SUPER-RESOLUTION OF TIME-SPLITTING METHODS FOR THE DIRAC EQUATION IN THE NONRELATIVISTIC LIMIT 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 limit 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 limit regime, the solution propagates waves with $O(\varepsilon^2)$ wavelength in time. Surprisingly, we find out that the splitting methods exhibit super-resolution, in the sense of breaking the resolution constraint under the Shannon’s sampling theorem, i.e. the methods can capture the solutions accurately even if the time step size $\tau$ is much larger than the sampled wavelength at $O(\varepsilon^2)$. $S_1$ shows $1/2$ order convergence uniformly with respect to $\epsilon$, $S_1$ 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 $\tau$ and uniformly convergent with $3/2$ order rate for non-resonant time step size. Finally, numerical examples are reported to validate our findings.

Key words. Dirac equation, super-resolution, nonrelativistic limit regime, time-splitting, uniform error bound

1. Introduction. The splitting technique introduced by Trotter in 1959 [46] has been widely applied in analysis and numerical simulation [2,9,10,12,20], 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 [31,47] and are superior in many applications. Developments of splitting type methods in solving partial differential equations (PDEs) include utilization in Schrödinger/nonlinear Schrödinger equations [2,9,10,19,20,37,45], Dirac/nonlinear Dirac equations [7,13,36], Maxwell-Dirac system [11,32], Zakharov system [12,13,28,34,35], Stokes equation [18], and Enrenfest dynamics [25], etc.

When dealing with oscillatory problems, the splitting method usually performs much better than traditional numerical methods [9,31]. For instance, in order to obtain “correct” observables of the Schrödinger equation in the semiclassical limit 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 limit regime [21] and the Enrenfest dynamics [25]. However, in general, splitting methods still suffer from the mesh size/time step constraints related to the high frequencies in the aforementioned problems, i.e. they need to obey the resolution constraint determined by the Shannon’s sampling theorem [43] – 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 limit 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, which is highly nontrivial. In the rest of the paper, we will discuss the oscillatory Dirac equation in the nonrelativistic limit regime, with conventional time splitting numerical approach and its super-resolution properties.

Proposed by British physicist Paul Dirac in 1928 [23], 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 \[12, 26, 39, 40\], as well as the relativistic effects of molecules in super intense lasers, e.g., attosecond lasers \[16, 27\]. Mathematically, the \(d\)-dimensional \((d = 1, 2, 3)\) Dirac equation with external electro-magnetic potentials \[7, 14\] for the complex spinor vector field \(\Psi := \Psi(t, x) = (\psi_1(t, x), \psi_2(t, x), \psi_3(t, x), \psi_4(t, x))^T \in \mathbb{C}^4\) can be written as

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

with initial value

\[
(1.2) \quad \Psi(t = 0, x) = \Psi_0(x), \quad x \in \mathbb{R}^d,
\]

where \(i = \sqrt{-1}\), \(t\) is time, \(x = (x_1, \ldots, x_d)^T \in \mathbb{R}^d\) is the spatial coordinate vector, \(\partial_j = \frac{\partial}{\partial x_j}\) \((j = 1, \ldots, d)\), \(V := V(t, x)\) and \(A_j := A_j(t, x)\) \((j = 1, \ldots, d)\) 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 limit 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 \(4 \times 4\) matrices \(\alpha_1, \alpha_2, \alpha_3\) and \(\beta\) are

\[
(1.3) \quad \alpha_1 = \begin{pmatrix} 0 & \sigma_1 \\ \sigma_1 & 0 \end{pmatrix}, \quad \alpha_2 = \begin{pmatrix} 0 & \sigma_2 \\ \sigma_2 & 0 \end{pmatrix}, \quad \alpha_3 = \begin{pmatrix} 0 & \sigma_3 \\ \sigma_3 & 0 \end{pmatrix}, \quad \beta = \begin{pmatrix} I_2 & 0 \\ 0 & -I_2 \end{pmatrix},
\]

where \(\sigma_1, \sigma_2, \sigma_3\) are the Pauli matrices

\[
(1.4) \quad \sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix},
\]

In 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 \[21, 22, 24, 29, 30, 42\] and references therein. In the numerical aspect, many accurate and efficient numerical methods have been proposed and analyzed \[3, 38\], such as the finite difference time domain (FDTD) methods \[13, 41\], time-splitting Fourier pseudospectral (TSFP) method \[7, 32\], exponential wave integrator Fourier pseudospectral (EWI-FP) method \[7\], and the Gaussian beam method \[35\], etc.

In the nonrelativistic limit regime, as \(\varepsilon \to 0^+\), the Dirac equation (1.1) converges to Pauli equation \[15, 33\] or Schrödinger equation \[5, 15\], and the solution propagates waves with wavelength \(O(\varepsilon^2)\) in time and \(O(1)\) in space, respectively. The highly oscillatory nature of the solution in time brings severe difficulties in numerical computation in the nonrelativistic limit regime, i.e. when \(0 < \varepsilon \ll 1\). In fact, it would cause the time step size \(\tau\) strictly dependent on \(\varepsilon\) in order to capture the solution accurately. Rigorous error estimates were established for the finite difference time domain method (FDTD), exponential wave integrator Fourier pseudospectral method (EWI-FP) and 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 \(S_{4c}\) 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 limit regime, where the errors are uniform with respect to \(\varepsilon \in (0, 1)\) \[6\], allowing for \(\varepsilon\)-independent time step \(\tau\).
From the analysis in [7], the error bounds for second order Strang splitting TSFP (also called as \( S_2 \) later in this paper) depends on the small parameter \( \varepsilon \) as \( \tau^2 / \varepsilon^4 \). Surprisingly, through our extensive numerical experiments, we find out that if the magnetic potentials \( A_j \equiv 0 \) for \( j = 1, \ldots, d \) in (1.1), the errors of TSFP are then independent of \( \varepsilon \) and uniform w.r.t. \( \varepsilon \), i.e., \( S_2 \) for Dirac equation (1.1) without magnetic potentials \( A_j \) has super-resolution w.r.t. \( \varepsilon \). In such case, (1.1) reduces to

\[
(1.5) \quad i \partial_t \Psi(t, x) = \left( -\frac{i}{\varepsilon} \sum_{j=1}^{d} \alpha_j \partial_j + \frac{1}{\varepsilon^2} \beta + V(t, x) I_4 \right) \Psi(t, x), \quad x \in \mathbb{R}^d, \quad d = 1, 2, 3, \quad t > 0,
\]

with the initial value given in (1.2). In lower dimensions \( (d = 1, 2) \), the four component Dirac equation (1.3) can be reduced to the following two-component form for \( \Phi(t, x) = (\phi_1(t, x), \phi_2(t, x))^T \in \mathbb{C}^2 [7] \):

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

with initial value

\[
(1.7) \quad \Phi(t = 0, x) = \Phi_0(x), \quad x \in \mathbb{R}^d, \quad d = 1, 2.
\]

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 \( \tau \) is much larger than the sampled wavelength at \( O(\varepsilon^2) \), i.e. they exhibit super-resolution in the sense of breaking the resolution constraint under the Shannon’s sampling theorem [43]. This super-resolution property of the splitting methods makes them more efficient and reliable for solving the Dirac equation without magnetic potentials in the nonrelativistic limit regime, compared to other numerical approaches in the literature. In the sequel, 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 limit regime without magnetic potential, and state the main results. In section 3 and section 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, \( A \preceq B \) is used with the meaning that there exists a generic constant \( C > 0 \) independent of \( \varepsilon \) and \( \tau \), such that \( |A| \leq C B \). \( A \preceq_\delta B \) has a similar meaning that there exists a constant \( C_\delta > 0 \) dependent on \( \delta \) but independent of \( \varepsilon \) and \( \tau \), such that \( |A| \leq C_\delta B \).

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 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.
2.1. Time-splitting methods. Denote the Hermitian operator
\[
T^\varepsilon = -i\varepsilon \sigma_1 \partial_x + \sigma_3, \quad x \in \mathbb{R},
\]
and the Dirac equation \((1.6)\) in 1D can be written as
\[
i\partial_t \Phi(t, x) = \frac{1}{\varepsilon^2} T^\varepsilon \Phi(t, x) + V(t, x) \Phi(t, x), \quad x \in \mathbb{R},
\]
with initial value
\[
\Phi(0, x) = \Phi_0(x), \quad x \in \mathbb{R}.
\]

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 \([46]\)
\[
\Phi^{n+1}(x) = e^{-\frac{i\tau}{2} T^\varepsilon} e^{-i \int_{t_n}^{t_{n+1}} V(s, x) \, ds} \Phi^n(x), \quad \text{with} \quad \Phi^0(x) = \Phi_0(x), \quad x \in \mathbb{R}.
\]

**Second-order splitting (Strang splitting).** The discrete-in-time second-order splitting \((S_2)\) is written as \([44]\)
\[
\Phi^{n+1}(x) = e^{-\frac{i\tau}{2} T^\varepsilon} e^{-i \int_{t_n}^{t_{n+1}} V(s, x) \, ds} e^{-\frac{i\tau}{2} T^\varepsilon} \Phi^n(x), \quad \text{with} \quad \Phi^0(x) = \Phi_0(x), \quad x \in \mathbb{R}.
\]

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
\[
(A) \quad V(t, x) \in W^{m, \infty}([0, T]; L^\infty(\mathbb{R})) \cap L^\infty([0, T]; W^{2m+m_*, \infty}(\mathbb{R})), \quad m \in \mathbb{N}^*, \quad m_* \in \{0, 1\}.
\]
In addition, we assume the exact solution \(\Phi(t, x)\) satisfies
\[
(B) \quad \Phi(t, x) \in L^\infty([0, T]; (H^{2m+m_*}(\mathbb{R}))^2), \quad m \in \mathbb{N}^*, \quad m_* \in \{0, 1\}.
\]
We remark here that if the initial value \(\Phi_0(x) \in (H^{2m+m_*}(\mathbb{R}))^2\), 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
\[
e^n(x) = \Phi(t_n, x) - \Phi^n(x), \quad 0 \leq n \leq \frac{T}{\tau},
\]
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
\[
(2.7) \quad \|e^n(x)\|_{L^2} \lesssim \tau + \varepsilon, \quad \|e^n(x)\|_{L^2} \lesssim \tau + \tau/\varepsilon, \quad 0 \leq n \leq \frac{T}{\tau}.
\]
As a result, there is a uniform error bound for $S_1$

\[ \| e^n(x) \|_{L^2} \lesssim \tau + \max_{0 < \varepsilon \leq 1} \min \{ \varepsilon, \tau / \varepsilon \} \lesssim \sqrt{\tau}, \quad 0 \leq n \leq \frac{T}{\tau}. \]

**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

\[ \| e^n(x) \|_{L^2} \lesssim \tau^2 + \varepsilon, \quad \| e^n(x) \|_{L^2} \lesssim \tau^2 / \varepsilon^3, \quad 0 \leq n \leq \frac{T}{\tau}. \]

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

\[ \| e^n(x) \|_{L^2} \lesssim \tau^2 + \max_{0 < \varepsilon \leq 1} \min \{ \varepsilon, \tau^2 / \varepsilon^3 \} \lesssim \sqrt{\tau}, \quad 0 \leq n \leq \frac{T}{\tau}. \]

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

\[ \| e^n(x) \|_{L^2} \leq C_1 \| \Phi_0(x) \|_{H^2} \left( \tau + \max_{0 < \varepsilon \leq 1} \min \{ \varepsilon, \tau / \varepsilon \} \right), \quad 0 \leq n \leq \frac{T}{\tau}, \]

and the error estimates in Theorem 2.2 can be restated as

\[ \| e^n(x) \|_{L^2} \leq C_2 \| \Phi_0(x) \|_{H^4} \left( \tau^2 + \max_{0 < \varepsilon \leq 1} \min \{ \varepsilon, \tau^2 / \varepsilon^3 \} \right), \quad 0 \leq n \leq \frac{T}{\tau}, \]

where $C_1$ and $C_2$ are constants depending only on $V(t, x)$ and $T$.

