Absorbing layers for the Dirac equation

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Abstract

This work is devoted to the construction of perfectly matched layers (PML) for the Dirac equation, that not only arises in relativistic quantum mechanics but also in the dynamics of electrons in graphene or in topological insulators. While the resulting equations are stable at the continuous level, some care is necessary in order to obtain a stable scheme at the discrete level. This is related to the so-called fermion doubling problem. For this matter, we consider the numerical scheme introduced by Hammer et al. [19], and combine it with the discretized PML equations. We state some arguments for the stability of the resulting scheme, and perform simulations in two dimensions. The perfectly matched layers are shown to exhibit, in various configurations, superior absorption than the absorbing potential method and the so-called transport-like boundary conditions.

1 Introduction

The Dirac equation, introduced in 1928 by P. A. Dirac in the context of relativistic quantum mechanics [14], has recently found applications in the description of new nanostructures. One of which is graphene, where the electrons dynamics is described at the so-called Dirac points by a massless Dirac equation [13]. Another example is given by the family of topological insulators [17], where edge electrons are described by

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a Dirac equation with a varying mass of non-constant sign. This results in the so-called protected states that enjoy very weak backscattering. See e.g. [21, 26] for classical references on graphene and topological insulators.

The design of such nanostructures is improved by modeling and numerical simulations. This imposes that the equations of interest are solved on a finite domain and that appropriate conditions have to be defined at the boundary of the domain. In the context of semiconductors, it is crucial to allow for electron flow across the device, and to avoid unphysical reflections at the boundary of the (artificial) numerical domain. Inadequate boundary conditions would result for example in untruthful Intensity-Voltage curves that are one of the main characteristics of the structure. Similar problems arise in scattering problems, for instance in relativistic heavy ion collisions, where the equations can only be solved on a finite domain.

This led to the concept of absorbing boundary conditions, for which several approaches can be found in the literature for various equations such as the Schrödinger or Helmholtz equations. In the semiconductor context, a classical method is to divide the device into two zones, the injection zone and an active zone where the important physical effects take place. One supposes then that the coefficients are constant (for instance the potential) in the injection zone, so that the Schrödinger or the Helmholtz equations can be solved exactly and exact boundary conditions can be defined at the interface between the two zones. The technique works both for time-dependent and stationary problems, see e.g. [15, 1, 4, 5, 10, 9] for a few references in a vast literature, and was applied for instance for the simulation of a resonant tunneling diode in [25]. In the time-dependent case, calculations are fairly involved since the boundary conditions involve a memory kernel that needs to be conveniently discretized for stability purposes [1, 6]. Exact absorbing boundary conditions for the one-dimensional Dirac equation were derived in [18]. The approach can be generalized to some non-constant potentials and various geometries using pseudo-differential calculus, see e.g. [2]. This latter technique was extended to the Dirac equation in [3].

An alternative method is to surround the domain of computation by unphysical absorbing layers in order to minimize reflections at the boundary. A simple related technique is to impose a complex potential in the layers in order to absorb particles. Another technique was introduced by Bérenger in [11, 12] in the context of wave propagation, the celebrated perfectly matched layers (PML). They consist in augmenting the system with a set of well-chosen equations in the layers that lead to perfect absorption at the continuous level. When the corresponding equations are discretized on a finite domain, there are though some unavoidable errors that generate some reflections. PML were constructed for many systems, for instance the wave equation, Maxwell’s equations, linearized Euler’s equation or the Schrödinger equation [11, 12, 27, 30]. The advantage
of the PML compared to other methods is their great simplicity, that leads to a minimal intrusion in the code while still offering a very good absorption.

The purpose of this work is to construct PML for the Dirac equation and to evaluate their performance compared to two standard techniques, the absorbing potential method, and the so-called outflow or transport-like boundary conditions, see [22], Chapter 7. The latter ones are obtained by a simple upwind discretization of one-dimensional advection equations. The choice of the discretization of the Dirac equation augmented with the PML is crucial for the comparison of the absorbing methods. Indeed, while we will see that the PML are stable at the continuous level, an inadequate numerical scheme can potentially lead to a spurious behavior and exponential growth in the layers. This is related to the so-called fermion doubling problem, which is a consequence of a non-monotonic discrete dispersion relation [28, 23]. We will base our discretization on the work of [19] where the derived scheme is immune to the fermion-doubling problem, so that stability at the discrete level can be expected.

The paper is structured as follows: in section 2, we construct the PML for the three dimensional Dirac equation and explore their stability; in section 3, we discretize the two-dimensional Dirac equation including the PML following [19], and argue about the stability of resulting scheme; in section 4 we present some simulations in 2D that show the superior absorption of the PML in various configurations, from low to high frequency waves, for normal to grazing incidence; finally, a conclusion is offered in section 5.

2 Perfectly matched layers for the 3D Dirac equation

This section is devoted to the derivation of the PML equations and an analysis of stability.

The 3D Dirac equation. The three dimensional Dirac equation reads

\[ i\hbar \partial_t \Psi = \mathcal{H} \Psi, \]  

where the spinor \( \Psi \in \mathbb{C}^4 \), \( \hbar \) is the reduced Planck constant, and the Hamiltonian is given by, for \( x = (x_1, x_2, x_3) \),

\[ \mathcal{H} = -i\hbar c \sum_{j=1}^{3} \alpha_j \partial x_j + mc^2 \beta + V(x) \mathbb{I}_4. \]
Above, $c$ is the speed of light, $m$ is the mass of the considered particle, $V$ some potential profile in $L^\infty(\mathbb{R}^3)$ (e.g. a potential barrier, or a Klein step), $I_n$ is the identity matrix in $\mathbb{R}^{n \times n}$, and $\alpha_1, \alpha_2, \alpha_3, \beta$ are hermitian matrices defined by

$$
\alpha_j = \sigma_1 \otimes \sigma_j = \begin{pmatrix} 0 & \sigma_j \\ \sigma_j & 0 \end{pmatrix}, \quad \beta = \sigma_3 \otimes I_2 = \begin{pmatrix} I_2 & 0 \\ 0 & -I_2 \end{pmatrix}.
$$

