\tilde{p}_3(\tau)| \lesssim \min\{\tau^2/\varepsilon^2, \tau^3/\varepsilon^4\}$ (Taylor expansion up to the linear or the quadratic term),

$$
\|\tilde{I}_2^n(x)\|_{L^2} \lesssim \min\{\tau\varepsilon, \tau^2/\varepsilon\}, \quad \|\tilde{I}_4^n(x)\|_{L^2} \lesssim \min\{\tau\varepsilon, \tau^2/\varepsilon\}. \tag{4.30}
$$

Now, we proceed to treat $\tilde{I}_1^n$ and $\tilde{I}_3^n$. For $\tilde{I}_1^n(x)$, it is similar to (4.17) which has been analyzed in the S_1 case. Using the same idea (details omitted for brevity here), and the fact that $|\tilde{p}_1(\tau)| = \left|\int_0^\tau e^{i(2s-\tau)/\varepsilon^2}ds - \tau\right| \lesssim \min\{\tau, \tau^2/\varepsilon^2\}$ as well as $\Pi_\pm^\varepsilon V(t_k)\Pi_\mp^\varepsilon = O(\varepsilon)$, under the regularity assumptions, we can get for $\tau \in \mathcal{A}_\delta(\varepsilon)$,

$$
\|\tilde{I}_1^n(x)\|_{L^2} \lesssim \min\{\tau, \tau^2/\varepsilon^2\}\left(\sum_{k=0}^{n-1}\tau\varepsilon/\delta + \varepsilon/\delta\right) \lesssim_\delta \min\{\tau\varepsilon, \tau^2/\varepsilon\}. \tag{4.31}
$$

Similarly, noticing $|\tilde{p}_2(\tau)|, |\tilde{p}_3(\tau)| \le \tau^2$, we can get

$$
\|\tilde{I}_3^n(x)\|_{L^2} \lesssim \tau^2\left(\sum_{k=0}^{n-1}\tau\varepsilon/\delta + \varepsilon/\delta\right) \lesssim_\delta \tau^2\varepsilon. \tag{4.32}
$$

Combining the estimates for $\tilde{I}_j^n$ $(j = 1,2,3,4)$, we have

$$
\left\|\sum_{k=0}^n S_e(t_{n+1};t_{k+1})\tilde{\eta}_{2+}^k(x)\right\|_{L^2} \le \sum_{j=1}^4 \|\tilde{I}_j^n(x)\|_{L^2} \lesssim_\delta \min\{\tau\varepsilon, \tau^2/\varepsilon\}. \tag{4.33}
$$

For $\sum_{k=0}^n S_e(t_{n+1};t_{k+1})\tilde{\eta}_{2-}^k(x)$, we can have the same results as

$$
\left\|\sum_{k=0}^n S_e(t_{n+1};t_{k+1})\tilde{\eta}_{2-}^k(x)\right\|_{L^2} \lesssim_\delta \min\{\tau\varepsilon, \tau^2/\varepsilon\}, \tag{4.34}
$$

which yield the following results in view of (4.33) and (4.29)

$$
\left\|\sum_{k=0}^n S_e(t_{n+1};t_{k+1})\tilde{\eta}_2^k(x)\right\|_{L^2} \lesssim_\delta \min\{\tau\varepsilon, \tau^2/\varepsilon\}. \tag{4.35}
$$

The same technique works for $S_e(t_{n+1};t_{k+1})\tilde{\eta}_3^k(x)$ and we can get

$$
\left\|\sum_{k=0}^n S_e(t_{n+1};t_{k+1})\tilde{\eta}_3^k(x)\right\|_{L^2} \lesssim_\delta \min\{\tau\varepsilon, \tau^2/\varepsilon\}. \tag{4.36}
$$

Plugging these results into (4.28), we have

$$\|\mathbf{e}^{n+1}(x)\|_{L^2} \lesssim_\delta \tau^2 + \sum_{k=0}^{n} \tau \|\mathbf{e}^k(x)\|_{L^2} + \min\{\tau\varepsilon, \tau^2/\varepsilon\}. \tag{4.37}$$

Gronwall's inequality then implies for τ satisfying $\tau \in \mathcal{A}_\delta(\varepsilon)$,

$$\|\mathbf{e}^{n+1}(x)\|_{L^2} \lesssim_\delta \tau^2 + \min\{\tau\varepsilon, \tau^2/\varepsilon\}, \quad 0 \le n \le \frac{T}{\tau} - 1. \tag{4.38}$$

This completes the proof for Theorem 2.5. □

5. Numerical results

In this section, we report three numerical examples to verify our theorems. For spatial discretization, we use Fourier pseudospectral method.