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

### 2.3. Improved uniform error bounds for non-resonant time steps.

In the Dirac equation \[ (1.6) \] or \[ (1.3) \], the leading term is $\frac{1}{\varepsilon} \sigma_3 \Psi$ or $\frac{1}{\varepsilon} \beta \Psi$, which suggests the solution exhibits almost periodicity in time with periods $2k\pi \varepsilon^2$ ($k \in \mathbb{N}$, the periods of $e^{-i\sigma_3 \varepsilon^2}$ and $e^{-i\beta \varepsilon^2}$). From numerical results, we observe the errors behave much better compared to the results in Theorems 2.1 & 2.2, when $2\tau$ is away from the leading temporal oscillation periods $2k\pi \varepsilon^2$. In fact, for given $0 < \delta \leq 1$, define

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

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 2.3.** Let $\Phi^n(x)$ be the numerical approximation obtained from $S_1$ \[ (2.4) \]. If the time step size $\tau$ is non-resonant, i.e. there exists $0 < \delta \leq 1$, 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

\[ \| e^n(x) \|_{L^2} \lesssim \delta \tau, \quad 0 \leq n \leq \frac{T}{\tau}. \]
Theorem 2.4. Let $\Phi^n(x)$ be the numerical approximation obtained from $S_2$ (2.5). If the time step size $\tau$ is non-resonant, i.e. there exists $0 < \delta \leq 1$, such that $\tau \in A_\delta(\varepsilon)$, under the assumptions (A) and (B) with $m = 2$ and $m_\ast = 1$, 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

\begin{align}
\|e^n(x)\|_{L^2} \lesssim & \; \tau^2 + \tau \varepsilon, \quad \|e^n(x)\|_{L^2} \lesssim \delta \tau^2 + \tau^2 / \varepsilon, \quad 0 \leq n \leq \frac{T}{\tau}.
\end{align}

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

\begin{align}
\|e^n(x)\|_{L^2} \lesssim & \; \max_{0 < \varepsilon \leq 1} \min\{\tau \varepsilon, \tau^2 / \varepsilon\} \lesssim \tau^{3/2}, \quad 0 \leq n \leq \frac{T}{\tau}.
\end{align}

Remark 2.2. In Theorems 2.3 and 2.4, the constants in the error estimates depend on $\delta$ and the proof in the paper suggests that the constants are bounded from above by $\frac{T}{\tau} C$ and $\frac{2}{\tau} C$ with some common factor $C$ independent of $\delta$ and $\tau$. The optimality of the uniform error bounds in Theorems 2.3 and 2.4 will be verified by numerical examples presented in section 5.

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 $T^\varepsilon$ is diagonalizable in the phase space (Fourier domain), it can be decomposed as [6, 7, 15]

\begin{align}
T^\varepsilon = \sqrt{I - \varepsilon^2 \Delta} \Pi^\varepsilon_+ - \sqrt{I - \varepsilon^2 \Delta} \Pi^\varepsilon_-, \quad \Pi^\varepsilon_+ = \text{diag}(1, 0), \quad \Pi^\varepsilon_- = \text{diag}(0, 1),
\end{align}

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

\begin{align}
\Pi^\varepsilon_+ = & \; \frac{1}{2} \left[ I_2 + (I_2 - \varepsilon^2 \Delta)^{-1/2} T^\varepsilon \right], \quad \Pi^\varepsilon_- = \frac{1}{2} \left[ I_2 - (I_2 - \varepsilon^2 \Delta)^{-1/2} T^\varepsilon \right].
\end{align}

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

\begin{align}
\Pi^\varepsilon_+ = & \; I_2 + \varepsilon R_1 = I_2 + \frac{\varepsilon}{2} \sigma_1 \partial_x + \varepsilon^2 R_2, \quad \Pi^\varepsilon_- = I_2 - \frac{\varepsilon}{2} \sigma_1 \partial_x - \varepsilon^2 R_2,
\end{align}

\begin{align}
\Pi^0_+ = & \; \text{diag}(1, 0), \quad \Pi^0_- = \text{diag}(0, 1),
\end{align}

Fig. 2.1. Illustration of non-resonant time steps $A_\delta(\varepsilon)$ with $\delta = 0.15$ for (a) $\varepsilon = 1$ and (b) $\varepsilon = 0.5$. 

(a) $\varepsilon = 1$

\begin{center}
\begin{tikzpicture}
\draw[->,>=latex,thick] (-2,0) -- (2,0) node[below] {$2\pi$};
\foreach \x in {0,pi/2,pi,3*pi/2,2*pi}
\draw[thick] \x cm -- (\x cm,0);
\draw[->,>=latex,thick] (-2,0) -- (2,0) node[below] {$2\pi$};
\foreach \x in {0,pi/2,pi,3*pi/2,2*pi}
\draw[thick] \x cm -- (\x cm,0);
\draw[->,>=latex,thick] (-2,0) -- (2,0) node[below] {$2\pi$};
\foreach \x in {0,pi/2,pi,3*pi/2,2*pi}
\draw[thick] \x cm -- (\x cm,0);
\draw[->,>=latex,thick] (-2,0) -- (2,0) node[below] {$2\pi$};
\foreach \x in {0,pi/2,pi,3*pi/2,2*pi}
\draw[thick] \x cm -- (\x cm,0);
\draw[->,>=latex,thick] (-2,0) -- (2,0) node[below] {$2\pi$};
\foreach \x in {0,pi/2,pi,3*pi/2,2*pi}
\draw[thick] \x cm -- (\x cm,0);
\draw[->,>=latex,thick] (-2,0) -- (2,0) node[below] {$2\pi$};
\foreach \x in {0,pi/2,pi,3*pi/2,2*pi}
\draw[thick] \x cm -- (\x cm,0);
\draw[->,>=latex,thick] (-2,0) -- (2,0) node[below] {$2\pi$};
\foreach \x in {0,pi/2,pi,3*pi/2,2*pi}
\draw[thick] \x cm -- (\x cm,0);
\draw[->,>=latex,thick] (-2,0) -- (2,0) node[below] {$2\pi$};
\foreach \x in {0,pi/2,pi,3*pi/2,2*pi}
\draw[thick] \x cm -- (\x cm,0);
\draw[->,>=latex,thick] (-2,0) -- (2,0) node[below] {$2\pi$};
\foreach \x in {0,pi/2,pi,3*pi/2,2*pi}
\draw[thick] \x cm -- (\x cm,0);
\end{tikzpicture}
\end{center}
where \( \mathcal{R}_1 : (H^m(\mathbb{R}))^2 \to (H^{m-1}(\mathbb{R}))^2 \) for \( m \geq 1, m \in \mathbb{N}^* \), and \( \mathcal{R}_2 : (H^m(\mathbb{R}))^2 \to (H^{m-2}(\mathbb{R}))^2 \) for \( m \geq 2, m \in \mathbb{N}^* \) are uniformly bounded operators with respect to \( \varepsilon \).

To help capture the features of solutions, denote

\[
(3.5) \quad \mathcal{D}^\varepsilon = \frac{1}{\varepsilon^2} (\sqrt{I_d - \varepsilon^2 \Delta} - I_d) = -(\sqrt{I_d - \varepsilon^2 \Delta} + I_d)^{-1} \Delta,
\]

where \( \mathcal{D}^\varepsilon \) is a uniformly bounded operator with respect to \( \varepsilon \) from \( (H^m(\mathbb{R}))^2 \) to \( (H^{m-2}(\mathbb{R}))^2 \) for \( m \geq 2 \), then we have the decomposition for the unitary evolution operator \( e^{it\mathcal{D}^\varepsilon} \) as

\[
(3.6) \quad e^{\frac{it}{\varepsilon^2} \mathcal{D}^\varepsilon} = e^{\frac{it}{\varepsilon^2} (\sqrt{I_d - \varepsilon^2 \Delta} \Pi_+ - \sqrt{I_d - \varepsilon^2 \Delta} \Pi_-)} = e^{it/\varepsilon^2} e^{it\mathcal{D}^\varepsilon} \Pi_+ + e^{-it/\varepsilon^2} e^{-it\mathcal{D}^\varepsilon} \Pi_-.
\]

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 \( \Phi(t) := \Phi(t, x) \) in 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

\[
(3.7) \quad e^{n+1}(x) = e^{-\frac{it}{\varepsilon^2} \mathcal{D}^\varepsilon} e^{-i \int_{t_n}^{t_{n+1}} V(s, x) ds} e^n(x) + \eta^n(x) + \eta^n_2(x), \quad 0 \leq n \leq \frac{T}{\tau} - 1,
\]

with \( \|\eta^n_1(x)\|_{L^2} \lesssim \tau^2 \), \( \eta^n_2(x) = -i e^{\frac{it}{\varepsilon^2} \mathcal{D}^\varepsilon} \left( \int_0^t f^n_2(s) ds - \tau f^n_2(0) \right) \), where

\[
(3.8) \quad f^n_2(s) = e^{i2s/\varepsilon^2} e^{is\mathcal{D}^\varepsilon} \Pi_+ \left( V(t_n) \Pi_- e^{is\mathcal{D}^\varepsilon} \Phi(t_n) \right) + e^{-i2s/\varepsilon^2} e^{-is\mathcal{D}^\varepsilon} \Pi_- \left( V(t_n) \Pi_+ e^{-is\mathcal{D}^\varepsilon} \Phi(t_n) \right).
\]

**Proof.** From the definition of \( e^n(x) \), noticing the Lie-Trotter splitting formula [2.4], we have

\[
(3.9) \quad e^{n+1}(x) = e^{-\frac{it}{\varepsilon^2} \mathcal{D}^\varepsilon} e^{-i \int_{t_n}^{t_{n+1}} V(s, x) ds} e^n(x) + \eta^n(x), \quad 0 \leq n \leq \frac{T}{\tau} - 1, \quad x \in \mathbb{R},
\]

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

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

Noticing [2.2], applying Duhamel’s principle, we derive

\[
(3.11) \quad \Phi(t_{n+1}, x) = e^{-\frac{it}{\varepsilon^2} \mathcal{D}^\varepsilon} \Phi(t_n, x) - i \int_{t_n}^{t_{n+1}} e^{-\frac{i(t-s)}{\varepsilon^2} \mathcal{D}^\varepsilon} V(t_n + s, x) \Phi(t_n + s, x) ds,
\]

while Taylor expansion gives

\[
(3.12) \quad e^{-\frac{it}{\varepsilon^2} \mathcal{D}^\varepsilon} e^{-i \int_{t_n}^{t_{n+1}} V(s, x) ds} \Phi(t_n, x) = e^{-\frac{it}{\varepsilon^2} \mathcal{D}^\varepsilon} \left( 1 - i \int_{t_n}^{t_{n+1}} V(s, x) ds + O(\tau^2) \right) \Phi(t_n, x).
\]

Combining [3.11], [3.12] and [3.10], we get

\[
(3.13) \quad \eta^n(x) = i e^{-\frac{it}{\varepsilon^2} \mathcal{D}^\varepsilon} V(t_n, x) \Phi(t_n, x) - i \int_{t_n}^{t_{n+1}} e^{-\frac{i(t-s)}{\varepsilon^2} \mathcal{D}^\varepsilon} \left( V(t_n, x) e^{-\frac{it}{\varepsilon^2} \mathcal{D}^\varepsilon} \Phi(t_n, x) \right) ds + \sum_{j=1}^{2} R_j^n(x),
\]

where
where
\[ R_1^n(x) = e^{-\frac{it}{\lambda^2}T^x} (\lambda_1^n(x) + \lambda_2^n(x)) \Phi(t_n, x), \]
\[ R_2^n(x) = -i \int_0^t e^{-\frac{i(t-s)}{\lambda^2}T^x} (V(t_n)\lambda_4^n(s)) \, ds - i \int_0^t e^{-\frac{i(t-s)}{\lambda^2}T^x} (\lambda_3^n(s)\Phi(t_n + s, x)) \, ds, \]
with
\[ (3.14) \quad \lambda_1^n(x) = e^{-i \int_{t_n}^{t_n+1} V(s,x) \, ds} \left( 1 - i \int_{t_n}^{t_n+1} V(s,x) \, ds \right), \]
\[ (3.15) \quad \lambda_2^n(x) = -i \int_{t_n}^{t_n+1} V(s,x) \, ds + i\tau V(t_n, x), \quad \lambda_3^n(s,x) = V(t_n + s, x) - V(t_n, x), \quad 0 \leq s \leq \tau, \]
\[ (3.16) \quad \lambda_4^n(x) = -i \int_0^\tau e^{-\frac{i(t_n-s)}{\lambda^2}T^x} (V(t_n+w,x)\Phi(t_n+w,x)) \, dw, \quad 0 \leq s \leq \tau. \]