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

**Absorbing layers.** We introduce first some notation: We suppose the domain of interest (the physical domain) is the cartesian product $D = [x_{1,L}, x_{1,R}] \times [x_{2,L}, x_{2,R}] \times [x_{3,L}, x_{3,R}]$, and we denote by $\Sigma(z)$ a continuous, positive, non-decreasing (non-linear) function, satisfying $\Sigma(z) = 0$ for $z \leq 0$. For $\omega$ the dual Fourier variable of the time $t$, absorbing layers surrounding $D$ in all directions are obtained with the classical complex non-linear change of variables

$$
x_j \to x_j + \frac{i}{\omega}(\mu_{j,L}(x_j) + \mu_{j,R}(x_j)), \quad j \in \{1, 2, 3\},
$$

where

$$
\mu_{j,L}(z) = \int_{x_{j,L}}^{z} \Sigma(x_{j,L} - u)du \quad \text{and} \quad \mu_{j,R}(z) = \int_{x_{j,R}}^{z} \Sigma(u - x_{j,R})du.
$$

We assumed for simplicity that all layers in all directions have the same absorbing function $\Sigma$. Note that by construction, $\mu_{j,L} = \mu_{j,R} = 0$ in the domain $D$. In the absorbing layers, the above change of variables turns the partial differentiation operator $\partial_{x_j}$ into a pseudo-differential operator $\partial_{x_j}^{AL}$ formally given by

$$
\partial_{x_j}^{AL} \varphi(t, x) = \left( \frac{\partial_t}{\partial_t + \sigma_j(x_j)} \right) \partial_{x_j} \varphi(t, x) = \frac{1}{2\pi} \int_{\mathbb{R}} \frac{\omega e^{i\omega t}}{\omega - i\sigma_j(x_j)} \partial_{x_j} \hat{\varphi}(\omega, x) d\omega,
$$

where $\hat{\varphi}(\omega, x)$ is the Fourier transform of $\varphi$ in the $t$ variable and

$$
\sigma_j(z) = \Sigma(x_{j,L} - z) + \Sigma(z - x_{j,R}).
$$
See [29] for an introduction on pseudo-differential operators. The operator $\partial^AL_{x_j}$ is conveniently recast in terms of $\partial_{x_j}$ as

$$
(\partial^AL_{x_j} - \partial_{x_j})\varphi(t, x) = \frac{i\sigma_j(x_j)}{2\pi} \int_\mathbb{R} \frac{e^{i\omega} \partial_{x_j} \hat{\varphi}(\omega, x) d\omega}{\omega - i\sigma_j(x_j)} \quad \colon= \xi_j(t, x),
$$

where direct computations show that $\xi_j$ satisfies

$$
\partial_t \xi_j + \sigma_j(x_j)\xi_j = -\sigma_j(x_j)\partial_{x_j} \varphi, \quad j \in \{1, 2, 3\}.
$$

Introducing the components of the spinor $\Psi = (\Psi_1, \Psi_2, \Psi_3, \Psi_4)^T$ (the $(\cdot)^T$ sign means transposition), the above change of variables and calculations lead to a modified Hamiltonian $\mathcal{H}^L$ that reads

$$
\mathcal{H}^L = -i\hbar c \sum_{j=1}^3 \alpha_j \partial^AL_{x_j} + mc^2 \beta + V(x)\Pi_4,
$$

which can be expressed as

$$
\mathcal{H}^L \Psi = \mathcal{H} \Psi + S, \quad S = -i\hbar c \sum_{j=1}^3 \alpha_j \xi_j,
$$

where the vectors $\xi_j = (\xi_{jk})_{k \in \{1, 2, 3, 4\}} \in \mathbb{C}^4$ satisfy

$$
\partial_t \xi_{jk} + \sigma_j \xi_{jk} = -\sigma_j \partial_{x_j} \Psi_k, \quad \sigma_j = \sigma_j(x_j).
$$

An initial condition needs to be added to (4), and it is natural to impose $\xi_{jk}(0) = 0$ when $\Psi(t = 0)$ is supported in $D$. The introduction of absorbing layers therefore only results in the addition of terms involving the functions $\xi_{jk}$ in the Hamiltonian, which makes the approach very easy to implement and not very intrusive.

We investigate now the stability of the modified Dirac equation.

**Stability.** It is not difficult to show that the system

$$
i\hbar \partial_t \Psi = \mathcal{H}^L \Psi, \quad \Psi(t = 0, \cdot) = \Psi_0,
$$

where $\Psi_0 \in (H^1(\mathbb{R}^3))^4$ (the usual Sobolev space), is well-posed in $H^1(\mathbb{R}^3)$. We have indeed the following lemma, whose proof is given for convenience in the Appendix in the case $V = 0$. The proof carries over to the case $V \in W^{1,\infty}(\mathbb{R}^3)$ with minor modifications.
Lemma 2.1 Assume that the function $\Sigma$ used in the construction of the PML is bounded, and that $V = 0$. Then, the solution $\Psi$ to (5) satisfies the estimate:

$$
\|\Psi(t, \cdot)\|_{H^1} \leq C\|\Psi_0\|_{H^1} e^{Ct}, \quad \forall t > 0,
$$

(6)

where $C$ is a positive constant and

$$
\|\Psi\|^2_{H^1} = \sum_{i=1}^{4} \|\Psi_i\|^2_{H^1(\mathbb{R}^3)}.
$$

According to the definition given in [8], the system is actually said to be weakly well-posed. The above bound is not a good estimate of the stability since it allows for exponentially growing solutions. The appropriate notion of stability for the PML is given in [8], and (5) is said to be weakly stable if it is weakly well-posed and if it satisfies in addition an estimate of the type, for some $s \geq 0$,

$$
\|\Psi(t, \cdot)\|_{L^2} \leq C(1 + t)^s \|\Psi_0\|_{H^s}, \quad \forall t > 0.
$$

(7)

Getting (7) is much more involved than (6) since it requires some control on exponential solutions. Our goal here is not to give of complete proof of stability but only to give the main arguments. The standard technique introduced in [8] consists in freezing the coefficient $\sigma(x)$ and using a plane wave analysis. We follow here a similar but slightly different route, we directly perform the change of variables (2) in the plane wave solutions to (1) instead of working with the perturbed dispersion relation. Plane wave solutions of (1) for $V = 0$ have the form

$$
\Psi(t, x, k) = e^{ik \cdot x - \omega(k)t} e_+(k) + e^{ik \cdot x + \omega(k)t} e_-(k),
$$