In the first two 1D examples, we choose the electric potential in (2.2) as

$$V(t,x) = \frac{1-x}{1+x^2}, \quad x \in \mathbb{R}, \quad t \ge 0, \tag{5.1}$$

and the initial data in (2.3) for the first two examples in 1D as

$$\phi_1(0,x) = e^{-\frac{x^2}{2}}, \quad \phi_2(0,x) = e^{-\frac{(x-1)^2}{2}}, \quad x \in \mathbb{R}. \tag{5.2}$$

In the last example, which is a 2D problem, we choose the electric potential in (1.5) as the honeycomb lattice potential with $\mathbf{x} = (x_1, x_2)^T \in \mathbb{R}^2$

$$V(t,\mathbf{x}) = \cos(-\frac{4\pi}{\sqrt{3}}x_1) + \cos(\frac{2\pi}{\sqrt{3}}x_1 + 2\pi x_2) + \cos(\frac{2\pi}{\sqrt{3}}x_1 - 2\pi x_2), \tag{5.3}$$

and the initial data in (1.2) are chosen as

$$\psi_1(0,\mathbf{x}) = e^{-\frac{x_1^2+x_2^2}{2}}, \quad \psi_2(0,\mathbf{x}) = e^{-\frac{(x_1-1)^2+x_2^2}{2}}, \tag{5.4}$$

$$\psi_3(0,\mathbf{x}) = e^{-\frac{(x_1+1)^2+(x_2+1)^2}{2}}, \quad \psi_4(0,\mathbf{x}) = e^{-\frac{x_1^2+(x_2-1)^2}{2}}. \tag{5.5}$$

In the 1D numerical simulations, as a common practice, we truncate the whole space onto a sufficiently large bounded domain $\Omega = (a,b)$, and assume periodic boundary conditions. The mesh size is chosen as $h := \triangle x = \frac{b-a}{M}$ with M being an even positive integer. Then the grid points can be denoted as $x_j := a + jh$ for $j = 0, 1, \ldots, M$.

To show the numerical results, we introduce the discrete l^2 errors of the numerical solution. Let $\Phi^n = (\Phi_0^n, \Phi_1^n, \ldots, \Phi_{M-1}^n, \Phi_M^n)^T$ be the numerical solution obtained by a numerical method with time step τ and ε as well as a very fine mesh size h at time $t = t_n$, and let $\Phi(t,x)$ be the exact solution. Then the relative discrete l^2 error is quantified as

$$e^{\varepsilon,\tau}(t_n) = \frac{\|\Phi^n - \Phi(t_n,\cdot)\|_{l^2}}{\|\Phi(t_n,\cdot)\|_{l^2}} = \frac{\sqrt{h\sum_{j=0}^{M-1}|\Phi_j^n - \Phi(t_n,x_j)|^2}}{\sqrt{h\sum_{j=0}^{M-1}|\Phi(t_n,x_j)|^2}}, \tag{5.6}$$

and $e^{\varepsilon,\tau}(t_n)$ should be close to the L^2 errors (with normalized probability density of the wave function) in Theorems 2.1, 2.2, 2.4, and 2.5 for fine spatial mesh sizes h.

For the 2D example, with similar notation (equal mesh size h and grid points along each direction), the relative discrete l^2 error could be defined as

$$e^{\varepsilon,\tau}(t_n) = \frac{\|\Psi^n - \Psi(t_n,\cdot)\|_{l^2}}{\|\Psi(t_n,\cdot)\|_{l^2}} = \frac{h\sqrt{\sum_{j=0}^{M^2-1}|\Psi_j^n - \Psi(t_n,\mathbf{x}_j)|^2}}{h\sqrt{\sum_{j=0}^{M^2-1}|\Psi(t_n,\mathbf{x}_j)|^2}}. \tag{5.7}$$

Example 1. We first test the uniform error bounds for the splitting methods. In this example, we choose resonant time step size, that is, for small enough chosen ε, there is a positive k_0, such that $\tau = k_0\varepsilon\pi$.

The bounded computational domain is set as $\Omega = (-32, 32)$. Because we are only concerned with the temporal errors in this paper, during the computation, the spatial mesh size is always set to be $h = \frac{1}{16}$ so that the spatial error is negligible. As there is no exact solution available, for comparison, we use a numerical "exact" solution generated by the S_2 method with a very fine time step size $\tau_e = 2\pi \times 10^{-6}$.

Tables 5.1 and 5.2 show the numerical errors $e^{\varepsilon,\tau}(t = 2\pi)$ with different ε and time step size τ for S_1 and S_2, respectively.

TABLE 5.1. Discrete l^2 temporal errors $e^{\varepsilon,\tau}(t = 2\pi)$ for the wave function with resonant time step size, S_1 method.