It is easy to see that for \( 0 \leq n \leq \frac{T}{\lambda^2} - 1 \),
\[ \|\lambda_1^n(x)\|_{L^\infty} \lesssim \tau^2\|V(t,x)\|^2_{L^\infty(L^\infty)}, \quad \|\lambda_2^n(x)\|_{L^\infty([0,T];L^2)} \lesssim \tau\|V(t,x)\|_{L^\infty(L^\infty)}\|\Phi(t,x)\|_{L^\infty((L^2)^2)}, \]
\[ \|\lambda_3^n(x)\|_{L^\infty} \lesssim \tau^2\|\partial_t V(t,x)\|_{L^\infty(L^\infty)}, \quad \|\lambda_4^n(x)\|_{L^\infty([0,T];L^\infty)} \lesssim \tau\|\partial_t V(t,x)\|_{L^\infty(L^\infty)}. \]

As a consequence, we obtain the following bounds for \( 0 \leq n \leq \frac{T}{\lambda^2} - 1 \),
\[ (3.17) \quad \|R_1^n(x)\|_{L^2} \lesssim (\|\lambda_1^n(x)\|_{L^\infty} + \|\lambda_2^n(x)\|_{L^\infty})\|\Phi(t_n)\|_{L^2} \lesssim \tau^2, \]
\[ (3.18) \quad \|R_2^n(x)\|_{L^2} \lesssim \tau \left( \|V(t_n)\|_{L^\infty}\|\lambda_4^n(x)\|_{L^\infty([0,T];L^2)} + \|\lambda_3^n(x)\|_{L^\infty([0,T];L^\infty)}\|\Phi(t_n)\|_{L^\infty((L^2)^2)} \right) \lesssim \tau^2. \]

Recalling \( \eta^n_2(x) \) given in Lemma 3.1, we introduce
\[ f^n(s) := f^n(s,x) = e^{-\frac{is}{\lambda^2}T^x} \left( V(t_n,x)e^{-\frac{it}{\lambda^2}T^x}\Phi(t_n, x) \right) = f^n_1(s) + f^n_2(s), \quad 0 \leq s \leq \tau, \]
with \( f^n_2 \) given in 3.8 and \( f^n_1 \) from the decomposition 3.6 as
\[ f^n_1(s) = e^{isD^s} \Pi_+ \left( V(t_n)e^{-isD^s}\Pi_+ \Phi(t_n) \right) + e^{-isD^s} \Pi_- \left( V(t_n)e^{isD^s}\Pi_- \Phi(t_n) \right), \]
and then \( \eta^n(x) \) can be written as
\[ (3.20) \quad \eta^n(x) = -ie^{-\frac{is}{\lambda^2}T^x} \left( \int_0^\tau (f^n_1(s) + f^n_2(s)) \, ds - \tau (f^n_1(0) + f^n_2(0)) \right) + R^n_1(x) + R^n_2(x). \]

Now, it is easy to verify that \( \eta^n(x) = \eta^n_1(x) + \eta^n_2(x) \) with \( \eta^n_2(x) \) given in Lemma 3.1 if we let
\[ (3.21) \quad \eta^n_1(x) = -ie^{-\frac{is}{\lambda^2}T^x} \left( \int_0^\tau f^n_1(s) \, ds - \tau f^n_1(0) \right) + R^n_1(x) + R^n_2(x). \]

Noticing that
\[ \left\| e^{-\frac{is}{\lambda^2}T^x} \left( \int_0^\tau f^n_1(s) \, ds - \tau f^n_1(0) \right) \right\|_{L^2} \lesssim \tau^2\|\partial_t f^n_1(\cdot)\|_{L^\infty([0,T];(L^2)^2)} \]
\[ \lesssim \tau^2 \left( \|V(t_n)\|_{L^\infty}\|\Phi(t_n)\|_{H^2} + \|V(t_n)\|_{W^{2,\infty}}\|\Phi(t_n)\|_{H^2} \right), \]
recalling the regularity assumptions $(A)$ and $(B)$, combining (3.21) and (3.18), we can get

$$\|\eta^n_1(x)\|_{L^2} \leq \|R^n_1(x)\|_{L^2} + \|R^n_2(x)\|_{L^2} + \left\| e^{-\frac{\tau}{2}T^*} \left( \int_0^T f^n_1(s) ds - \tau f^n_1(0) \right) \right\|_{L^2} \lesssim \tau^2,$$

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 $m_\ast = 0$, we have

$$e^{n+1}_t(x) = e^{-\frac{\tau}{2}T^*} e^{-i \int_{t_{n+1}}^{t_n+1} V(s,x) ds} e^{-\frac{i\tau}{2} T^*} e^n(x) + \eta^n_1(x) + \eta^n_2(x) + \eta^n_3(x), \quad 0 \leq n \leq \frac{T}{\tau} - 1,$$

with

$$\|\eta^n_1(x)\|_{L^2} \lesssim \tau^3,$n^n_2(x) = -ie^{-\frac{i\tau}{2} T^*} \left( \int_0^\tau f^n_2(s) ds - \tau f^n_2(\tau/2) \right),$$

$$\eta^n_3(x) = -e^{-\frac{i\tau}{2} T^*} \left( \int_0^\tau \int_0^\tau \sum_{j=2}^{4} g^n_j(s,w) dw ds - \frac{\tau^2}{2} \sum_{j=2}^{4} g^n_j(\tau/2,\tau/2) \right),$$

where

$$f^n_2(s) = e^{\frac{i\tau}{2} T^*} e^{isD^s} \Pi_+^e (V(t_n + s) e^{isD^s} \Pi_+^e \Phi(t_n)) + e^{-\frac{i\tau}{2} T^*} e^{-isD^s} \Pi_+^e (V(t_n + s) e^{-isD^s} \Pi_+^e \Phi(t_n)),$$

$$g^n_2(s,w) = e^{2w/2} e^{isD^s} \Pi_+^e \left( V(t_n) e^{-i(s-w)D^s} \Pi_+^e \Phi(t_n) \right),$$

$$g^n_3(s,w) = e^{2(s-w)/2} e^{isD^s} \Pi_-^e \left( V(t_n) e^{-i(s-w)D^s} \Pi_-^e \Phi(t_n) \right),$$

$$g^n_4(s,w) = e^{2s/2} e^{isD^s} \Pi_+^e \left( V(t_n) e^{-i(s-w)D^s} \Pi_+^e \Phi(t_n) \right).$$

**Proof.** From the definition of $e^n(x)$, noticing the Strang splitting formula (2.4), we have

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

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

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

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

$$\Phi(t_{n+1}) = e^{-\frac{\tau}{2}T^*} \Phi(t_n,x) - \int_0^\tau e^{-\frac{i\tau}{2} T^*} \left( V(t_n + s,x) e^{-\frac{i\tau}{2} T^*} \Phi(t_n,x) \right) ds$$

$$- \int_0^\tau \int_0^\tau e^{-\frac{i\tau}{2} T^*} \left( V(t_n + s,x) e^{-\frac{i\tau}{2} T^*} (V(t_n + w,x) \Phi(t_n + w,x)) \right) dw ds,$$
\(e^{-i \int_{t_n}^{t_n+1} V(s,x) \, ds} e^{-\frac{i \tau x}{\varepsilon} T^x} \Phi(t_n,x)\)

\[
(3.32) \quad = e^{-\frac{i \tau x}{\varepsilon} T^x} \left(1 - i \int_0^\tau V(t_n+s,x) \, ds - \frac{1}{2} \left(\int_0^\tau V(t_n+s,x) \, ds\right)^2 + O(\tau^3)\right) e^{-\frac{i \tau x}{\varepsilon} T^x} \Phi(t_n,x).
\]

Denoting

\[
(3.33) \quad f^n(s) = e^{\frac{i \tau x}{\varepsilon} T^x} \left(V(t_n+s,x) e^{-\frac{i \tau x}{\varepsilon} T^x} \Phi(t_n,x)\right), \quad 0 \leq s \leq \tau,
\]
\[
(3.34) \quad g^n(s,w) = e^{\frac{i \tau x}{\varepsilon} T^x} \left(V(t_n,x) e^{-\frac{i \tau x}{\varepsilon} T^x} \left(V(t_n,x) e^{\frac{i \tau x}{\varepsilon} T^x} \Phi(t_n,x)\right)\right), \quad 0 \leq s, w \leq \tau,
\]

in view of (3.31) and (3.32), \(\eta^n(x)\) (3.30) can be written as

\[
(3.35) \quad \eta^n(x) = -e^{\frac{i \tau x}{\varepsilon} T^x} \left[i \int_0^\tau f^n(s) \, ds - i \tau f^n \left(\frac{\tau}{2}\right) + \int_0^\tau \int_0^s g^n(s,w) \, dw \, ds - \frac{\tau^2}{2} g^n \left(\frac{\tau^2}{2}, \frac{\tau}{2}\right)\right] + \sum_{j=1}^2 R^n_j(x),
\]

where

\[
(3.36) \quad R^n_1(x) = -e^{\frac{i \tau x}{\varepsilon} T^x} (\lambda^n_1(x) + \lambda^n_2(x)) e^{-\frac{i \tau x}{\varepsilon} T^x} \Phi(t_n,x),
\]
\[
(3.37) \quad R^n_2(x) = -\int_0^\tau \int_0^s e^{-\frac{(\tau-s) x}{\varepsilon} T^x} \left(V(t_n+s,x) e^{-\frac{(\tau-s) x}{\varepsilon} T^x} (V(t_n+w,x) \lambda^n_3(w,x))\right) \, dw \, ds,
\]

with

\[
\lambda^n_1(x) = -i \left(\int_0^\tau V(t_n+s,x) \, ds - \tau V(t_n+\frac{\tau}{2},x)\right) - \frac{1}{2} \left(\int_0^\tau V(t_n+s,x) \, ds\right)^2 - \tau^2 V^2(t_n,x),
\]
\[
\lambda^n_2(x) = e^{-i \int_0^\tau V(t_n+s,x) \, ds} - 1 + i \int_0^\tau V(t_n+s,x) \, ds + \frac{1}{2} \left(\int_0^\tau V(t_n+s,x) \, ds\right)^2,
\]
\[
\lambda^n_3(w,x) = -i \int_0^w e^{-\frac{(w-s) x}{\varepsilon} T^x} (V(t_n+u,x) \Phi(t_n+u,x)) \, du.
\]

It is easy to check that

\[
\|\lambda^n_1(x)\|_{L^\infty} \lesssim \tau^3 \|\partial_t V(t,x)\|_{L^\infty(L^\infty)} + \tau^3 \|\partial_t V(t,x)\|_{L^\infty(L^\infty)} \|V(t,x)\|_{L^\infty(L^\infty)},
\]
\[
\|\lambda^n_2(x)\|_{L^\infty} \lesssim \tau^2 \|V(t,x)\|_{L^2(L^\infty)}, \quad \|\lambda^n_3(w,x)\|_{L^\infty([0,\tau];L^2)} \lesssim \tau \|V(t,x)\|_{L^\infty(L^\infty)} \|\Phi\|_{L^\infty(L^2)},
\]

which immediately implies that

\[
(3.38) \quad \|R^n_1(x)\|_{L^2} \lesssim (\|\lambda^n_1(x)\|_{L^\infty} + \|\lambda^n_2(x)\|_{L^\infty}) \|\Phi(t_n)\|_{L^2} \lesssim \tau^3,
\]
\[
(3.39) \quad \|R^n_2(x)\|_{L^2} \lesssim \tau^2 \|V(t,x)\|_{L^2(L^\infty)} \|\lambda^n_3(w,x)\|_{L^\infty([0,\tau];L^2)} \lesssim \tau^3.
\]

In view of (3.6), recalling the definitions of \(f^n_2(s)\) and \(g^n_j(s,w)\) \((j = 2,3,4)\) given in Lemma (3.2), we introduce \(f^n_1(s)\) and \(g^n_1(s,w)\) such that

\[
(3.40) \quad f^n(s) = f^n_1(s) + f^n_2(s), \quad g^n(s,w) = \sum_{j=1}^4 g^n_j(s,w)
\]
where

\[ f^n_1(s) = e^{isD^r} \Pi^+_\varepsilon \left( V(t_n + s) e^{-isD^r} \Pi^+ \Phi(t_n) \right) + e^{-isD^r} \Pi^- \left( V(t_n + s) e^{isD^r} \Pi^- \Phi(t_n) \right), \]
\[ g^n_1(s, w) = e^{isD^r} \Pi^+ \left( V(t_n) e^{-i(s-w)D^r} \Pi^+ \left( V(t_n) e^{-iwD^r} \Pi^+ \Phi(t_n) \right) \right) \]
\[ + e^{-isD^r} \Pi^- \left( V(t_n) e^{i(s-w)D^r} \Pi^- \left( V(t_n) e^{iwD^r} \Pi^- \Phi(t_n) \right) \right). \]