(8)

where $e_\pm$ are two linearly independent vectors in $\mathbb{C}^4$, and the dispersion relation is

$$
\omega(k) = \sqrt{m^2 c^4 + c^2 |k|^2}.
$$

The vector $e_+$ is associated with particles with positive energies while $e_-$ with the ones with negative energies. The group velocity of a positive energy wave packet is

$$
v_+(k) = \nabla_k \omega(k) = \frac{c^2 k}{\omega(k)},
$$

with the opposite sign for $v_-$ for negative energy. Plane wave solutions for the modified Dirac equation (5) are obtained by performing the change of variables (2) in (8). This yields, introducing the group velocities $v_\pm$ defined above,

$$
\Psi^{AL}(t, x, k) = e^{ik \cdot x - v_+(k) \mu(x)/c^2 - i\omega(k)t} e_+(k) + e^{ik \cdot x - v_-(k) \mu(x)/c^2 + i\omega(k)t} e_-(k),
$$

(9)
where we have defined the vector $\mu(x) = (\mu_{j,L}(x_j) + \mu_{j,R}(x_j))_{j \in \{1,2,3\}}$. The latter expression shows not only that there are no reflections since $\Psi^{AL} = \Psi$ for $x \in D$, but also that the PML are stable (in the sense of (7), i.e. there are no exponentially growing solutions): consider for instance right going particles (whether with positive or negative energies) with positive group velocities $v_{\pm}$ along the $x_j$ direction; then these particles always travel to the right in the layer and are exponentially absorbed with no reflection since $\mu_j(x_j) = \mu_{j,R}(x_j) \geq 0$. Instabilities would occur if there existed left-going particles in the right layer, which is not the case. A similar analysis holds for left-going particles.

The stability could have been directly obtained by applying the stability criterion given [8]: denoting by $S_{\pm}(k) = \pm k/\omega(k)$ the slowness vectors of positive and negative energy particles, stability of the PML in the direction $x_j$ (i.e. stability of the wave component traveling along the $x_j$ direction) occurs as soon as

$$(S_{\pm}(k))_j \times (v_{\pm}(k))_j \geq 0. \quad (10)$$

This is straightforwardly verified as

$$(S_{\pm}(k))_j \times (v_{\pm}(k))_j = \left( \frac{ck_j}{\omega(k)} \right)^2.$$  

In order to evaluate the performance of the PML and to compare with other methods, we will solve the Dirac equation in two spatial dimensions. We need for this to pay attention to the discretization scheme in order to avoid inward going particles in the layers and therefore numerical instabilities. This is the object of the next section.

## 3 Discretization of the 2D Dirac equation

In the 2D setting, the spinor reduces to a two dimensional vector. We discretize first the 2D Dirac equation and then consider the stability of the obtained scheme. We start by simplifying the notation and write $x = x_1$, $y = x_2$ as well as $\Psi = (u, v)^T$. We suppose for simplicity that the layers are symmetric around the origin so that, with the notation of the previous section, $x_{j,L} = -x_{j,R} < 0$ for $j = 1, 2$. As a consequence, we have $\sigma_j(x) \equiv \sigma(x)$, and the 2D Dirac equation reads

$$\partial_t u = -c\partial_x v + ic\partial_y v + \left( \frac{V + mc^2}{ih} \right) u - c\eta^x - c\eta^y \quad (11)$$

$$\partial_t v = -c\partial_x u - ic\partial_y u + \left( \frac{V - mc^2}{ih} \right) v - c\xi^x - c\xi^y, \quad (12)$$
where the absorbing functions $\eta^x, \eta^y, \xi^x, \xi^y$ verify

$$
\partial_t \xi^x + \sigma(x)\xi^x = -\sigma(x)\partial_x u, \quad \partial_t \xi^y + \sigma(y)\xi^y = -\sigma(y)\partial_y u,
$$
$$
\partial_t \eta^x + \sigma(x)\eta^x = -\sigma(x)\partial_x v, \quad \partial_t \eta^y + \sigma(y)\eta^y = -\sigma(y)\partial_y v,
$$
augmented with vanishing initial conditions. The upper indices in $\eta$ and $\xi$ refer to the direction along which particles are absorbed by the layer. We set in the sequel $c = h = 1$.

The discretization of (11)-(12) is not straightforward since basic finite differences schemes can potentially lead to instabilities in the PML, even though the continuous equation is stable: it is indeed well-known that centered finite differences approximations used e.g. in the Crank-Nicolson scheme lead to the so-called fermion doubling problem [28, 23]. The latter is a consequence of the non-monotonic discrete dispersion relation of such schemes: along one branch of the dispersion curve, higher energy particles are created with a group velocity opposite to those with lower energies. This is a critical point for the PML: consider for instance particles with positive energies in the right layer; there are no instabilities at the continuous level since the group velocity is positive, and there is then exponential absorption; at the discrete level, particles with negative group velocities are created, which results in the violation of the stability condition (10) and exponential growth.

There are several ways to overcome such a difficulty. Modifications of the dispersion relation by a change of variables have been introduced in [7, 20, 24] for several equations such as the linearized Euler equation, resulting in a monotonic dispersion curve. Such an approach would require here a change of variables adapted to the discretization scheme.