$e^{\varepsilon,\tau}(t=2\pi)$	$\tau_0=\pi/4$	$\tau_0/4$	$\tau_0/4^2$	$\tau_0/4^3$	$\tau_0/4^4$	$\tau_0/4^5$
$\varepsilon_0=1$	4.84E-1	**1.27E-1**	3.20E-2	8.03E-3	2.01E-3	5.02E-4
order	–	**0.97**	0.99	1.00	1.00	1.00
$\varepsilon_0/2$	6.79E-1	1.21E-1	**3.10E-2**	7.78E-3	1.95E-3	4.87E-4
order	–	1.24	**0.98**	1.00	1.00	1.00
$\varepsilon_0/2^2$	5.78E-1	2.71E-1	3.07E-2	**7.76E-3**	1.95E-3	4.87E-4
order	–	0.55	1.57	**0.99**	1.00	1.00
$\varepsilon_0/2^3$	**5.33E-1**	1.85E-1	1.21E-1	7.75E-3	**1.95E-3**	4.87E-4
order	–	0.76	0.30	1.98	**1.00**	1.00
$\varepsilon_0/2^4$	5.13E-1	1.48E-1	7.02E-2	5.76E-2	1.95E-3	**4.88E-4**
order	–	0.90	0.54	0.14	2.44	**1.00**
$\varepsilon_0/2^5$	5.04E-1	**1.34E-1**	4.70E-2	3.07E-2	2.82E-2	4.88E-4
order	–	**0.96**	0.75	0.31	0.06	2.93
$\varepsilon_0/2^7$	4.98E-1	1.25E-1	**3.37E-2**	1.18E-2	7.68E-3	7.05E-3
order	–	1.00	**0.95**	0.76	0.31	0.06
$\varepsilon_0/2^9$	4.97E-1	1.24E-1	3.17E-2	**8.46E-3**	2.95E-3	1.92E-3
order	–	1.00	0.98	**0.95**	0.76	0.31
$\varepsilon_0/2^{11}$	4.96E-1	1.23E-1	3.13E-2	7.94E-3	**2.12E-3**	7.37E-4
order	–	1.00	0.99	0.99	**0.95**	0.76
$\max_{0<\varepsilon\le1} e^{\varepsilon,\tau}(t=2\pi)$	6.79E-1	2.71E-1	1.21E-1	5.76E-2	2.82E-2	1.39E-2
order	–	0.66	0.58	0.54	0.52	0.51

In Tables 5.1 and 5.2, the last two rows show the largest error of each column for fixed τ. They both give 1/2 order of convergence, which coincides well with Theorems 2.1 and 2.2. More specifically, in Table 5.1, we can see when $\tau \gtrsim \varepsilon$ (below the lower bolded line), there is first order convergence, which agrees with the error bound $\|\Phi(t_n, x) - \Phi^n(x)\|_{L^2} \lesssim \tau + \varepsilon$. When $\tau \lesssim \varepsilon^2$ (above the upper bolded line), we observe first order convergence, which matches the other error

TABLE 5.2. Discrete l^2 temporal errors $e^{\varepsilon,\tau}(t=2\pi)$ for the wave function with resonant time step size, S_2 method.

$e^{\varepsilon,\tau}(t=2\pi)$	$\tau_0=\pi/4$	$\tau_0/4^2$	$\tau_0/4^3$	$\tau_0/4^4$	$\tau_0/4^5$	$\tau_0/4^6$
$\varepsilon_0=1$	8.08E-2	**4.44E-3**	2.76E-4	1.73E-5	1.08E-6	6.74E-8
order	–	**2.09**	2.00	2.00	2.00	2.00
$\varepsilon_0/2$	4.13E-1	9.66E-3	**5.73E-4**	3.57E-5	2.23E-6	1.39E-7
order	–	2.71	**2.04**	2.00	2.00	2.00
$\varepsilon_0/2^2$	2.63E-1	2.15E-1	1.21E-3	**7.22E-5**	4.50E-6	2.81E-7
order	–	0.15	3.74	**2.03**	2.00	2.00
$\varepsilon_0/2^3$	**2.08E-1**	1.10E-1	1.10E-1	1.51E-4	**9.05E-6**	5.64E-7
order	–	0.46	0.00	4.75	**2.03**	2.00
$\varepsilon_0/2^4$	1.92E-1	5.56E-2	5.51E-2	5.51E-2	1.89E-5	**1.13E-6**
order	–	0.89	0.01	0.00	5.76	**2.03**
$\varepsilon_0/2^5$	1.88E-1	2.85E-2	2.76E-2	2.76E-2	2.76E-2	2.36E-6
order	–	1.36	0.02	0.00	0.00	6.76
$\varepsilon_0/2^6$	1.87E-1	1.55E-2	1.38E-2	1.38E-2	1.38E-2	1.38E-2
order	–	1.79	0.08	0.00	0.00	0.00
$\varepsilon_0/2^7$	1.87E-1	**9.86E-3**	6.92E-3	6.90E-3	6.90E-3	6.90E-3
order	–	**2.12**	0.26	0.00	0.00	0.00
$\varepsilon_0/2^{11}$	1.87E-1	6.97E-3	**5.93E-4**	4.32E-4	4.31E-4	4.31E-4
order	–	2.37	**1.78**	0.23	0.00	0.00
$\varepsilon_0/2^{15}$	1.87E-1	6.95E-3	4.03E-4	**3.75E-5**	2.71E-5	2.70E-5
order	–	2.37	2.05	**1.71**	0.23	0.00
$\max_{0<\varepsilon\leq 1} e^{\varepsilon,\tau}(t=2\pi)$	4.13E-1	2.15E-1	1.10E-1	5.51E-2	2.76E-2	1.38E-2
order	–	0.47	0.49	0.50	0.50	0.50