Denote

\[ \zeta^n_1(x) = -ie^{-\frac{\tau}{2}T^r} \left( \int_0^t f^n_1(s) \, ds - \tau f^n_1(\tau/2) \right), \]
\[ \zeta^n_2(x) = -e^{-\frac{\tau}{2}T^r} \left( \int_0^\tau \int_0^s g^n_1(s, w) \, dw \, ds - \frac{\tau^2}{2} g^n_1(\tau/2, \tau/2) \right), \]

then it is easy to show that

\[ \| \zeta^n_1(x) \|_{L^2} \lesssim \tau^3 \| \partial_{ss} f_1(s) \|_{L^2} \lesssim \tau^3, \quad \| \zeta^n_2(x) \|_{L^2} \lesssim \tau^3 \left( \| \partial_s g_1(s, w) \|_{L^2} + \| \partial_w g_1(s, w) \|_{L^2} \right), \]

by noticing that \( V \in L^\infty(W^{2m, \infty}) \) and \( \Phi(t, x) \in L^\infty((H^2)^2) \) with \( m = 2 \) as well as the fact that \( D^r : (H^1)^2 \to (H^{l-2})^2 (l > 2) \) is uniformly bounded w.r.t. \( \varepsilon \). Recalling (3.38)-(3.41) and \( \eta_3^n (j = 2, 3) \) given in Lemma 3.2, we have

\[ \eta^n(x) = \eta^n_1(x) + \eta^n_2(x) + \eta^n_3(x), \]

where \( \eta^n_2(x) \) and \( \eta^n_3(x) \) are given in Lemma 3.2 and

\[ \eta^n_1(x) = R^n_1(x) + R^n_2(x) + \zeta^n_1(x) + \zeta^n_2(x). \]

Combining (3.38), (3.39) and (3.41), we can get

\[ \| \eta^n_1(x) \|_{L^2} \leq \| R^n_1(x) \|_{L^2} + \| R^n_2(x) \|_{L^2} + \| \zeta^n_1(x) \|_{L^2} + \| \zeta^n_2(x) \|_{L^2} \lesssim \tau^3, \]

which completes the proof. \( \square \)

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

\[ \| e^{n+1}(x) \|_{L^2} \leq \| e^n(x) \|_{L^2} + \| \eta^n_1(x) \|_{L^2} + \| \eta^n_2(x) \|_{L^2}, \quad 0 \leq n \leq \frac{T}{\tau} - 1, \]

with \( e^n(x) = 0, \| \eta^n_1(x) \|_{L^2} \lesssim \tau^2 \) and \( \eta^n_2(x) = -ie^{-\frac{\tau}{2}T^r} \left( \int_0^\tau f^n_2(s) \, ds - \tau f^n_2(0) \right), \) where \( f^n_2(s) \) is defined in (3.8).

To analyze \( f^n_2(s) \), using (3.39) and (3.41), we expand \( \Pi^+ V(t_n) \Pi^- \) and \( \Pi^- V(t_n) \Pi^+ \) to get

\[ \Pi^+ V(t_n) \Pi^- = \Pi^0_+ V(t_n) \left( \Pi^0_- - \varepsilon R_1 \right) + \varepsilon R_1 V(t_n) \Pi^- = -\varepsilon \Pi^0_+ V(t_n) R_1 + \varepsilon R_1 V(t_n) \Pi^-, \]
\[ \Pi^- V(t_n) \Pi^+ = \Pi^0_- V(t_n) \left( \Pi^0_+ + \varepsilon R_1 \right) - \varepsilon R_1 V(t_n) \Pi^+ = \varepsilon \Pi^0_- V(t_n) R_1 - \varepsilon R_1 V(t_n) \Pi^+. \]
As $R_1 : (H^m)^2 \to (H^{m-1})^2$ is uniformly bounded with respect to $\varepsilon \in (0, 1]$, we have

\begin{align}
(3.45) & \quad \left\| \Pi_+ \left( V(t_n) \Pi_+ e^{i\varepsilon \tau \Phi(t_n)} \right) \right\|_{L^2} \lesssim \varepsilon \left( \| \partial_x V(t_n) \|_{L^\infty} \| \Phi(t_n) \|_{L^2} + \| V(t_n) \|_{L^\infty} \| \partial_x \Phi(t_n) \|_{L^2} \right), \\
(3.46) & \quad \left\| \Pi_+ \left( V(t_n) \Pi_+ e^{i\varepsilon \tau \Phi(t_n)} \right) \right\|_{L^2} \lesssim \varepsilon \left( \| \partial_x V(t_n) \|_{L^\infty} \| \Phi(t_n) \|_{L^2} + \| V(t_n) \|_{L^\infty} \| \partial_x \Phi(t_n) \|_{L^2} \right).
\end{align}

Noticing the assumptions (A) and (B) with $m = 1$ and $m_* = 0$, we obtain from (3.8)

\begin{align}
(3.47) & \quad \| 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, \quad 0 \leq s \leq \tau.
\end{align}

As a result, from the first inequality, we get

\begin{align}
(3.48) & \quad \left\| \int_0^\tau f_2^n(s) \, ds - \tau f_2^n(0) \right\|_{L^2} \lesssim \tau \varepsilon.
\end{align}

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

\begin{align}
(3.49) & \quad \left\| \int_0^\tau f_2^n(s) \, ds - \tau f_2^n(0) \right\|_{L^2} = \left\| \int_0^\tau \int_0^s \partial_w f_2^n(w) \, dw \, ds \right\|_{L^2} \lesssim \tau^2 / \varepsilon.
\end{align}

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

\begin{align}
(3.50) & \quad \| \eta_2^n(x) \|_{L^2} \lesssim \min\{\tau \varepsilon, \tau^2 / \varepsilon\}.
\end{align}

Then from (3.44) and $e^0 = 0$, we get

\begin{align}
\| e^{n+1}(x) \|_{L^2} \leq & \left\| e^0(x) \right\|_{L^2} + \sum_{k=0}^n \| \eta_k^n(x) \|_{L^2} + \sum_{k=0}^n \| \eta_k^2(x) \|_{L^2} \\
\lesssim & n \tau^2 + n \min\{\tau \varepsilon, \tau^2 / \varepsilon\} \lesssim \tau + \min\{\tau \varepsilon, \tau^2 / \varepsilon\}, \quad 0 \leq n \leq \frac{T}{\tau} - 1,
\end{align}

which gives the desired results. \( \square \)

**Proof of Theorem 2.2**

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

\begin{align}
(3.51) & \quad \| e^{n+1}(x) \|_{L^2} \leq \left\| e^n(x) \right\|_{L^2} + \| \eta_k^n(x) \|_{L^2} + \| \eta_k^2(x) \|_{L^2} + \| \eta_k^3(x) \|_{L^2},
\end{align}

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

Through similar computations in the $S_1$ case, under the hypothesis of Theorem 2.2 we can show that

\begin{align}
\| f_2^n(s) \|_{L^2} \lesssim & \varepsilon, \quad \| \partial_s f_2^n(s) \|_{L^2} \lesssim \varepsilon / \varepsilon^2 = 1 / \varepsilon, \quad 0 \leq s \leq \tau; \\
\| g_j^n(s, w) \|_{L^2} \lesssim & \varepsilon, \quad \| \partial_s g_j^n(s, w) \|_{L^2} \lesssim 1 / \varepsilon, \quad 0 \leq s, w \leq \tau, \quad j = 2, 3, 4.
\end{align}

As a result, we have

\begin{align}
\left\| \int_0^\tau f_2^n(s) \, ds - \tau f_2^n(\tau / 2) \right\|_{L^2} \lesssim & \tau \varepsilon, \quad \left\| \int_0^\tau \int_0^s g_j^n(s, w) \, dw \, ds - \frac{\tau^2}{2} g_j^n(\tau/2, \tau/2) \right\|_{L^2} \lesssim \tau^2 \varepsilon, \quad j = 2, 3, 4.
\end{align}

On the other hand, Taylor expansion will lead to

\begin{align}
\left\| \int_0^\tau f_2^n(s) \, ds - \tau f_2^n(\tau / 2) \right\|_{L^2} \lesssim & \tau^3 / \varepsilon^3, \quad \left\| \int_0^\tau \int_0^s g_j^n(s, w) \, dw \, ds - \frac{\tau^2}{2} g_j^n(\tau/2, \tau/2) \right\|_{L^2} \lesssim \tau^3 / \varepsilon, \quad j = 2, 3, 4.
\end{align}
The two estimates above together with (3.23) and (3.24) imply
\[
\|\eta^n_2(x)\|_{L^2} + \|\eta^n_2(x)\|_{L^2} \lesssim \min\{\tau \varepsilon, \tau^3 / \varepsilon^3\}.
\]
Recalling (3.51), we can get
\[
\|e^{n+1}(x)\|_{L^2} \leq \|e^0(x)\|_{L^2} + \sum_{k=0}^n \|\eta^k_1(x)\|_{L^2} + \sum_{k=0}^n \|\eta^k_2(x)\|_{L^2} + \sum_{k=0}^n \|\eta^k_3(x)\|_{L^2}
\]
\[
\lesssim n \tau^3 + n \min\{\tau \varepsilon, \tau^3 / \varepsilon^3\} \lesssim \tau^2 + \min\{\varepsilon, \tau^2 / \varepsilon^3\}, \quad 0 \leq n \leq \frac{T}{\tau} - 1,
\]
which gives the desired result.

4. Proof of Theorems 2.3 and 2.4

If the time step size \(\tau\) is away from the resonance, i.e. for given \(\varepsilon\), there is a \(\delta > 0\), such that \(\tau \in A_\delta(\varepsilon)\), we can show improved uniform error bounds for the splitting methods given in Theorems 2.3 & 2.4 from Lemmas 3.1 & 3.2, as observed in our extensive numerical tests.

Proof of Theorem 2.3

Proof. We divide the proof into three steps.

Step 1 (Explicit representation of the error). From Lemma 3.1, we have
\[
e^{n+1}(x) = e^{-i \frac{\tau^2}{2} T^\varepsilon} e^{-i \frac{\tau}{\delta} V} ds e^n(x) + \eta^n_1(x) + \eta^n_2(x), \quad 0 \leq n \leq \frac{T}{\tau} - 1,
\]
with \(\|\eta^n_1(x)\|_{L^2} \lesssim \tau^2\), \(e^0 = 0\) and
\[
\eta^n_2(x) = -i e^{-i \tau s / \varepsilon^2} \left( \int_0^\tau f^n_2(s) ds - \tau f^n_2(0) \right).
\]
where
\[
f^n_2(s) = e^{i 2s / \varepsilon^2} e^{i s D^\varepsilon} \left( V(t^n) \Pi^\varepsilon e^{i s D^\varepsilon} \Phi(t^n) \right)
\]
Denote the numerical solution propagator \(S_{n,\tau} := e^{-i \frac{\tau^2}{2} T^\varepsilon} e^{-i \frac{\tau}{\delta} V} ds\) for \(n \geq 0\), then \(\Phi \in C^2\),
\[
\left\|S_{n,\tau} \Phi\right\|_{L^2} = \left\|\Phi\right\|_{L^2}, \quad \left\|S_{n,\tau} \Phi\right\|_{H^m} \leq e^{C\tau \|V(t,x)\|_{L^\infty(0,T;W^m,\infty)}} \left\|\Phi\right\|_{H^m}, \quad m \geq 1,
\]
for some generic constant \(C > 0\) and
\[
e^{n+1}(x) = S_{n,\tau} e^n(x) + (\eta^n_1(x) + \eta^n_2(x))
\]
\[
= S_{n,\tau} (S_{n-1,\tau} e^{n-1}(x)) + S_{n,\tau} \left( \eta^{n-1}_1(x) + \eta^{n-1}_2(x) \right) + (\eta^n_1(x) + \eta^n_2(x))
\]
\[
= \ldots
\]
\[
= S_{n,\tau} S_{n-1,\tau} \ldots S_{0,\tau} e^0(x) + \sum_{k=0}^n S_{n,\tau} S_{n+k,\tau} \left( \eta^k_1(x) + \eta^k_2(x) \right),
\]
where for \(k = n\), we take \(S_{n,\tau} \ldots S_{n+k,\tau} S_{n+1,\tau} = Id\). Since \(S_{n,\tau}\) preserves the \(L^2\) norm, noticing \(\|\eta^n_1(x)\|_{L^2} \lesssim \tau^2\), \(k = 0, 1, \ldots, n\), we have
\[
\left\|\sum_{k=0}^n S_{n,\tau} \ldots S_{k+1,\tau} \eta^k_1(x)\right\|_{L^2} \lesssim \sum_{k=0}^n \tau^2 \lesssim \tau,
\]
which leads to

\[(4.6) \quad \|e^{n+1}(x)\|_{L^2} \lesssim \tau + \left\| \sum_{k=0}^{n} S_{n,\tau}...S_{k+1,\tau} \eta^k_2(x) \right\|_{L^2}.
\]