We follow a different route and rather consider a particular scheme that exhibits a monotonic dispersion relation. The discretization was introduced in [19] and is based on an explicit leapfrog scheme doubly staggered in time and in space. The discretized versions of $(u, v)$ are then obtained as follows: $u$ has components both on the standard grid and on the staggered grid in both spatial directions, as well as on the staggered time grid; while $v$ has components on the standard time grid and on staggered grids in one direction only; that is

$$
u \equiv (u_{i,j}^{n+\frac{1}{2}}, u_{i-\frac{1}{2},j}^{n+\frac{1}{2}}), \quad v \equiv (v_{i-\frac{1}{2},j}^{n}, v_{i,j-\frac{1}{2}}^{n}).
$$
Above, the index $n$ (resp. $i$ and $j$) refers to the discretization in time (resp. in the directions $x$ and $y$). The two components of $u$ and $v$ are evolved alternatively and the scheme of [19] reads, for a cartesian grid with uniform stepsizes $(\Delta t, \Delta x, \Delta y)$ and accounting for the absorbing functions:
\[ \begin{align*}
v_{i,j}^{n+1} &= \left( \frac{2i - \Delta t(m - V_1)}{2i + \Delta t(m - V_1)} \right) v_{i,j}^{n} + \frac{2i \Delta t}{\Delta x(2i + \Delta t(m - V_1))} \left( u_{i,j}^{n+\frac{1}{2}} - u_{i-1,j}^{n+\frac{1}{2}} \right) \\
&\quad + \frac{2\Delta t}{\Delta y(2i + \Delta t(m - V_1))} \left( u_{i,j+\frac{1}{2}}^{n+\frac{1}{2}} - u_{i-\frac{1}{2},j+\frac{1}{2}}^{n+\frac{1}{2}} \right) \\
&\quad - \frac{2i \Delta t}{(2i + \Delta t(m - V_1))} \left( \xi_{i,j}^n + i\xi_{i,j}^{n+\frac{1}{2}} \right) \\
\end{align*} \]

\[ \begin{align*}
v_{i,j-\frac{1}{2}}^{n+1} &= \left( \frac{2i - \Delta t(m - V_2)}{2i + \Delta t(m - V_2)} \right) v_{i,j-\frac{1}{2}}^{n} + \frac{2i \Delta t}{\Delta x(2i + \Delta t(m - V_2))} \left( u_{i+\frac{1}{2},j-\frac{1}{2}}^{n+\frac{1}{2}} - u_{i-\frac{1}{2},j-\frac{1}{2}}^{n+\frac{1}{2}} \right) \\
&\quad + \frac{2\Delta t}{\Delta y(2i + \Delta t(m - V_2))} \left( u_{i,j}^{n+\frac{1}{2}} - u_{i,j-1}^{n+\frac{1}{2}} \right) \\
&\quad - \frac{2i \Delta t}{(2i + \Delta t(m - V_2))} \left( \xi_{i,j-\frac{1}{2}}^{n} + i\xi_{i,j-\frac{1}{2}}^{n+\frac{1}{2}} \right) \\
\end{align*} \]

\[ \begin{align*}
u_{i,j}^{n+\frac{3}{2}} &= \left( \frac{2i + \Delta t(m + V_3)}{2i - \Delta t(m + V_3)} \right) u_{i,j}^{n+\frac{1}{2}} - \frac{2i \Delta t}{\Delta x(2i - \Delta t(m + V_3))} \left( v_{i+\frac{1}{2},j}^{n+1} - v_{i-\frac{1}{2},j}^{n+1} \right) \\
&\quad - \frac{2\Delta t}{\Delta y(2i - \Delta t(m + V_3))} \left( y_{i,j}^{n+1} - y_{i,j+\frac{1}{2}}^{n+1} \right) \\
&\quad - \frac{2i \Delta t}{(2i - \Delta t(m + V_3))} \left( \eta_{i,j} + i\eta_{i,j}^{n+1} \right) \\
\end{align*} \]

\[ \begin{align*}
u_{i-\frac{1}{2},j}^{n+\frac{3}{2}} &= \left( \frac{2i + \Delta t(m + V_4)}{2i - \Delta t(m + V_4)} \right) u_{i-\frac{1}{2},j+1}^{n+\frac{1}{2}} - \frac{2i \Delta t}{\Delta x(2i - \Delta t(m + V_4))} \left( v_{i-\frac{1}{2},j}^{n+1} - v_{i-\frac{1}{2},j-\frac{1}{2}}^{n+1} \right) \\
&\quad - \frac{2\Delta t}{\Delta y(2i - \Delta t(m + V_4))} \left( y_{i,j}^{n+1} - y_{i-\frac{1}{2},j}^{n+1} \right) \\
&\quad - \frac{2i \Delta t}{(2i - \Delta t(m + V_4))} \left( \eta_{i-\frac{1}{2},j} - i\eta_{i-\frac{1}{2},j+\frac{1}{2}}^{n+1} \right) \\
\end{align*} \]

where the potential \( V \) might here depend on time and

\[ \begin{align*}
V_1 &= V_{i-\frac{1}{2},j}^{n+\frac{1}{2}}, \quad V_2 = V_{i,j-\frac{1}{2}}^{n+\frac{1}{2}}, \quad V_3 = V_{i,j}^{n+1}, \quad V_4 = V_{i-\frac{1}{2},j-\frac{1}{2}}^{n+1}.
\end{align*} \]

The scheme is explicit and globally of second order in time and space. It is not self-starting, and one can use for the initialization a locally second order scheme of the
form

\[
\begin{align*}
\frac{1}{2} u_{i,j} &= \left(1 - \frac{i\Delta t(m + V_{2})}{2}\right) u_{i,j} - \frac{\Delta t}{2\Delta x} (v_{i+\frac{1}{2},j} - v_{i-\frac{1}{2},j}) + \frac{i\Delta t}{2\Delta y} (v_{i,j+\frac{1}{2}} - v_{i,j-\frac{1}{2}}) \\
\frac{1}{2} u_{i-\frac{1}{2},j-\frac{1}{2}} &= \left(1 - \frac{i\Delta t(m + V_{1})}{2}\right) u_{i-\frac{1}{2},j-\frac{1}{2}} - \frac{\Delta t}{2\Delta x} (v_{i-\frac{1}{2},j-\frac{1}{2}} - v_{i-\frac{3}{2},j-\frac{3}{2}}) + \frac{i\Delta t}{2\Delta y} (v_{i-\frac{1}{2},j-\frac{1}{2}} - v_{i-\frac{1}{2},j-\frac{1}{2}-1}).
\end{align*}
\]

The absorbing functions are discretized as follows: consider first \(\xi^x\); we solve its corresponding equation between \(t\) and \(t + \Delta t\) and obtain

\[
\xi^x(t + \Delta t, x, y) = e^{-\sigma(x)\Delta t\xi^x(t, x, y)} - \sigma(x) \int_0^{\Delta t} e^{-\sigma(x)(t-s)} \partial_x u(s + t, x, y) ds. \tag{13}
\]