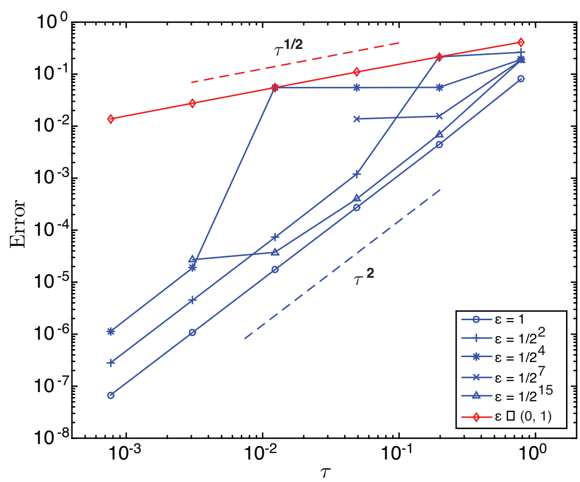

FIGURE 5.2. Order plot for S_2 using resonant time steps.

bound $\|\Phi(t_n,x)-\Phi^n(x)\|_{L^2} \lesssim \tau+\tau/\varepsilon$. Similarly, in Table 5.2, the second order convergence can be clearly observed when $\tau \lesssim \varepsilon^2$ (above the upper bolded line) or when $\tau \gtrsim \sqrt{\varepsilon}$ (below the lower bolded line), which fits well with the two error bounds $\|\Phi(t_n,x)-\Phi^n(x)\|_{L^2} \lesssim \tau^2+\tau^2/\varepsilon^3$ and $\|\Phi(t_n,x)-\Phi^n(x)\|_{L^2} \lesssim \tau^2+\varepsilon$.

Moreover, Figure 5.2 gives the order plot for S_2 under resonant time steps. It could be clearly observed that when ε is relatively large, there is second order convergence for small time step sizes; and when ε is relatively small, there is second order convergence for large time step sizes. Overall, there is a 1/2 order uniform convergence, which corresponds well with Theorem 2.2.

Through the results of this example, we successfully validate the uniform error bounds for the splitting methods in Theorems 2.1 and 2.2.

Example 2. In this example, we test the improved uniform error bounds for nonresonant time step size. Here we choose $\tau \in \mathcal{A}_\delta(\varepsilon)$ for some given ε and $0<\delta\le 1$.

The bounded computational domain is set as $\Omega=(-16,16)$. The numerical "exact" solution is computed by the S_2 method with a very small time step $\tau_e = 8\times 10^{-6}$. Spatial mesh size is fixed as $h=1/16$ for all the numerical simulations.

Tables 5.3 and 5.4 show the numerical errors $e^{\varepsilon,\tau}(t=4)$ with different ε and time step size τ for S_1 and S_2, respectively.

TABLE 5.3. Discrete l^2 temporal errors $e^{\varepsilon,\tau}(t=4)$ for the wave function with nonresonant time step size, S_1 method.

$e^{\varepsilon,\tau}(t=4)$	$\tau_0=1/2$	$\tau_0/2$	$\tau_0/2^2$	$\tau_0/2^3$	$\tau_0/2^4$	$\tau_0/2^5$	$\tau_0/2^6$
$\varepsilon_0=1$	3.51E-1	1.78E-1	8.96E-2	4.50E-2	2.25E-2	1.13E-2	5.64E-3
order	–	0.98	0.99	0.99	1.00	1.00	1.00
$\varepsilon_0/2$	3.52E-1	1.65E-1	8.34E-2	4.20E-2	2.11E-2	1.05E-2	5.28E-3
order	–	1.10	0.98	0.99	1.00	1.00	1.00
$\varepsilon_0/2^2$	3.25E-1	1.64E-1	8.04E-2	4.07E-2	2.05E-2	1.03E-2	5.15E-3
order	–	0.99	1.03	0.98	0.99	1.00	1.00
$\varepsilon_0/2^3$	3.24E-1	1.69E-1	8.10E-2	4.13E-2	2.02E-2	1.02E-2	5.13E-3
order	–	0.94	1.06	0.97	1.03	0.99	0.99
$\varepsilon_0/2^4$	3.12E-1	1.61E-1	8.24E-2	4.22E-2	2.05E-2	1.03E-2	5.10E-3
order	–	0.95	0.97	0.97	1.04	0.99	1.02
$\varepsilon_0/2^5$	3.25E-1	1.61E-1	8.10E-2	4.10E-2	2.07E-2	1.04E-2	5.13E-3
order	–	1.02	0.99	0.98	0.99	0.98	1.02
$\varepsilon_0/2^6$	3.19E-1	1.63E-1	8.43E-2	4.09E-2	2.05E-2	1.03E-2	5.16E-3
order	–	0.97	0.95	1.04	1.00	0.99	0.99
$\varepsilon_0/2^7$	3.18E-1	1.60E-1	8.10E-2	4.06E-2	2.05E-2	1.03E-2	5.13E-3
order	–	0.99	0.99	0.99	0.99	0.99	1.00
$\max_{0<\varepsilon\le 1} e^{\varepsilon,\tau}$	3.52E-1	1.78E-1	8.96E-2	4.50E-2	2.25E-2	1.13E-2	5.64E-3
order	–	0.98	0.99	0.99	1.00	1.00	1.00