The improved estimates rely on the refined analysis of the terms involving \(\eta^k_2\) in (4.6). To this aim, we introduce the following approximation of \(\eta^k_2\) to focus on the most relevant terms,

\[(4.7) \quad \tilde{\eta}^k_2(x) = \int_0^T \tilde{f}_2^k(s)ds - \tau \tilde{f}_2^k(0), \quad k = 0, 1, \ldots, n,
\]

with

\[(4.8) \quad \tilde{f}_2^k(s) = e^{i2s/\varepsilon^2} \Pi_+ (V(t_k)\Pi_- \Phi(t_k)) + e^{-i2s/\varepsilon^2} \Pi_- (V(t_k)\Pi_+ \Phi(t_k)),
\]

then it is easy to verify that (using Taylor expansion \(e^{i\tau D^r} = Id + O(\tau D^r))

\[(4.9) \quad \|\eta^k_2(x) - \tilde{\eta}^k_2(x)\|_{L^2} \lesssim \tau^2 \|V(t_k)\|_{H^2} \|\Phi(t_k)\|_{H^2} \lesssim \tau^2.
\]

As a result, from (4.6), we have

\[(4.10) \quad \|e^{n+1}(x)\|_{L^2} \lesssim \tau + \sum_{k=0}^{n} \left\| S_{n,\tau}...S_{k+1,\tau} (\eta^k_2(x) - \tilde{\eta}^k_2(x)) \right\|_{L^2} + \left\| \sum_{k=0}^{n} S_{n,\tau}...S_{k+1,\tau} \tilde{\eta}^k_2(x) \right\|_{L^2}
\]

**Step 2** (Representation of the error using the exact solution flow). Denote \(S_{\varepsilon}(t; t_k) (k = 0, 1, \ldots, n)\) to be the exact solution operator of the Dirac equation, acting on some \(\Phi(x) = (\phi_1(x), \phi_2(x))^T \in \mathbb{C}^2\) so that \(S_{\varepsilon}(t; t_k)\Phi(x)\) is the exact solution \(\Psi(t, x)\) at time \(t\) of

\[(4.11) \quad \left\{ \begin{array}{l}
i\partial_t \Psi(t, x) = \frac{T^r}{\varepsilon^2} \Psi(t, x) + V(t, x)\Psi(t, x), \\
\Psi(t_k, x) = \Phi(x).
\end{array} \right.
\]

and the following properties hold true for \(t \geq t_k\) and some generic constant \(C > 0\)

\[(4.12) \quad \left\| S_{\varepsilon}(t; t_k)\Phi \right\|_{L^2} = \|\Phi\|_{L^2}, \quad \left\| S_{\varepsilon}(t; t_k)\Phi \right\|_{H^m} \leq e^{C(t-t_k)}\|V(t, x)\|_{L_{[0,\tau]}^{\infty}} \|\Phi\|_{H^m}, \quad m \geq 1.
\]

It is convenient to write \(\tilde{\eta}^k_2(x) [4.7]\) as

\[(4.13) \quad \tilde{\eta}^k_2(x) = \left( \int_0^T e^{i2s/\varepsilon^2} ds - \tau \right) \Pi_+ (V(t_k)\Pi_- \Phi(t_k)) + \left( \int_0^T e^{-i2s/\varepsilon^2} ds - \tau \right) \Pi_- (V(t_k)\Pi_+ \Phi(t_k)),
\]

and by the inequality \(\int_0^T e^{i2s/\varepsilon^2} ds - \tau + \int_0^T e^{-i2s/\varepsilon^2} ds - \tau \leq 4\tau\) and similar computations in (3.35)-

\[(3.40),\) it follows that

\[(4.14) \quad \|\tilde{\eta}^k_2\|_{H^2} \lesssim \tau \varepsilon \|V(t_k)\|_{W^{3,\infty}} \|\Phi(t_k)\|_{H^3} \lesssim \varepsilon \tau.
\]
Recalling the error bounds in Theorem 2.1 and Remark 2.1, we have
\begin{equation}
\| (S_{n,\tau} \ldots S_{k+1,\tau} - S_c(t_{n+1};t_{k+1})) \tilde{n}_2^k(x) \|_{L^2} \lesssim (\tau + \frac{T}{\varepsilon}) \| \tilde{n}_2^k \|_{H^2} \lesssim (\tau + \frac{T}{\varepsilon}) \varepsilon \tau \lesssim \tau^2,
\end{equation}
and
\begin{equation}
\| e^{n+1}(x) \|_{L^2} \lesssim \tau + \sum_{k=0}^n \| (S_{n,\tau} \ldots S_{k+1,\tau} - S_c(t_{n+1};t_{k+1})) \tilde{n}_2^k(x) \|_{L^2} + \sum_{k=0}^n \| S_c(t_{n+1};t_{k+1}) \tilde{n}_2^k(x) \|_{L^2}
\leq \tau + \sum_{k=0}^n \| (S_{n,\tau} \ldots S_{k+1,\tau} - S_c(t_{n+1};t_{k+1})) \tilde{n}_2^k(x) \|_{L^2} + \sum_{k=0}^n \| S_c(t_{n+1};t_{k+1}) \tilde{n}_2^k(x) \|_{L^2}
\end{equation}
Noticing (4.15), we have
\begin{equation}
S_c(t_{n+1};t_{k+1}) \tilde{n}_2^k(x) = \left( \int_0^T e^{i2s/\varepsilon^2} ds - \tau \right) S_c(t_{n+1};t_{k+1}) \Pi^\varepsilon_+ V(t_k) \Pi^\varepsilon_- S_c(t_{k};t_{0}) \Phi(0)
+ \left( \int_0^T e^{-i2s/\varepsilon^2} ds - \tau \right) S_c(t_{n+1};t_{k+1}) \Pi^\varepsilon_- V(t_k) \Pi^\varepsilon_+ S_c(t_{k};t_{0}) \Phi(0),
\end{equation}
and it remains to estimate $S_c$ part in (4.16).

**Step 3** (Improved error bounds for non-resonant time steps). From [6], we know that the exact solution of Dirac equation is structured as follows
\begin{equation}
S_c(t_{n};t_k) \bar{\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_c^n \bar{\Phi}(x),
\end{equation}
where $R_c^n : (L^2)^2 \to (L^2)^2$ is the residue operator and $\| R_c^n \bar{\Phi}(x) \|_{L^2} \lesssim \varepsilon^2 \| \bar{\Phi}(x) \|_{H^2} (0 \leq k \leq n)$, and
\begin{equation}
\begin{cases}
i \partial_t \Psi_{\pm}(t, x) = \pm D^\varepsilon \Psi_{\pm}(t, x) + \Pi^\varepsilon_\pm (V(t) \Psi_{\pm}(t, x)), \\
\Psi_{\pm}(t, x) = \Pi^\varepsilon_\pm \bar{\Phi}(x).
\end{cases}
\end{equation}
Denote $S^\varepsilon_+(t; t_k) \bar{\Phi}(x) = \Psi_+(t, x)$, $S^\varepsilon_-(t; t_k) \bar{\Phi}(x) = \Psi_-(t, x)$ to be the solution propagator of the above equation for $\Psi_+(t, x)$, $\Psi_-(t, x)$, respectively, and $S^\varepsilon_\pm$ share the same properties in (4.12). Plugging (4.18) into (4.17), we derive
\begin{equation}
\sum_{k=0}^n S_c(t_{n+1};t_{k+1}) \tilde{n}_2^k(x)
= \sum_{k=0}^n \sum_{\sigma = \pm} \left( e^{-i(t_{n+1} - t_{k+1})/\varepsilon^2} S^\varepsilon_+(t_{n+1};t_{k+1}) + e^{i(t_{n+1} - t_{k+1})/\varepsilon^2} S^\varepsilon_-(t_{n+1};t_{k+1}) + R_c^n \right) \Pi^\varepsilon_\sigma V(t_k) \Pi^\varepsilon_\sigma 
+ \left( e^{-i(t_{n+1} - t_{k+1})/\varepsilon^2} S^\varepsilon_+(t_{n+1};t_{k+1}) + e^{i(t_{n+1} - t_{k+1})/\varepsilon^2} S^\varepsilon_-(t_{n+1};t_{k+1}) + R_c^n \right) \bar{\Phi}(0) \left( \int_0^T e^{i\sigma 2s/\varepsilon^2} ds - \tau \right)
+ \sum_{k=0}^n \sum_{\sigma = \pm} e^{i\sigma (t_{n+1} - t_{k+1})/\varepsilon^2} S^\varepsilon_\sigma(t_{n+1};t_{k+1}) \Pi^\varepsilon_\sigma V(t_k) \Pi^\varepsilon_\sigma e^{i\sigma \frac{t_{n+1}-t_{k+1}}{\varepsilon^2}} S^\varepsilon_\sigma(t_{k+1};t_{0}) \bar{\Phi}(0) \left( \int_0^T e^{i\sigma 2s/\varepsilon^2} ds - \tau \right)
\end{equation}
\begin{equation}
= I_1^n(x) + I_2^n(x),
\end{equation}
where \( \sigma^* = + \) if \( \sigma = - \) and \( \sigma^* = - \) if \( \sigma = + \),

\[
I_1^n(x) = \sum_{k=0}^{n} \sum_{\sigma = \pm} e^{-i\theta_{n+1} - 2k} S_c^\sigma(t_{n+1}; t_{k+1}) \Pi_+^\sigma V(t_k) \Pi_+^\sigma e^{-i\epsilon \frac{t_k - t_{k+1}}{2}} S_c^\sigma(t_{k}; t_0) \Phi(0) \left( \int_0^\tau e^{i\epsilon 2s/\epsilon^2} ds - \tau \right),
\]

\[
I_2^n(x) = \sum_{k=0}^{n} \sum_{\sigma = \pm} (R_{k+1}^n + \Pi_+^\sigma V(t_k) \Pi_+^\sigma \Phi(t_k) + S_c(t_{n+1}; t_{k+1}) \Pi_+^\sigma V(t_k) \Pi_+^\sigma R_0^k \Phi(0)) \left( \int_0^\tau e^{i\epsilon 2s/\epsilon^2} ds - \tau \right).
\]

As \( \left| \int_0^\tau e^{i\epsilon 2s/\epsilon^2} ds - \tau \right| \lesssim \tau^2/\epsilon^2 \) by Taylor expansion, we have

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

Denote \( p_\pm(\tau) = \int_0^\tau e^{i\epsilon 2s/\epsilon^2} ds - \tau \) and we can rewrite \( I_1^n(x) \) as

\[
I_1^n(x) = \sum_{k=0}^{n} \sum_{\sigma = \pm} e^{-i\theta_{n+1} - 2k - \tau} S_c^\sigma(t_{n+1}; t_{k+1}) \Pi_+^\sigma V(t_k) \Pi_+^\sigma S_c^\sigma(t_{k}; t_0) \Phi(0) p_\sigma(\tau),
\]

\[
= p_+(\tau) \sum_{k=0}^{n} (\theta_k - \theta_{k-1}) S_c^+(t_{n+1}; t_{k+1}) \Pi_+^\sigma V(t_k) \Pi_+^\sigma S_c^-(t_{k}; t_0) \Phi(0)
\]

\[
+ p_-(\tau) \sum_{k=0}^{n} (\theta_k - \theta_{k-1}) S_c^-(t_{n+1}; t_{k+1}) \Pi_+^\sigma V(t_k) \Pi_+^\sigma S_c^+(t_{k}; t_0) \Phi(0)
\]

\[
= \gamma_1^n(x) + \gamma_2^n(x),
\]

where \( \bar{\theta} \) is the complex conjugate of \( \theta \) and

\[
(4.20) \ \theta_k = \sum_{l=0}^{k} e^{-i(t_{n+1} - 2l)} / \epsilon^2 = \frac{e^{-i\tau / \epsilon^2} - e^{-i(n - 2k - 2) / \epsilon^2}}{1 - e^{2i\tau / \epsilon^2}}, \ \theta_{-1} = 0, \ \epsilon \leq k \leq n,
\]

\[
(4.21) \ \gamma_1^n(x) = p_+(\tau) \sum_{k=0}^{n} (\theta_k - \theta_{k-1}) S_c^+(t_{n+1}; t_{k+1}) \Pi_+^\sigma V(t_k) \Pi_+^\sigma S_c^-(t_{k}; t_0) \Phi(0),
\]

\[
(4.22) \ \gamma_2^n(x) = p_-(\tau) \sum_{k=0}^{n} (\theta_k - \theta_{k-1}) S_c^-(t_{n+1}; t_{k+1}) \Pi_+^\sigma V(t_k) \Pi_+^\sigma S_c^+(t_{k}; t_0) \Phi(0).
\]