We then replace \(\partial_x u(s + t, x, y)\) in the integral by

\[
\partial_x u(s + t, x, y) \simeq \partial_x u(t + \Delta t/2, x, y) \simeq \frac{1}{2} \left( \partial_x u(t, x, y) + \partial_x u(t + \Delta t, x, y) \right),
\]

which leads to the following second order discretization of (13):

\[
\xi^x(t_{n+\frac{1}{2}}, x, y) = e^{-\sigma(x)\Delta t\xi^x(t_{n-\frac{1}{2}}, x, y)} - \frac{(e^{-\sigma(x)\Delta t} - 1)}{2} \left( \partial_x u(t_{n+\frac{1}{2}}, x, y) + \partial_x u(t_{n-\frac{1}{2}}, x, y) \right).
\]

We then discretize the spatial derivatives of \(u\) with the same centered approximation as in the numerical scheme, and we obtain, with the notation \(\sigma_{i-\frac{1}{2}} = \sigma(x_{i-\frac{1}{2}})\) and \(\sigma_i = \sigma(x_i)\), for the \(\xi^x, \xi^y\) appearing in the first equation on \(u_{i-\frac{1}{2},j}^n\):

\[
\begin{align*}
\xi^x_{i-\frac{1}{2},j}^{n+\frac{1}{2}} &= e^{-\sigma_{i-\frac{1}{2}}\Delta t} \xi^x_{i-\frac{1}{2},j}^{n-\frac{1}{2}} + \frac{(e^{-\sigma_{i-\frac{1}{2}}\Delta t} - 1)}{2\Delta x} \left( u_{i+\frac{1}{2},j}^n - u_{i-\frac{1}{2},j}^n \right) + \frac{(e^{-\sigma_{i-\frac{1}{2}}\Delta t} - 1)}{2\Delta y} \left( u_{i,j+\frac{1}{2}}^n - u_{i,j-\frac{1}{2}}^n \right) \\
\xi^y_{i-\frac{1}{2},j}^{n+\frac{1}{2}} &= e^{-\sigma_{i-\frac{1}{2}}\Delta t} \xi^y_{i-\frac{1}{2},j}^{n-\frac{1}{2}} + \frac{(e^{-\sigma_{i-\frac{1}{2}}\Delta t} - 1)}{2\Delta y} \left( u_{i,j+\frac{1}{2}}^n - u_{i,j-\frac{1}{2}}^n \right) + \frac{(e^{-\sigma_{i-\frac{1}{2}}\Delta t} - 1)}{2\Delta y} \left( u_{i,j+\frac{1}{2}}^n - u_{i,j-\frac{1}{2}}^n \right).
\end{align*}
\]

For the equation on \(v_{i-\frac{1}{2},j}^{n+\frac{1}{2}}\), we find

\[
\begin{align*}
\xi^x_{i,j-\frac{1}{2}}^{n+\frac{1}{2}} &= e^{-\sigma_{i,j-\frac{1}{2}}\Delta t} \xi^x_{i,j-\frac{1}{2}}^{n-\frac{1}{2}} + \frac{(e^{-\sigma_{i,j-\frac{1}{2}}\Delta t} - 1)}{2\Delta x} \left( u_{i+\frac{1}{2},j-\frac{1}{2}}^n - u_{i-\frac{1}{2},j-\frac{1}{2}}^n \right) + \frac{(e^{-\sigma_{i,j-\frac{1}{2}}\Delta t} - 1)}{2\Delta y} \left( u_{i,j-\frac{1}{2}}^n - u_{i,j-\frac{1}{2}}^n \right) \\
\xi^y_{i,j-\frac{1}{2}}^{n+\frac{1}{2}} &= e^{-\sigma_{i,j-\frac{1}{2}}\Delta t} \xi^y_{i,j-\frac{1}{2}}^{n-\frac{1}{2}} + \frac{(e^{-\sigma_{i,j-\frac{1}{2}}\Delta t} - 1)}{2\Delta y} \left( u_{i,j-\frac{1}{2}}^n - u_{i,j-\frac{1}{2}}^n \right) + \frac{(e^{-\sigma_{i,j-\frac{1}{2}}\Delta t} - 1)}{2\Delta y} \left( u_{i,j-\frac{1}{2}}^n - u_{i,j-\frac{1}{2}}^n \right).
\end{align*}
\]
Proceeding similarly, we have for the equation on \( u_{i,j}^{n+\frac{1}{2}} \):

\[
\eta_{x,j}^{\ast n+1} = e^{-\sigma_i \Delta t} \eta_{x,j}^{\ast n} + \frac{(e^{-\sigma_i \Delta t} - 1)}{2\Delta x} \left( v_{i+\frac{1}{2},j}^{n+1} - v_{i-\frac{1}{2},j}^{n+1} + v_{i+\frac{1}{2},j}^{n} - v_{i-\frac{1}{2},j}^{n} \right)
\]

\[
\eta_{y,j}^{\ast n+1} = e^{-\sigma_j \Delta t} \eta_{y,j}^{\ast n} + \frac{(e^{-\sigma_j \Delta t} - 1)}{2\Delta y} \left( v_{i,j+\frac{1}{2}}^{n+1} - v_{i,j-\frac{1}{2}}^{n+1} + v_{i,j+\frac{1}{2}}^{n} - v_{i,j-\frac{1}{2}}^{n} \right),
\]

and for the one on \( u_{i-\frac{1}{2},j-\frac{1}{2}}^{n+\frac{1}{2}} \):

\[
\eta_{x,j-\frac{1}{2}}^{\ast n+1} = e^{-\sigma_i \Delta t} \eta_{x,j-\frac{1}{2}}^{\ast n} + \frac{(e^{-\sigma_i \Delta t} - 1)}{2\Delta x} \left( v_{i,j-\frac{1}{2}}^{n+1} - v_{i-1,j-\frac{1}{2}}^{n+1} + v_{i,j-\frac{1}{2}}^{n} - v_{i-1,j-\frac{1}{2}}^{n} \right)
\]

\[
\eta_{y,j-\frac{1}{2}}^{\ast n+1} = e^{-\sigma_j \Delta t} \eta_{y,j-\frac{1}{2}}^{\ast n} + \frac{(e^{-\sigma_j \Delta t} - 1)}{2\Delta y} \left( v_{i-\frac{1}{2},j}^{n+1} - v_{i-\frac{1}{2},j-1}^{n+1} + v_{i-\frac{1}{2},j}^{n} - v_{i-\frac{1}{2},j-1}^{n} \right).
\]