In Table 5.3, we could see that overall, for fixed time step size τ, the error $e^{\varepsilon,\tau}(t=4)$ does not change with different ε. This verifies the uniform first order

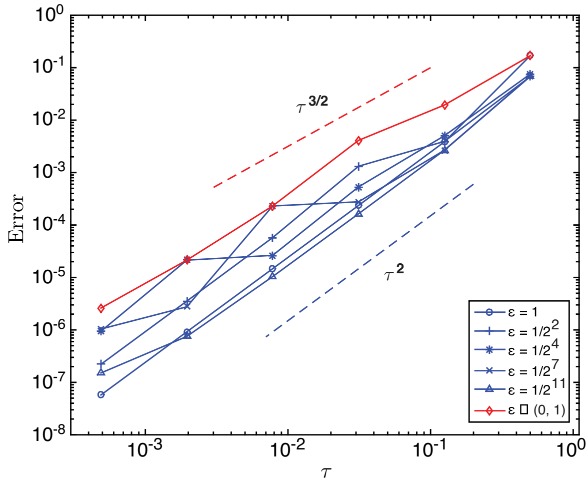

FIGURE 5.3. Order plot for S_2 using nonresonant time steps.

TABLE 5.4. Discrete l^2 temporal errors $e^{\varepsilon,\tau}(t=4)$ for the wave function with nonresonant time step size, S_2 method.

$e^{\varepsilon,\tau}(t=4)$	$\tau_0 = 1/2$	$\tau_0/4$	$\tau_0/4^2$	$\tau_0/4^3$	$\tau_0/4^4$	$\tau_0/4^5$
$\varepsilon_0 = 1/2$	1.69E-1	3.85E-3	**2.36E-4**	1.47E-5	9.20E-7	5.75E-8
order	–	2.73	**2.01**	2.00	2.00	2.00
$\varepsilon_0/2$	9.79E-2	1.16E-2	4.61E-4	**2.83E-5**	1.77E-6	1.10E-7
order	–	1.54	2.33	**2.01**	2.00	2.00
$\varepsilon_0/2^2$	6.76E-2	3.93E-3	1.32E-3	5.76E-5	**3.54E-6**	2.21E-7
order	–	2.05	0.78	2.26	**2.01**	2.00
$\varepsilon_0/2^3$	7.86E-2	4.49E-3	2.63E-4	1.72E-4	7.59E-6	**4.67E-7**
order	–	2.06	2.05	0.31	2.25	**2.01**
$\varepsilon_0/2^4$	7.55E-2	5.04E-3	5.33E-4	2.64E-5	2.14E-5	9.43E-7
order	–	1.95	1.62	2.17	0.15	2.25
$\varepsilon_0/2^5$	**7.01E-2**	1.94E-2	2.38E-4	6.50E-5	3.02E-6	2.61E-6
order	–	0.93	3.18	0.94	2.22	0.10
$\varepsilon_0/2^7$	6.84E-2	**2.67E-3**	2.77E-4	2.31E-4	2.76E-6	1.04E-6
order	–	**2.34**	1.64	0.13	3.19	0.70
$\varepsilon_0/2^9$	6.84E-2	2.67E-3	**1.65E-4**	1.03E-5	2.08E-6	2.10E-6
order	–	2.34	**2.01**	2.00	1.15	-0.00
$\varepsilon_0/2^{11}$	6.84E-2	2.67E-3	1.66E-4	**1.03E-5**	6.53E-7	4.53E-8
order	–	2.34	2.00	**2.00**	1.99	1.92
$\varepsilon_0/2^{13}$	6.84E-2	2.67E-3	1.64E-4	1.04E-5	**7.51E-7**	1.51E-7
order	–	2.34	2.01	1.99	**1.89**	1.16
$\max_{0<\varepsilon\le 1} e^{\varepsilon,\tau}(t=4)$	1.69E-1	1.94E-2	4.11E-3	2.31E-4	2.14E-5	2.61E-6
order	–	1.56	1.12	2.08	1.72	1.52