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

\[
|\theta_k| \leq \frac{1}{\delta}, \ k = 0, 1, ..., n.
\]

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

\[
\| \gamma_1^n(x) \|_{L^2} \leq 2\tau \left\| \sum_{k=0}^{n} \theta_k \left( S_c^+(t_{n+1}; t_{k+1}) \Pi_+^\sigma V(t_k) \Pi_+^\sigma S_c^-(t_{k}; t_0) - S_c^+(t_{n+1}; t_{k+2}) \Pi_+^\sigma V(t_{k+1}) \Pi_+^\sigma S_c^-(t_{k+1}; t_0) \right) \Phi(0) \right\|_{L^2}
\]

\[
+ \tau \| \theta_h S_c^+(t_{n+1}; t_{h+1}) \Pi_+^\sigma V(t_h) \Pi_+^\sigma S_c^-(t_{h}; t_0) \Phi(0) \|_{L^2}
\]

\[
\lesssim \tau \sum_{k=0}^{n-1} \frac{\tau}{\delta} + \tau / \delta \lesssim \delta \tau,
\]

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where we have used the triangle inequality and properties of the solution flows $S_e^\pm$ to deduce that

<table>
<thead>
<tr>
<th>$| (S_e^+ (t_{n+1};t_{k+1})) \Pi_e^+ V(t_k) \Pi_e^- S_e^- (t_k; t_0) - S_e^+ (t_{n+1};t_{k+2}) \Pi_e^+ V(t_k) \Pi_e^- S_e^- (t_k; t_0) | L^2$</th>
<th>(4.24)</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\leq | S_e^+ (t_{n+1};t_{k+1}) \Pi_e^+ (V(t_k) - V(t_{k+1})) \Pi_e^- S_e^- (t_k; t_0) + V(t_{k+1}) \Pi_e^- S_e^- (t_k; t_0) - S_e^- (t_{n+1};t_{k+1}) | L^2$</td>
<td>(4.25)</td>
</tr>
<tr>
<td>$\leq | \tau | \partial_t V | L^\infty(L^2) | | (0,T) | L^2 | L^\infty([t_{k+1},t_{n+1}];(L^2)^2)$</td>
<td>(4.26)</td>
</tr>
<tr>
<td>$| \tau | \partial_t (S_e^+ (t_{n+1};t)) \Pi_e^+ V(t_k) \Pi_e^- S_e^- (t_k; t_0) | L^\infty([t_{k+1},t_{n+1}];(L^2)^2)$</td>
<td>(4.27)</td>
</tr>
</tbody>
</table>

Similarly, we could get $\| \gamma^2(x) \| L^2 \leq \delta$ and hence $\| I_1^2(x) \| L^2 \leq \delta$. In summary, we have

| $\| e^{n+1}(x) \| L^2 \leq \| I_1^n(x) \| L^2 + \| I_2^n(x) \| L^2 \leq \delta$ | (4.28) |

which gives the desired results. \( \square \)

**Proof of Theorem 2.4**

**Proof.** We divide the proof into two steps.

1. **Step 1** (Representation of the error using the exact solution flow). From Lemma 3.2, we have

| $e^{n+1}(x) = e^{-\frac{i}{2\pi} T^e} e^{-i f^{n+1}_j V(s,x) ds} e^{-\frac{i}{2\pi} T^e} e^n(x) + \eta_1^n(x) + \eta_2^n(x) + \eta_3^n(x), \quad 0 \leq n \leq \frac{T}{\epsilon} - 1,$ | (4.23) |

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

| $\| \eta_1^n(x) \| L^2 \leq \tau^3, \quad \eta_2^n(x) = -i e^{-\frac{i}{2\pi} T^e} \left( \int_0^\tau f_2^n(s) ds - \tau f_2^n(\tau/2) \right), \quad \eta_3^n(x) = -e^{-\frac{i}{2\pi} T^e} \left( \int_0^\tau \int_0^s \sum_{j=2}^4 g_j^n(s,w) dw ds - \frac{\tau^2}{2} \sum_{j=2}^4 g_j^n(\tau/2,\tau/2) \right), \quad$ | (4.24) |

where $f_2^n$ and $g_j^n$ \((j = 2, 3, 4)\) are given in (3.25)-(3.28).

Denote the second order splitting integrator $S_{n,\tau} = e^{-\frac{i}{2\pi} T^e} e^{-i f^{n+1}_j V(s,x) ds} e^{-\frac{i}{2\pi} T^e}$ for $n \geq 0$, and $S_e(t; t_k)$ to be the exact solution flow for the Dirac equation (2.2), then $S_{n,\tau}$ enjoys the similar properties as those in the first order Lie-Trotter splitting case (4.4) and we can get

| $e^{n+1}(x) = S_e(t_{n+1}; t_n) e^n(x) + \eta_1^n(x) + \eta_2^n(x) + \eta_3^n(x) + (S_{n,\tau} - S_e(t_{n+1}; t_n)) e^n(x)$ | (4.25) |

| $= \ldots$ |

| $= S_e(t_{n+1}; t_0) e^n(x) + \sum_{k=0}^n S_e(t_{n+1}; t_{k+1})(\eta_1^k(x) + \eta_2^k(x) + \eta_3^k(x))$ | (4.26) |

| $+ \sum_{k=0}^n S_e(t_{n+1}; t_{k+1})(S_{k,\tau} - S_e(t_{k+1}; t_k)) e^k(x).$ |

By Duhamel’s principle, it is straightforward to compute

| $(S_{k,\tau} - S_e(t_{k+1}; t_k)) \Phi(x) = e^{-\frac{i}{2\pi} T^e} (e^{-i f^{k+1}_{k+1} V(s,x) ds} - 1)e^{-\frac{i}{2\pi} T^e}$ |

| $- i \int_0^\tau e^{-\frac{i}{2\pi} (s-x) T^e} V(t_k + s, x) S_e(t_k + s; t_k) \Phi(x) ds.$ | (4.27) |
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 \( S_e(t; t_k) \) \( \text{(4.12)} \), we obtain from \( \text{(4.27)} \)

\[
\left\| (S_k, \tau) - S_e(t_k; t_k) \right\|_{L^2} \leq \tau \left\| V(t, x) \right\|_{L^\infty([t_k, t_{k+1}]; L^\infty)} \left\| \Phi \right\|_{L^2} + \tau \left\| V(t, x) \right\|_{L^\infty([t_k, t_{k+1}]; L^\infty)} \left\| \Phi \right\|_{L^2} \lesssim \tau \left\| \Phi \right\|_{L^2},
\]

and

\[
\| S_e(t_{n+1}; t_k) - S_e(t_k; t_k) \|_{L^2} \lesssim \tau \left\| \Phi \right\|_{L^2}, \quad k = 0, \ldots, n.
\]

Noticing \( \| \Phi^0 \|_{L^2} = 0 \), combining \( \text{(4.28)} \) and \( \text{(4.26)} \), recalling \( \left\| \Phi_t^0 \right\|_{L^2} \lesssim \tau^3 \), we can control

\[
\left\| \Phi^{n+1} \right\|_{L^2} \lesssim \tau + \sum_{k=0}^n \left\| S_e(t_{n+1}; t_k) - S_e(t_k; t_k) \right\|_{L^2} + \sum_{j=1}^3 \left\| \sum_{k=0}^n S_e(t_{n+1}; t_k) \left( \eta_j^k(x) \right) \right\|_{L^2}.
\]

Similar to the Lie-Trotter splitting \( S_1 \), the key to establish the improved error bounds for non-resonant \( \tau \) is to derive refined estimates for the terms involving \( \eta_j^k \) \( (j = 2, 3) \) in \( \text{(4.29)} \). To this purpose, we introduce the approximations \( \tilde{\eta}_j^k(x) \) of \( \eta_j^k(x) \) \( (l = 2, 3, k = 0, 1, \ldots, n) \) as

\[
\tilde{\eta}_j^k(x) = \int_0^\tau \tilde{f}_j^k(s) ds - \tau \tilde{f}_j^k(\tau/2), \quad \tilde{\eta}_j^k(x) = \int_0^\tau \int_0^\tau \frac{4}{2} \sum_{j=2}^4 \tilde{g}_j^k(s, w) dw ds - \frac{\tau^2}{2} \sum_{j=2}^4 \tilde{g}_j^k(\tau/2, \tau/2),
\]

where we expand \( V(t_k + s, x) = V(t_k, x) + s \partial_t V(t_k, x) + O(s^2) \) and \( e^{i s \partial^e} = \text{Id} + i s \partial^e + O(s^2) \) up to the linear term in \( f_j^k(s, w) \) \( \text{(3.25)} \) and the zeroth order term in \( g_j^k(s, w) \) \( (j = 2, 3, 4) \) \( \text{(3.26)} - \text{(3.28)} \), respectively,

\[
\tilde{f}_j^k(s) = \text{se}^{i 2 s e^2 \partial^e} \left( i \partial^e \Pi_+^e (V(t_k) \Pi_+^e \Phi(t_k)) + i \Pi_+^e (V(t_k) \partial^e \Pi_+^e \Phi(t_k)) \right) + \text{se}^{-i 2 s e^2 \partial^e} \left( i \partial^e \Pi_-^e (V(t_k) \Pi_-^e \Phi(t_k)) + i \Pi_-^e (V(t_k) \partial^e \Pi_-^e \Phi(t_k)) \right) + e^{i 2 s e^2 \partial^e} \Pi_+^e (V(t_k) \Pi_+^e \Phi(t_k)) + e^{-i 2 s e^2 \partial^e} \Pi_-^e (V(t_k) \Pi_-^e \Phi(t_k)).
\]

Using Taylor expansion in \( f_j^k(s, w) \) \( \text{(3.25)} \) and \( g_j^k(s, w) \) \( (j = 2, 3, 4) \) \( \text{(3.26)} - \text{(3.28)} \) as well as properties of \( \partial^e \), it is not difficult to check that

\[
\| \Phi_j^k(x) - \tilde{\Phi}_j^k(x) \|_{L^2} \lesssim \tau^3 \left( \left\| V(t, x) \right\|_{W^{2, \infty}([0, T]; L^\infty)} \left\| \Phi(t_k) \right\|_{L^2} + \left\| \partial_t V(t, x) \right\|_{W^{1, \infty}([0, T]; H^2)} \left\| \Phi(t_k) \right\|_{H^2} + \left\| V(t, x) \right\|_{L^\infty([0, T]; H^s)} \left\| \Phi(t_k) \right\|_{H^s} \right) \lesssim \tau^3,
\]

\[
\| \Phi_j^k(x) - \tilde{\Phi}_j^k(x) \|_{L^2} \lesssim \tau^3 \left\| V(t_n, x) \right\|_{W^{2, \infty}([0, T]; L^\infty)}^2 \left\| \Phi(t_k) \right\|_{H^s} \lesssim \tau^3.
\]
which would yield for \( k \leq n \leq \frac{T}{\tau} - 1 \),
\[
\| S_c(t_{n+1}; t_{k+1}) \tilde{\eta}^k_2(x) - S_c(t_{n+1}; t_{k+1}) \tilde{\eta}^k_2(x) \|_{L^2} \lesssim \| \eta^k_2(x) - \tilde{\eta}^k_2(x) \|_{L^2} \lesssim \tau^3,
\]
(4.31)
\[
\| S_c(t_{n+1}; t_{k+1}) \tilde{\eta}^k_3(x) - S_c(t_{n+1}; t_{k+1}) \tilde{\eta}^k_3(x) \|_{L^2} \lesssim \| \eta^k_3(x) - \tilde{\eta}^k_3(x) \|_{L^2} \lesssim \tau^3.
\]
(4.32)

Plugging the above inequalities into (4.29), we derive
\[
\| e^{n+1}(x) \|_{L^2} \lesssim \tau^2 + \sum_{k=0}^n \tau^3 + \sum_{j=2}^3 \left( \sum_{k=0}^n \| S_c(t_{n+1}; t_{k+1}) \tilde{\eta}^k_2(x) \|_{L^2} + \sum_{k=0}^n \tau \| e^k(x) \|_{L^2} \right)
\]
(4.33)
\[
\lesssim \tau^2 + \sum_{k=0}^n \| S_c(t_{n+1}; t_{k+1}) \tilde{\eta}^k_2(x) \|_{L^2} + \sum_{k=0}^n \tau \| e^k(x) \|_{L^2}.
\]

**Step 2** (Improved estimates for non-resonant time steps). It remains to show the estimates on the terms related to \( \tilde{\eta}^k_2 \) and \( \tilde{\eta}^k_3 \). The arguments will be similar to those in the proof of the Lie-Trotter splitting case Theorem 2.3 so we only sketch the proof below. Taking \( \tilde{\eta}^k_2 \) for example, we write
\[
\tilde{\eta}^k_2(s) = \tilde{\eta}^k_{2+}(s) + \tilde{\eta}^k_{2-}(s),
\]
(4.34)
\[
\tilde{\eta}^k_{2\pm}(s) = \int_0^\tau \tilde{f}^k_{2\pm}(s) ds - \tau \tilde{f}^k_{2\pm} (\tau/2), \quad k = 0, 1, ..., n,
\]
with
\[
\tilde{f}^k_{2\pm}(s) = \pm s e^{\pm i 2k / \tau^2} (i D^x \Pi^\perp_k (V(t_k) \Pi^+ \Phi(t_k)) + i \Pi^\perp_k (V(t_k) D^x \Pi^+ \Phi(t_k))) \pm \Pi^\perp_k (\partial_t V(t_k) \Pi^+ \Phi(t_k))
\]
and \( \tilde{f}^k_{2\pm}(s) = \tilde{f}^n_{2\pm}(s) + \tilde{f}^n_{2\pm}(-s) \).