The continuous equations posed on the whole space are thus approximated by the discrete equations on \( (u_{i,j}^{n+\frac{1}{2}}, u_{i-\frac{1}{2},j-\frac{1}{2}}^{n+\frac{1}{2}}) \) and \( (v_{i,j}^{n+\frac{1}{2}}, v_{i-\frac{1}{2},j-\frac{1}{2}}^{n+\frac{1}{2}}) \), with each component defined on a bounded domain with \( N_x \times N_y \) spatial grid points, and augmented with homogeneous Dirichlet boundary conditions, i.e.

\[
v_{i-\frac{1}{2},1}^{n+\frac{1}{2}} = v_{i-\frac{1}{2},N_y}^{n+\frac{1}{2}} = u_{i,1} = u_{i,N_y} = v_{1,j-\frac{1}{2}}^{n+\frac{1}{2}} = v_{N_x,j-\frac{1}{2}}^{n+\frac{1}{2}} = u_{1,j} = u_{N_x,j} = 0.
\]

**Stability.** For \( \Delta x = \Delta y \), it is shown in [19] that in absence of PML, the scheme of the last section is stable whenever \( \Delta t \leq \Delta x/\sqrt{2} \). When the PML are included, we proceed as in the continuous case and do not give a full proof of stability but only its main ingredients: we look at discrete plane waves after the change of variables (2). When \( V \) is a constant (zero here for simplicity) and \( m = c = \hbar = 1 \), we find

\[
\Psi^{AL}(t, \bar{x}, k) = e^{ik\bar{x}-k\cdot\mu(\bar{x})/\omega(k)-i\omega(k)t} e_+(k) + e^{ik\bar{x}-k\cdot\mu(\bar{x})/\omega + i\omega(k)t} e_-(k),
\]

where \( k = (k_x, k_y), \bar{x} = (j_x \Delta x, j_y \Delta y), t = j_t \Delta t, (j_x, j_y, j_t) \) are integers and \( e_\pm \) are two linearly independent vectors. The discrete dispersion relation given in [19] is, in the positive energy \( \omega \geq 0 \) case,

\[
\sin \frac{\Delta t}{2} \omega(k) = \sqrt{\frac{\Delta t}{2 + \Delta t} \left( 1 + \left( \frac{2}{\Delta x} \sin \frac{k_x \Delta x}{2} \right)^2 + \left( \frac{2}{\Delta y} \sin \frac{k_y \Delta y}{2} \right)^2 \right)},
\]

(15)
with a negative sign on the right for negative energy particles. As in the continuous case, we need the components of the vector \( k/\omega \) to have the same sign as the components of the group velocity in order to ensure stability. The fact that, for \( \beta = x, y \),

\[
\partial_\beta \omega(k) = \frac{4}{\Delta t(2 + \Delta t)} \frac{\Delta t \sin(k_\beta \Delta \beta)}{\Delta \beta \sin(\omega(k) \Delta t)},
\]

leads to

\[
\frac{k_\beta \partial_\beta \omega(k)}{\omega(k)} = \frac{4}{\Delta t(2 + \Delta t)} \left( \frac{k_\beta}{\omega(k)} \right)^2 \frac{\text{sinc}(k_\beta \Delta \beta)}{\text{sinc}(\omega(k) \Delta t)} \geq 0,
\]

which is non-negative since \( k_\beta \in (-\frac{\pi}{\Delta \beta}, \frac{\pi}{\Delta \beta}) \) and \( \text{sinc}(\omega(k) \Delta t) \geq 0 \) thanks to (15) and \( \omega \geq 0 \). The latter inequality holds as well for the negative energy case, which shows that particles always travel outwards in the layer and there is no exponential blow up.

Using the previous scheme, we evaluate in the following section the performance of the PML in comparison to the absorbing potential technique and the transport-like (outflow) boundary conditions.

4 Numerical simulations

This section is devoted to the numerical simulations. As mentioned earlier, we consider two methods to compare with the PML, which we present now in more detail: the absorbing potential approach, which simply consists in imposing a complex potential in the layers, and we will use for the computations the scheme of the last section with \( V(x) = -i\sigma(x) \), where \( \sigma \) is the same function as in the PML; and the so-called transport-like boundary conditions. These conditions are based on a splitting of the Dirac equation as in [16] and on a first-order upwind discretization of the advection operators in the \( x \) and \( y \) directions. More precisely, we split the Hamiltonian into

\[
\mathcal{H} = \mathcal{H}_x + \mathcal{H}_y + \mathcal{H}_0,
\]

where

\[
\mathcal{H}_x = -i\sigma_x \partial_x, \quad \mathcal{H}_y = -i\sigma_y \partial_y, \quad \mathcal{H}_0 = m\sigma_z + V\mathbb{1}_2.
\]

Above, we used the notation \( \sigma_x = \sigma_1, \sigma_y = \sigma_2, \sigma_z = \sigma_3 \). We let then evolve the spinor with a first-order Lie Splitting of the form

\[
\Psi^{n+1} = e^{-i\Delta t\mathcal{H}_x}e^{-i\Delta t\mathcal{H}_y}e^{-i\Delta t\mathcal{H}_0}\Psi^n.
\]
We consider a first-order splitting since the upwind scheme that we define further is first-order. The operator $e^{-i\Delta t\mathcal{H}_0}$ is local in $(x, y)$ and poses no difficulty, while the operators $e^{-i\Delta t\mathcal{H}_x}$ and $e^{-i\Delta t\mathcal{H}_y}$ are treated as follows: the Pauli matrices are diagonalized as

$$
\sigma_x = P_x D P_x^{-1}, \quad \sigma_y = P_y D P_y^{-1}, \quad D = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix},
$$

where

$$
P_x = P_x^{-1} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}, \quad P_y = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & -1 \\ i & i \end{pmatrix}, \quad P_y^{-1} = \frac{1}{\sqrt{2}} \begin{pmatrix} i & 1 \\ -i & 1 \end{pmatrix}.
$$