convergence in time for S_1 with nonresonant time step size, as stated in Theorem 2.4. In Table 5.4, the last two rows show the largest error of each column for fixed τ, which gives 3/2 order of convergence, consistent with Theorem 2.5. More specifically, in Table 5.4, we can observe the second order convergence when $\tau \gtrsim \varepsilon$ (below the lower bolded line) or when $\tau \lesssim \varepsilon^2$ (above the upper bolded line). The lower bolded diagonal line agrees with the error bound $\|\Phi(t_n,x) - \Phi^n(x)\|_{L^2} \lesssim \tau^2 + \tau\varepsilon$, and the upper bolded diagonal line matches the other error bound $\|\Phi(t_n,x) - \Phi^n(x)\|_{L^2} \lesssim \tau^2 + \tau^2/\varepsilon$.

Similar to the resonant time step case, Figure 5.3 exhibits the order plot for S_2 with nonresonant time step sizes. When ε is relatively large, there is second order uniform convergence for small time step sizes; and when ε is relatively small, there is second order uniform convergence for large time step sizes. Overall, there is uniform 3/2 order convergence in time, which corresponds well with Theorem 2.5.

TABLE 5.5. Discrete l^2 temporal errors $e^{\varepsilon,\tau}(t=2\pi)$ in 2D for the wave function with resonant time step size, S_2 method.

$e^{\varepsilon,\tau}(t=2\pi)$	$\tau_0=\pi/16$	$\tau_0/4$	$\tau_0/4^2$	$\tau_0/4^3$	$\tau_0/4^4$	$\tau_0/4^5$
$\varepsilon_0=1$	1.28E-1	**2.56E-3**	1.57E-4	9.78E-6	6.08E-7	3.41E-8
order	–	**2.82**	2.02	2.00	2.00	2.08
$\varepsilon_0/2$	4.33E-1	6.48E-3	**3.17E-4**	1.96E-5	1.22E-6	6.85E-8
order	–	3.03	**2.18**	2.01	2.00	2.08
$\varepsilon_0/2^2$	1.01	8.71E-2	6.99E-4	**3.92E-5**	2.42E-6	1.36E-7
order	–	1.76	3.48	**2.08**	2.01	2.08
$\varepsilon_0/2^3$	1.44	6.31E-2	2.55E-2	8.50E-5	**4.88E-6**	2.73E-7
order	–	2.26	0.65	4.11	**2.06**	2.08
$\varepsilon_0/2^4$	1.46	**5.52E-2**	1.14E-2	9.90E-3	1.07E-5	**5.58E-7**
order	–	**2.36**	1.14	0.10	4.93	**2.13**
$\varepsilon_0/2^8$	1.46	5.22E-2	**3.27E-3**	5.76E-4	5.35E-4	5.35E-4
order	–	2.40	**2.00**	1.25	0.05	0.00
$\varepsilon_0/2^{12}$	1.46	5.22E-2	3.22E-3	**2.40E-4**	1.39E-4	1.39E-4
order	–	2.40	2.01	**1.87**	0.39	0.00
$\varepsilon_0/2^{16}$	1.46	5.22E-2	3.22E-3	1.99E-4	**1.57E-5**	5.83E-6
order	–	2.40	2.01	2.01	**1.83**	0.72
$\max_{0<\varepsilon\le 1} e^{\varepsilon,\tau}$	1.46	8.71E-2	2.55E-2	9.90E-3	4.44E-3	2.16E-3
order	–	2.03	0.89	0.68	0.58	0.52

Through the results of this example, we successfully validate the improved uniform error bounds for the splitting methods in Theorems 2.4 and 2.5, with nonresonant time step sizes.

Example 3. In this example, we deal with a 2D problem. We test the uniform convergence for resonant and nonresonant time step sizes using S_2 for (1.5).

TABLE 5.6. Discrete l^2 temporal errors $e^{\varepsilon,\tau}(t=4)$ in 2D for the wave function with nonresonant time step size, S_2 method.