Recalling the structure of the exact solution to the Dirac equation in (4.18), we have for \( 0 \leq k \leq n \)
\[
S_c(t_n; t_k) \Phi(x) = e^{-i(t_n-t_k)/\tau^2} S^+_c(t_n; t_k) \Phi(x) + e^{i(t_n-t_k)/\tau^2} S^-_c(t_n; t_k) \Phi(x) + R^k_n \Phi(x),
\]
(4.35)
where the propagators \( S^\pm_c \) and the residue operator \( R^k_n : (L^2)^2 \rightarrow (L^2)^2 \) are defined in (4.18). Therefore, we can get
\[
\sum_{k=0}^n \| S_c(t_{n+1}; t_{k+1}) \tilde{\eta}^k_2(x) = \sum_{j=1}^4 \tilde{I}^j_2(x),
\]
with
\[
\tilde{I}^1_2(x) = \left( \int_0^\tau e^{i 2s / \tau^2} ds - \tau e^{i \tau / \tau^2} \right) \sum_{k=0}^n e^{-i(t_{n+1}-t_{k+1})/\tau^2} S^+_c(t_{n+1}; t_{k+1}) \Pi^+ \Phi(t_k),
\]
\[
\tilde{I}^2_2(x) = \left( \int_0^\tau e^{i 2s / \tau^2} ds - \tau e^{i \tau / \tau^2} \right) \sum_{k=0}^n \left( R^{n+1} \Pi^+ V(t_k) \Pi^+ \Phi(t_k) + S_c(t_{n+1}; t_{k+1}) \Pi^+ \Phi(t_k) \right),
\]
\[
\tilde{I}^3_2(x) = \left( \int_0^\tau e^{i 2s / \tau^2} ds - \tau e^{i \tau / \tau^2} \right) \sum_{k=0}^n e^{-i(t_{n+1}-t_{k+1})/2 \tau} S^+_c(t_{n+1}; t_{k+1}) (i D^x \Pi^+_c V(t_k) + \Pi^+_c \partial_t V(t_k)) \Phi(t_k),
\]
\[
\tilde{I}^4_2(x) = \left( \int_0^\tau e^{i 2s / \tau^2} ds - \tau e^{i \tau / \tau^2} \right) \sum_{k=0}^n \left( R^{n+1} \Pi^+ V(t_k) \Pi^+ \Phi(t_k) + \Pi^+_c \partial_t V(t_k) \right),
\]
\[
+ \sum_{k=0}^n \left( i D^x \Pi^+_c V(t_k) + \Pi^+_c \partial_t V(t_k) \right) \Pi^+_c \Phi(t_k).
\]
The residue terms $\tilde{I}_2^n$ and $\tilde{I}_4^n$ will be estimated first. Using the properties of $R_k^n$ and $S_{\varepsilon}$, noticing \[3.35 - 3.46\], we have
\[
\|R_k^{n+1} \Pi_\varepsilon^- V(t_k) \Pi_\varepsilon^- \Phi(t_k) + S_{\varepsilon}(t_{n+1}; t_{k+1}) \Pi_\varepsilon^+ V(t_k) \Pi_\varepsilon^+ R_0^k \Phi(0)\|_{L^2} \lesssim \varepsilon^3 \|V(t_k)\|_{W^{3,\infty}} (\|\Phi(t_k)\|_{H^3} + \|\Phi(0)\|_{H^3}),
\]
\[
\|R_k^{n+1}(i \partial x \Pi_\varepsilon^- V(t_k) + i \Pi_\varepsilon^- \partial_t V(t_k) \Pi_\varepsilon^- \Phi(t_k))\|_{L^2} \lesssim \varepsilon^3 \|V(t, x)\|_{W^{1,\infty}(0, T; W^{3,\infty})} \|\Phi(t_k)\|_{H^5},
\]
\[
\|S_{\varepsilon}(t_{n+1}; t_{k+1})(i \partial x \Pi_\varepsilon^+ V(t_k) + i \Pi_\varepsilon^+ \partial_t V(t_k)) \Pi_\varepsilon^+ R_0^k \Phi(0)\|_{L^2} \lesssim \varepsilon^3 \|V(t, x)\|_{W^{1,\infty}(0, T; W^{3,\infty})} \|\Phi(0)\|_{H^5},
\]
which will lead to the following conclusions in view of the fact that \(\left| \int_0^T e^{i t^2 / \varepsilon^2} / e^{i t / \varepsilon^2} \right| \leq \min\{\tau^2 / \varepsilon^2, \tau^3 / \varepsilon^4\}\) and \(\left| \int_0^\tau e^{i t^2 / \varepsilon^2} d\tau - \frac{t^2}{2} e^{i t / \varepsilon^2} \right| \lesssim \min\{\tau^2 / \varepsilon^2, \tau^3 / \varepsilon^4\}\) (Taylor expansion up to the linear or the quadratic term),
\[
\|\tilde{I}_2^n(x)\|_{L^2} \lesssim \min\{\tau \varepsilon, \tau^2 / \varepsilon\}, \quad \|\tilde{I}_4^n(x)\|_{L^2} \lesssim \min\{\tau \varepsilon, \tau^2 / \varepsilon\}.
\]
Now, we proceed to treat $\tilde{I}_1^n$ and $\tilde{I}_3^n$. For $\tilde{I}_1^n(x)$, it is similar to \[4.21\] which has been analyzed in the $S_1$ case. Using the same idea (details omitted for brevity here), and the fact that \(\left| \int_0^\tau e^{i t^2 / \varepsilon^2} - e^{i t / \varepsilon^2} \right| \lesssim \min\{\tau, \tau^2 / \varepsilon^2\}\) as well as $\Pi_\varepsilon^+ V(t_k) \Pi_\varepsilon^- = O(\varepsilon)$, under the regularity assumptions, we can get for $\tau \in \mathcal{A}_3(\varepsilon),$
\[
\|\tilde{I}_1^n(x)\|_{L^2} \lesssim \min\{\tau, \tau^2 / \varepsilon^2\}\left(\sum_{k=0}^{n-1} \tau \varepsilon / \delta + \varepsilon / \delta\right) \lesssim \delta \min\{\tau, \tau^2 / \varepsilon\}.
\]
Similarly, noticing \(\left| \int_0^\tau e^{i t^2 / \varepsilon^2} d\tau - \frac{t^2}{2} e^{i t / \varepsilon^2} \right| \leq \tau^2\), we can get
\[
\|\tilde{I}_3^n(x)\|_{L^2} \lesssim \tau^2 \left(\sum_{k=0}^{n-1} \tau \varepsilon / \delta + \varepsilon / \delta\right) \lesssim \delta \tau^2 \varepsilon.
\]
Combining the estimates for $\tilde{I}_j^n$ ($j = 1, 2, 3, 4$), we have
\[
\left\| \sum_{k=0}^{n} S_{\varepsilon}(t_{n+1}; t_{k+1}) \tilde{I}_2^k(x) \right\|_{L^2} \leq \sum_{j=1}^{4} \|\tilde{I}_j^n(x)\|_{L^2} \lesssim \delta \min\{\tau \varepsilon, \tau^2 / \varepsilon\}.
\]
For $\sum_{k=0}^{n} S_{\varepsilon}(t_{n+1}; t_{k+1}) \tilde{I}_2^k(x)$, we can have the same results as
\[
\left\| \sum_{k=0}^{n} S_{\varepsilon}(t_{n+1}; t_{k+1}) \tilde{I}_2^-k(x) \right\|_{L^2} \lesssim \delta \min\{\tau \varepsilon, \tau^2 / \varepsilon\},
\]
which yield the following results in view of \[4.39\] and \[4.34\]
\[
\left\| \sum_{k=0}^{n} S_{\varepsilon}(t_{n+1}; t_{k+1}) \tilde{I}_2^k(x) \right\|_{L^2} \lesssim \delta \min\{\tau \varepsilon, \tau^2 / \varepsilon\}.
\]
The same technique works for $S_{\varepsilon}(t_{n+1}; t_{k+1}) \tilde{I}_3^k(x)$ and we can get
\[
\left\| \sum_{k=0}^{n} S_{\varepsilon}(t_{n+1}; t_{k+1}) \tilde{I}_3^k(x) \right\|_{L^2} \lesssim \delta \min\{\tau \varepsilon, \tau^2 / \varepsilon\}.
\]
Plugging these results into (4.33), we have

\[(4.43) \quad \|e^{n+1}(x)\|_{L^2} \lesssim \delta \tau^2 + \sum_{k=0}^n \tau \|e^k(x)\|_{L^2} + \min\{\tau \varepsilon, \tau^2 / \varepsilon\}.\]

Gronwall’s inequality then implies for \(\tau\) satisfying \(\tau \in A_\delta(\varepsilon),\)

\[(4.44) \quad \|e^{n+1}(x)\|_{L^2} \lesssim \delta \tau^2 + \min\{\tau \varepsilon, \tau^2 / \varepsilon\}, \quad 0 \leq n \leq T - 1.\]

This completes the proof for Theorem 2.4.

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

In both examples, we choose the electric potential in (2.2) as

\[(5.1) \quad V(t, x) = \frac{1 - x}{1 + x^2}, \quad x \in \mathbb{R}, \quad t \geq 0,\]

and the initial data in (2.3) as

\[(5.2) \quad \phi_1(0, x) = e^{-x^2}, \quad \phi_2(0, x) = e^{-\left(x - 1\right)^2}, \quad x \in \mathbb{R}.\]

In the 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 \(h := \Delta x = \frac{b - a}{M}\) 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 \(\Phi^n = (\Phi^n_0, \Phi^n_1, \ldots, \Phi^n_{M-1}, \Phi^n_M)^T\) be the numerical solution obtained by a numerical method with time step \(\tau\) and \(\varepsilon\) as well as a very fine mesh size \(h\) at time \(t = t_n\), and \(\Phi(t, x)\) be the exact solution, then the discrete \(l^2\) error is quantified as

\[(5.3) \quad e^{\varepsilon, \tau}(t_n) = \|\Phi^n - \Phi(t_n, \cdot)\|_2 = \left(\sum_{j=0}^{M-1} h |\Phi(t_n, x_j) - \Phi^n_j|^2\right)^{1/2},\]

and \(e(t_n)\) should be close to the \(L^2\) errors in Theorems 2.1, 2.2, 2.3 & 2.4 for fine spatial mesh sizes \(h\).

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 \(\varepsilon\), 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 \(h = \frac{1}{M}\) 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 \(\tau_0 = 2\pi \times 10^{-6}\).

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

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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.