The solution $\Phi_{\beta}^{n+1} = e^{-i\Delta t\mathcal{H}_\beta} \Phi_{\beta}^n$, $\beta = x, y$, at $t = t_n + \Delta t$ of

$$
i\partial_t \Phi_{\beta} = \mathcal{H}_\beta \Phi_{\beta}, \quad \Phi_{\beta}(t_n) = \Phi_{\beta}^n,
$$

is then obtained from $\Phi_{\beta}(t) = P_{\beta}(U(t), W(t))^T$, where $(U, W)$ satisfy the advection equations

$$
\partial_t U + \partial_x U = 0, \quad \partial_t W - \partial_y W = 0.
$$

Transport-like boundary conditions follow from an upwind discretization of the latter equations, where information is passed from left to right for right-going particles and vice versa for left-going particles, so that no conditions are imposed at the boundary of the domain. The scheme reads for $\beta = x$:

$$
U_{i,j}^{n+1} = U_{i,j}^n - \frac{\Delta t}{\Delta x} (U_{i,j}^n - U_{i-1,j}^n), \quad W_{i,j}^{n+1} = W_{i,j}^n + \frac{\Delta t}{\Delta x} (W_{i+1,j}^n - W_{i,j}^n),
$$

(17)

with similar expressions when $\beta = y$.

**Parameters.** The Dirac equation is solved on a square (that we will denote by $D$) of side $L = 10$ centered at the origin, and the physical constants are set to one, $\hbar = c = m = 1$. The spatial grid is uniform with stepsize $\Delta x = \Delta y = 0.04$. The time stepsize is $\Delta t = \Delta x/2$ for the scheme of section 3 in order to satisfy the CFL, and it is $\Delta t = \Delta x = \Delta y$ for the upwind scheme (17), so that we are at the maximal CFL for 1D upwinding and minimize dispersion effects. The initial condition has the form $\Psi(t = 0) = (u_0, v_0)^T$ where $v_0 = 0$ and

$$
u_0(x, y) = e^{-\frac{|X-X_0|^2}{a^2}} e^{iK_0 \cdot X}, \quad X = (x, y).
$$
We set $a = 0.6$. The vectors $X_0 = (x_0, y_0)$ and $K_0 = k_0(\cos \theta, \sin \theta)$ will take several values. We want to evaluate the methods depending on the frequency of the oscillations and on the angle at which particles hit the boundaries. We then consider in total 13 types of initial conditions:

- “Low” frequency with $k_0 = 1.25\pi$, “medium” frequency with $k_0 = 2.5\pi$, and “high” frequency with $k_0 = 5\pi$. This corresponds respectively to 6.25, 12.5 and 25 wavelengths in the domain.
- Incidence angle $\theta = \frac{\pi}{2}, \frac{5\pi}{8}, \frac{6\pi}{8}, \frac{7\pi}{8}$ for each of the above frequencies. The case $\theta = \frac{\pi}{2}$ is normal incidence, while $\theta = \frac{7\pi}{8}$ is grazing incidence.
- A purely Gaussian initial condition with $k_0 = 0$.

We are only interested here in quantifying the reflection rates at the boundaries and not in the overall accuracy of the different methods. For this, we compute a reference solution $u_{\text{ref}}$ in a larger domain that has the same uniform stepsize as the smaller domain $D$. The domain is a square of side $2L = 20$. The grid is chosen such that the nodes of $D$ coincide with those of the larger domain. We then compute the error

$$E_\beta = \frac{\|u_{T,\beta} - u_{\text{ref}}^{T,\beta}\|_{L_2(D)}}{\|u_0\|_{L_2(D)}},$$

where $\beta$ stands for either the absorbing potential method (AP), the PML, or the transport-like boundary conditions. The parameter $T$ corresponds to the final time of the simulation.

For the absorbing potential method and the PML, the domain is surrounded with a layer a thickness $\ell$. The function $\Sigma$ in the definition of $\sigma$ is chosen as

$$\Sigma(x) = \begin{cases} 
0 & \text{if } x \leq 0 \\
\sigma_0 x^2 & \text{otherwise}.
\end{cases}$$

We will test several configurations with different thickness $\ell$ and absorption $\sigma_0$. We will consider $\ell = 2, 1.5, 1$, that is the layer is, respectively, 20%, 15% and 10% of the length of the domain $D$. The parameter $\sigma_0$ will take values that range from 0.1 to 10. The “interior” potential $V$ in $\mathcal{H}_0$ is set to zero in order to keep a precise control on the wavenumbers. Non-zero $V$ would modify locally the frequency and the direction. The numerical results below show that the optimal thickness $\ell$ and the optimal absorption
factor $\sigma_0$ are weakly dependent on the wavenumber and the incident angle. A consequence is that the PML will perform well for non-zero potentials without a fine tuning of $\ell$ and $\sigma_0$.

The results are depicted in figures 1-5. In all figures, the green line corresponds to the transport BC, the blue curves to the AP, and the red curves to the PML. The diamonds correspond to an absorbing layer of length $\ell = 2$, circles to $\ell = 1.5$, and squares to $\ell = 1$.

In figure 1 are represented the errors for a normal incidence $\theta = \pi/2$ for the three frequencies and the various configurations of the layers. The shape of the curves can easily be explained: we expect better absorption the larger the layer, and there exist optimal choices of $\sigma_0$, that we denote by $\sigma_{\text{opt}}$. When $\sigma_0 < \sigma_{\text{opt}}$, there is little reflection at the inner boundary of the layer since the contrast is small, but there is also little absorption so that the main contribution to the error is due to the reflected waves at the outer boundary of the layer. When $\sigma_0 > \sigma_{\text{opt}}$, waves are well absorbed in the layer, but reflections at the inner boundary are larger and constitute the main source of error. The choice $\sigma_{\text{opt}}$ the best trade off between the two effects.