$e^{\varepsilon,\tau}(t=4)$	$\tau_0 = 1/8$	$\tau_0/8$	$\tau_0/8^2$	$\tau_0/8^3$	$\tau_0/8^4$
$\varepsilon_0 = 1$	**9.41E-3**	1.43E-4	2.23E-6	3.47E-8	4.92E-10
order	–	2.01	2.00	2.00	2.05
$\varepsilon_0/2^{3/2}$	5.54E-2	**3.68E-4**	5.71E-6	8.91E-8	1.25E-9
order	–	**2.41**	2.00	2.00	2.05
$\varepsilon_0/2^3$	6.56E-1	1.23E-3	**1.61E-5**	2.50E-7	3.49E-9
order	–	3.02	**2.09**	2.00	2.05
$\varepsilon_0/2^{9/2}$	3.00E-1	3.29E-3	5.34E-5	**7.34E-7**	1.02E-8
order	–	2.17	1.98	**2.06**	2.05
$\varepsilon_0/2^6$	**2.77E-1**	3.35E-3	9.19E-5	2.13E-6	**2.64E-8**
order	–	2.12	1.73	1.81	**2.11**
$\varepsilon_0/2^9$	2.79E-1	**3.30E-3**	4.58E-4	1.64E-6	6.37E-8
order	–	**2.13**	0.95	2.71	1.56
$\varepsilon_0/2^{12}$	2.79E-1	3.27E-3	**5.08E-5**	8.57E-7	3.09E-7
order	–	2.14	**2.00**	1.96	0.49
$\varepsilon_0/2^{15}$	2.79E-1	3.27E-3	5.12E-5	**1.24E-6**	4.45E-7
order	–	2.14	2.00	**1.79**	0.49
$\max_{0<\varepsilon\le 1} e^{\varepsilon,\tau}(t=4)$	6.56E-1	1.70E-2	4.58E-4	1.02E-5	4.45E-7
order	–	1.76	1.74	1.83	1.51

The bounded computational domain is still set as $\Omega = (-10,10) \times (-10,10)$. The numerical "exact" solution is computed by the S_2 method with a very small time step $\tau_e = 2\pi \times 10^{-5}$ for resonant time steps, and $\tau_e = 10^{-5}$ for nonresonant time steps. Spatial mesh size is fixed as $h = 1/16$ for all the numerical simulations.

Tables 5.5 and 5.6 show the numerical errors under resonant and nonresonant time step sizes, respectively, with different ε.

The conclusions which could be drawn from Tables 5.5 and 5.6 are similar to those from Tables 5.2 and 5.4. The results validate that the theorems of super-resolution could be extended to two-dimensional, or even higher-dimensional cases.

6. Conclusion

The super-resolution property of time-splitting methods for the Dirac equation in the nonrelativistic regime without magnetic potentials were established. We rigorously proved the uniform error bounds, and the improved uniform error bounds with nonresonant time step for the Lie-Trotter splitting S_1 and the Strang splitting S_2. For S_1, we have two independent error bounds $\tau + \varepsilon$ and $\tau + \tau/\varepsilon$, resulting in a uniform 1/2 order convergence. Surprisingly, there will be first order improved uniform convergence if the time step size is nonresonant. For S_2, the uniform convergence rate is also 1/2, while the two different error bounds are $\tau^2 + \varepsilon$ and $\tau^2 + \tau^2/\varepsilon^3$, respectively. With nonresonant time step size, the convergence order can be improved to 3/2 for S_2, while the two independent error bounds become $\tau^2+\tau\varepsilon$ and $\tau^2+\tau^2/\varepsilon$. The numerical results agreed well with the theorems. In this paper, only the 1D case was presented, but indeed the results are still valid in higher dimensions, and the proofs can be easily generalized. Moreover, higher order time-splitting methods, like the S_4, $S_{4\mathrm{c}}$, $S_{4\mathrm{RK}}$ methods used in [14], also have the super-resolution property for the Dirac equation in the nonrelativistic regime in the absence of external magnetic potentials.

Appendix

In this section, we sketch the proofs of Theorems 2.1 and 2.4 for the Lie splitting S_1 applied to the four-vector Dirac equation (1.5) in higher dimensions $d=2,3$, as the arguments for the Lie (S_1)/Strang splitting (S_2) applied to the four-vector form (1.5)/two-vector form (1.6) would be similar. In such case, assumptions (A) and (B) are directly generalized to the high dimensions ($d=2,3$).

For $d=2,3$, the Lie-Trotter splitting S_1 for (1.5) is

$$\Psi^{n+1}(\mathbf{x})=e^{-\frac{i\tau}{\varepsilon^2}\mathcal{T}^\varepsilon}e^{-i\int_{t_n}^{t_{n+1}}V(s,\mathbf{x})\,ds}\Psi^n(\mathbf{x}),\quad \mathbf{x}=(x_1,\ldots,x_d)\in\mathbb{R}^d, \tag{0.1}$$

with $\Psi^0(x)=\Psi_0(x)\in\mathbb{C}^4$, where the free Dirac operator $\mathcal{T}^\varepsilon$ becomes

$$\mathcal{T}^\varepsilon=-\varepsilon\sum_{j=1}^{d}\alpha_j\partial_j+\beta \tag{0.2}$$