<table>
<thead>
<tr>
<th>$e^{\varepsilon,\tau}(t = 2\pi)$</th>
<th>$\tau_0/\pi$</th>
<th>$\tau_0/4$</th>
<th>$\tau_0/4^2$</th>
<th>$\tau_0/4^3$</th>
<th>$\tau_0/4^4$</th>
<th>$\tau_0/4^5$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\varepsilon_0 = 1$</td>
<td>4.84E-1</td>
<td>1.27E-1</td>
<td>3.20E-2</td>
<td>8.03E-3</td>
<td>2.01E-3</td>
<td>5.02E-4</td>
</tr>
<tr>
<td>order</td>
<td>0.97</td>
<td>0.99</td>
<td>1.00</td>
<td>1.00</td>
<td>1.00</td>
<td>1.00</td>
</tr>
<tr>
<td>$\varepsilon_0/2$</td>
<td>6.79E-1</td>
<td>1.23E-1</td>
<td>3.10E-2</td>
<td>7.78E-3</td>
<td>1.95E-3</td>
<td>4.87E-4</td>
</tr>
<tr>
<td>order</td>
<td>0.72</td>
<td>0.98</td>
<td>1.00</td>
<td>1.00</td>
<td>1.00</td>
<td>1.00</td>
</tr>
<tr>
<td>$\varepsilon_0/2^2$</td>
<td>5.78E-1</td>
<td>2.71E-1</td>
<td>3.07E-2</td>
<td>7.67E-3</td>
<td>1.95E-3</td>
<td>4.87E-4</td>
</tr>
<tr>
<td>order</td>
<td>0.55</td>
<td>0.99</td>
<td>1.00</td>
<td>1.00</td>
<td>1.00</td>
<td>1.00</td>
</tr>
<tr>
<td>$\varepsilon_0/2^3$</td>
<td>5.33E-1</td>
<td>1.85E-1</td>
<td>1.21E-1</td>
<td>7.75E-3</td>
<td>1.95E-3</td>
<td>4.87E-4</td>
</tr>
<tr>
<td>order</td>
<td>0.76</td>
<td>0.30</td>
<td>1.98</td>
<td>1.00</td>
<td>1.00</td>
<td>1.00</td>
</tr>
<tr>
<td>$\varepsilon_0/2^4$</td>
<td>5.13E-1</td>
<td>1.48E-1</td>
<td>7.02E-2</td>
<td>5.76E-2</td>
<td>1.95E-3</td>
<td>4.88E-4</td>
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<tr>
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<td>0.54</td>
<td>0.14</td>
<td>2.44</td>
<td>1.00</td>
<td>1.00</td>
</tr>
<tr>
<td>$\varepsilon_0/2^5$</td>
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<td>1.34E-1</td>
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<td>3.07E-2</td>
<td>2.82E-2</td>
<td>4.88E-4</td>
</tr>
<tr>
<td>order</td>
<td>0.96</td>
<td>0.75</td>
<td>0.31</td>
<td>0.06</td>
<td>2.93</td>
<td></td>
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<tr>
<td>$\varepsilon_0/2^6$</td>
<td>4.98E-1</td>
<td>1.25E-1</td>
<td>3.37E-2</td>
<td>1.18E-2</td>
<td>7.68E-3</td>
<td>7.05E-3</td>
</tr>
<tr>
<td>order</td>
<td>1.00</td>
<td>0.95</td>
<td>0.76</td>
<td>0.31</td>
<td>0.06</td>
<td>2.93</td>
</tr>
<tr>
<td>$\varepsilon_0/2^7$</td>
<td>4.97E-1</td>
<td>1.24E-1</td>
<td>3.17E-2</td>
<td>8.46E-3</td>
<td>2.95E-3</td>
<td>1.92E-3</td>
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<tr>
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<td>0.98</td>
<td>0.95</td>
<td>0.76</td>
<td>0.31</td>
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</tr>
<tr>
<td>$\varepsilon_0/2^8$</td>
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<td>1.23E-1</td>
<td>3.13E-2</td>
<td>9.46E-3</td>
<td>2.12E-3</td>
<td>7.37E-4</td>
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<tr>
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<td>0.99</td>
<td>0.95</td>
<td>0.76</td>
<td></td>
</tr>
<tr>
<td>$\varepsilon_0/2^9$</td>
<td>4.95E-1</td>
<td>1.22E-1</td>
<td>3.12E-2</td>
<td>1.95E-3</td>
<td>2.11E-3</td>
<td>7.36E-4</td>
</tr>
<tr>
<td>order</td>
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<td>0.99</td>
<td>0.99</td>
<td>0.95</td>
<td>0.76</td>
<td></td>
</tr>
</tbody>
</table>

In Tables 5.1 & 5.2, the last two rows show the largest error of each column for fixed $\tau$. They both give 1/2 order of convergence, which coincides well with Theorems 2.1 & 2.2. More specifically, in Table 5.1, we 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 bound $\|\Phi(t_n, x) - \Phi^n(x)\|_{L^2} \lesssim \tau + \tau^2/\varepsilon$. 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 $\|\Phi(t_n, x) - \Phi^n(x)\|_{L^2} \lesssim \tau^2 + \varepsilon$.

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

Example 2 In this example, we test the improved uniform error bounds for non-resonant time step size. Here we choose $\tau \in A_0(\varepsilon)$ for some given $\varepsilon$ and $0 < \delta \leq 1$.

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 $\tau_c = 8 \times 10^{-6}$. Spatial mesh size is fixed as...
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.

<table>
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<tr>
<th>$e^{\varepsilon,\tau}(t = 2\pi)$</th>
<th>$\tau_0 = \pi/4$</th>
<th>$\tau_0/2^3$</th>
<th>$\tau_0/4^3$</th>
<th>$\tau_0/4^5$</th>
<th>$\tau_0/4^6$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\varepsilon_0 = 1$</td>
<td>8.08E-2</td>
<td>2.76E-4</td>
<td>1.73E-5</td>
<td>1.08E-6</td>
<td>6.74E-8</td>
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<td>2.00</td>
<td>2.00</td>
<td>2.00</td>
</tr>
<tr>
<td>$\varepsilon_0/2$</td>
<td>4.13E-1</td>
<td>5.73E-4</td>
<td>3.57E-5</td>
<td>2.23E-6</td>
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<td>2.76E-2</td>
<td>2.76E-2</td>
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<td>2.71E-5</td>
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<td>1.71</td>
<td>0.23</td>
<td>0.00</td>
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<tr>
<td>$\max_{0&lt;\varepsilon \leq 1} e^{\varepsilon,\tau}(t = 2\pi)$</td>
<td>4.13E-1</td>
<td>2.15E-1</td>
<td>1.10E-1</td>
<td>5.51E-2</td>
<td>2.76E-2</td>
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<td>0.49</td>
<td>0.50</td>
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</table>

$h = 1/16$ for all the numerical simulations.

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

In Table 5.3 we could see that overall, for fixed time step size $\tau$, the error $e^{\varepsilon,\tau}(t = 4)$ does not change with different $\varepsilon$. This verifies the uniform first order convergence in time for $S_1$ with non-resonant time step size, as stated in Theorem 2.3. In Table 5.4, the last two rows show the largest error of each column for fixed $\tau$, which gives $3/2$ order of convergence, consistent with Theorem 2.4. 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 $\| \Phi(t_n, x) - \Phi^n(x) \|_{L^2} \lesssim \tau^2 + \tau^2 / \varepsilon$.

Through the results of this example, we successfully validate the improved uniform error bounds for the splitting methods in Theorem 2.3 and 2.4 with non-resonant time step size.
Table 5.3
Discrete $l^2$ temporal errors $e^{\varepsilon,\tau}(t = 4)$ for the wave function with non-resonant time step size, S1 method.

<table>
<thead>
<tr>
<th>$\varepsilon_0$</th>
<th>$\tau_0 = 1$</th>
<th>$\tau_0/2$</th>
<th>$\tau_0/2^2$</th>
<th>$\tau_0/2^3$</th>
<th>$\tau_0/2^4$</th>
<th>$\tau_0/2^5$</th>
<th>$\tau_0/2^6$</th>
<th>$\tau_0/2^7$</th>
</tr>
</thead>
<tbody>
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<td>$\varepsilon_0 = 1$</td>
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<td>3.51E-1</td>
<td>1.78E-1</td>
<td>8.96E-2</td>
<td>4.50E-2</td>
<td>2.25E-2</td>
<td>1.13E-2</td>
<td>5.64E-3</td>
</tr>
<tr>
<td>order</td>
<td>-</td>
<td>0.98</td>
<td>0.98</td>
<td>0.99</td>
<td>0.99</td>
<td>1.00</td>
<td>1.00</td>
<td>1.00</td>
</tr>
<tr>
<td>$\varepsilon_0/2$</td>
<td>6.52E-1</td>
<td>3.52E-1</td>
<td>1.65E-1</td>
<td>8.34E-2</td>
<td>4.20E-2</td>
<td>2.11E-2</td>
<td>1.05E-2</td>
<td>5.28E-3</td>
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<tr>
<td>order</td>
<td>-</td>
<td>0.89</td>
<td>1.10</td>
<td>0.98</td>
<td>0.99</td>
<td>1.00</td>
<td>1.00</td>
<td>1.00</td>
</tr>
<tr>
<td>$\varepsilon_0/2^2$</td>
<td>6.78E-1</td>
<td>3.25E-1</td>
<td>1.64E-1</td>
<td>8.04E-2</td>
<td>4.07E-2</td>
<td>2.05E-2</td>
<td>1.03E-2</td>
<td>5.15E-3</td>
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<td>order</td>
<td>-</td>
<td>1.06</td>
<td>0.99</td>
<td>1.03</td>
<td>0.98</td>
<td>0.99</td>
<td>1.00</td>
<td>1.00</td>
</tr>
<tr>
<td>$\varepsilon_0/2^3$</td>
<td>6.43E-1</td>
<td>3.24E-1</td>
<td>1.69E-1</td>
<td>8.10E-2</td>
<td>4.13E-2</td>
<td>2.02E-2</td>
<td>1.02E-2</td>
<td>5.13E-3</td>
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<tr>
<td>order</td>
<td>-</td>
<td>0.99</td>
<td>0.94</td>
<td>1.06</td>
<td>0.97</td>
<td>1.03</td>
<td>0.99</td>
<td>0.99</td>
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<td>$\varepsilon_0/2^4$</td>
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<td>3.12E-1</td>
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<td>8.24E-2</td>
<td>4.22E-2</td>
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<td>1.03E-2</td>
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<td>order</td>
<td>-</td>
<td>1.04</td>
<td>0.95</td>
<td>0.97</td>
<td>1.04</td>
<td>1.04</td>
<td>0.99</td>
<td>1.02</td>
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<td>$\varepsilon_0/2^5$</td>
<td>6.50E-1</td>
<td>3.25E-1</td>
<td>1.61E-1</td>
<td>8.10E-2</td>
<td>4.10E-2</td>
<td>2.07E-2</td>
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<td>1.02</td>
<td>0.99</td>
<td>0.98</td>
<td>0.99</td>
<td>0.98</td>
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<td>8.43E-2</td>
<td>4.09E-2</td>
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<td>0.95</td>
<td>1.04</td>
<td>1.00</td>
<td>0.99</td>
<td>0.99</td>
</tr>
<tr>
<td>$\varepsilon_0/2^7$</td>
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<td>3.18E-1</td>
<td>1.60E-1</td>
<td>8.10E-2</td>
<td>4.06E-2</td>
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<td>0.99</td>
<td>0.99</td>
<td>0.99</td>
<td>0.99</td>
<td>1.00</td>
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</table>

6. Conclusion. The super-resolution property of time-splitting methods for the Dirac equation in the nonrelativistic limit regime without magnetic potentials were established. We rigorously proved the uniform error bounds, and the improved uniform error bounds with non-resonant 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 non-resonant. 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 non-resonant 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 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 $S_4$, $S_{4c}$, $S_{HRK}$ methods used in [14], also have the super-resolution property for Dirac equation in the nonrelativistic limit regime in the absence of external magnetic potentials.

Acknowledgment
We acknowledge support from the Ministry of Education of Singapore grant R-146-000-223-112 (W. Bao and J. Yin) and the NSFC grant No. U1530401 and 11771036 (Y. Cai). This work was partially done when the first author was visiting the Courant Institute for Mathematical Sciences in 2018.
### Table 5.4

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

<table>
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<th>$e^{\varepsilon,\tau}(t = 4)$</th>
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<th>$\tau_0/4$</th>
<th>$\tau_0/4^2$</th>
<th>$\tau_0/4^3$</th>
<th>$\tau_0/4^4$</th>
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<td>2.00</td>
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<td>1.99</td>
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### REFERENCES


[27] A. H. C. Neto, F. Guinea, N. M. R. Peres, K. S. Novoselov and A. K. Geim, The electronic properties of...