and the decomposition (3.1) holds with projections $\Pi_\pm^\varepsilon$ given in (3.2) by replacing I_2 with I_4. Now, the following expansions for $\Pi_\pm^\varepsilon$ are valid [15]:

$$\Pi_+^\varepsilon=\Pi_+^0+\varepsilon\mathcal{R}_1=\Pi_+^0-i\frac{\varepsilon}{2}\sum_{j=1}^{d}\alpha_j\partial_j+\varepsilon^2\mathcal{R}_2,\quad \Pi_+^0=\mathrm{diag}(1,1,0,0), \tag{0.3}$$

$$\Pi_-^\varepsilon=\Pi_-^0-\varepsilon\mathcal{R}_1=\Pi_-^0+i\frac{\varepsilon}{2}\sum_{j=1}^{d}\alpha_j\partial_j-\varepsilon^2\mathcal{R}_2,\quad \Pi_-^0=\mathrm{diag}(0,0,1,1), \tag{0.4}$$

where $\mathcal{R}_1:(H^m(\mathbb{R}^d))^4\to(H^{m-1}(\mathbb{R}^d))^4$ for $m\geq1$, $m\in\mathbb{N}^*$, and $\mathcal{R}_2:(H^m(\mathbb{R}^d))^4\to(H^{m-2}(\mathbb{R}^d))^4$ for $m\geq2$, $m\in\mathbb{N}^*$ are uniformly bounded operators with respect to ε.

We introduce the error function similar to (2.6)

$$\mathbf{e}^n(\mathbf{x})=\Psi(t_n,\mathbf{x})-\Psi^n(\mathbf{x}),\quad 0\leq n\leq\frac{T}{\tau}, \tag{0.5}$$

and we will show the conclusions in Theorems 2.1 and 2.4 hold. The proof will be sketched as follows.

Step 1 (Local error decomposition). Following the computations in Lemma 3.1, we have

$$\mathbf{e}^{n+1}(\mathbf{x})=e^{-\frac{i\tau}{\varepsilon^2}\mathcal{T}^\varepsilon}e^{-i\int_{t_n}^{t_{n+1}}V(s,\mathbf{x})ds}\mathbf{e}^n(\mathbf{x})+\eta_1^n(\mathbf{x})+\eta_2^n(\mathbf{x}),\quad 0\leq n\leq\frac{T}{\tau}-1, \tag{0.6}$$

with $\|\eta_1^n(\mathbf{x})\|_{L^2}\lesssim\tau^2$, $\eta_2^n(x)=-ie^{-\frac{i\tau}{\varepsilon^2}\mathcal{T}^\varepsilon}\left(\int_0^\tau f_2^n(s)ds-\tau f_2^n(0)\right)$, where

$$\begin{aligned}f_2^n(s)=&e^{i2s/\varepsilon^2}e^{is\mathcal{D}^\varepsilon}\Pi_+^\varepsilon\left(V(t_n)\Pi_-^\varepsilon e^{is\mathcal{D}^\varepsilon}\Psi(t_n)\right)\\&+e^{-i2s/\varepsilon^2}e^{-is\mathcal{D}^\varepsilon}\Pi_-^\varepsilon\left(V(t_n)\Pi_+^\varepsilon e^{-is\mathcal{D}^\varepsilon}\Psi(t_n)\right).\end{aligned} \tag{0.7}$$

Step 2 (Theorem 2.1 for general time steps). Analogous to the proof of Theorem 2.1 in section 3, the estimates (3.45) and (3.45) hold true for the $d = 2, 3$ case by noticing the decompositions (0.3) and (0.4) and $\Pi^0_\pm V(\mathbf{x})\Pi^0_\mp = 0$. Then the proof of Theorem 2.1 for the $d = 2, 3$ case can be proceeded as the same in section 3.

Step 3 (Theorem 2.4 for nonresonant steps). Following the proof of Theorem 2.4 for $d = 1$ case in section 4, by using the similar estimates as (0.3) and (0.4) for the $d = 2, 3$ cases (observed in the above step), we can derive (4.11) for the high-dimensional cases. So (4.12) is valid. The rest of the proof for the high-dimensional case of Theorem 2.4 ($d = 2, 3$) can be carried out exactly the same as that in section 4, where only the solution structure (4.14) of the Dirac equation is used and such structure is valid in $d = 2, 3$ [6, 15].

As can be seen in the above generalizations to the higher dimensions $d = 2, 3$, the estimates (0.3) and (0.4) play the key roles, which ensures that $\Pi^\varepsilon_\pm V(t, \mathbf{x})\Pi^\varepsilon_\mp = O(\varepsilon)$ (valid for $d = 1, 2, 3$, two-vector form and/or four-vector form). However, such $O(\varepsilon)$ order estimates do not hold if electrical potential $V(t, \mathbf{x})$ is replaced by the external magnetic potentials and we can only obtain the stated results in this paper for the Dirac equation without magnetic potentials.

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