As is classical with absorbing conditions, it is clearly seen in figure 1 that higher frequencies are better absorbed than lower frequencies. Note that the errors for $k = 5\pi$ are identical for AP and the PML. This is a consequence of (i) the high frequency regime, (ii) the normal incidence, (iii) the fact that the absorbing potential is defined with $\sigma$, and is easily (unformally) explained as follows: consider expression (3) specialized to the 2D case,

$$
(\partial_y^{AL} - \partial_y)v(t, x, y) = \frac{i\sigma(y)}{2\pi} \int_{\mathbb{R}} \frac{e^{i\omega t}}{\omega - i\sigma(y)} \partial_y \hat{v}(\omega, x, y) d\omega.
$$

We will see that with the current choice of $K_0 = 5\pi(0, 1)$, we have

$$
(\partial_y^{AL} - \partial_y)v(t, x, y) \simeq i\sigma(y)u(t, x, y).
$$

Indeed, with our choice of initial conditions, the solutions $(u, v)$ are mostly supported around the wavenumber $K_0$. Using then the dispersion relation, we have $|w| = \sqrt{1 + |k|^2} \simeq |K_0| = 5\pi$. Let us compare now the energy $\omega$ with a typical $\sigma$. Since waves are exponentially decreasing in the PML, expression (18) has a significant amplitude only for some $y$ not too far from the interior boundary of the PML, say $y \leq L/2 + \ell_m$, where we recall that $L$ is the side length of the square. Let us pick $\ell_m = \ell/2$ for concreteness. The average value of $\sigma$ in $[0, \ell_m]$ for $\sigma_0 = 10$ is then equal to 3.3 for $\ell = 2$, which can be neglected compared to $|\omega| \simeq 5\pi$ in first approximation. We then replace the
denominator $\omega - i\sigma(y)$ in (18) simply by $\omega$. Moreover, taking the Fourier transform of (11) in $(t, x)$ leads to (denoting by $\hat{u}$ and $\hat{v}$ the Fourier transforms),

$$i\omega \hat{u}(\omega, k_x, y) \simeq -ik_x \hat{v}(\omega, k_x, y) + i \left(1 + \frac{\sigma(y)}{\omega}\right) \partial_y \hat{v}(\omega, k_x, y) + \hat{u}(\omega, k_x, y).$$

With the same argument as above, we can neglect the term in $\sigma(y)/\omega$. We can also neglect the $k_x$ contribution since $\hat{v}$ is supported around $K_0 = 5\pi(0, 1)$. This gives

$$\partial_y \hat{v}(\omega, x, y) \simeq \omega \hat{u}(\omega, x, y) + i\hat{u}(\omega, x, y).$$

Plugging this into (18) gives

$$(\partial_y^{\text{AL}} - \partial_y)v(t, x, y) \simeq \frac{i\sigma(y)}{2\pi} \int_{\mathbb{R}} e^{it\omega} \left(1 + \frac{i}{\omega}\right) \hat{u}(\omega, x, y) d\omega \simeq \frac{i\sigma(y)}{2\pi} \int_{\mathbb{R}} e^{it\omega} \hat{u}(\omega, x, y) d\omega,$$

which is the desired result. The same conclusion naturally holds for the layers in the $x$ direction.

For the optimal choice of $\sigma_0$, PML offer an optimal reflection rate of about 0.34%, 0.03%, 0.007% for $\ell = 2$ for low, medium and high frequencies, respectively. We find 0.53%, 0.07%, 0.015% for $\ell = 1.5$, and 1.3%, 0.27%, 0.1% for $\ell = 1$. Averaging over the three values of $\ell$, this is about 10 times and 5 times better than AP for low and medium frequencies, respectively. As explained above, the two methods provide identical results for large frequencies, which explains the decrease from 10 to 5 in efficiency factor between PML and AP.

Figures 2–4 correspond to $\theta = \frac{5\pi}{8}$, $\frac{6\pi}{8}$, $\frac{7\pi}{8}$. Results for the PML are very similar to the case $\theta = \frac{\pi}{2}$, with very slight variations in the errors. The results are also relatively stable for AP for $\theta = \frac{5\pi}{8}$, $\frac{6\pi}{8}$ for low and medium frequencies, and PML perform in average 10 times better. Some differences in the high frequency case appear since the incidence is not normal any longer. In the grazing case $\theta = \frac{7\pi}{8}$, PML offer now about 10, 15.5 and 16 times better absorption rates for low, medium and high frequencies after averaging over $\ell$.

Figure 5 corresponds to the purely Gaussian initial condition. In this case, waves with several frequencies and incidence angles have to be absorbed. Reflection rates for the PML are 0.4%, 0.9%, 1.7% for $\ell = 2, 1.5, 1$, with values about 10 times larger for the AP.

For all configurations, the transport-like boundary conditions present an error that ranges from 4% to 13%, with an average of 8%. This is significantly larger than the two other methods for an appropriate choice of $\sigma_0$, and not unexpected since outflow boundary conditions are a very basic type of absorbing boundary conditions.
Summary. Absorption in the PML depends very little on the incidence angle, but mostly on the frequency of the wave (and naturally on the layers characteristics). The worst reflection rate is 1.7% for the Gaussian initial condition with a small layer of thickness $\ell = 1$, and the best one is 0.007% for $\ell = 2$ and a high frequency wave with normal incidence. The AP yields relatively good results in regard to the simplicity of the technique, with, a few very particular cases excluded, reflection rates from 10 to 16 times higher than the PML. In particular, the PML perform much better for grazing angles. With much larger reflection rates, the transport-like BC are not competitive compared to the other two methods, the best rate about 20 times larger than the worst rate of the PML.

Figure 1: Comparison absorbing potential (AP)-PML-transport-like. The green line corresponds to the transport BC, the blue curve to the AP, and the red curve to the PML. The diamonds correspond to an absorbing layer of length $\ell = 2$, circles to $\ell = 1.5$, and squares to $\ell = 1$. The coefficient $\sigma_0$ is the strength of the absorption. The initial condition is centered at $[0, 2.8]$ and $T = 10$. Left: low frequency $k = 5\pi/4$; center: medium frequency $k = 5\pi/2$; right: high frequency $k = 5\pi$. Incidence angle $\theta = \pi/2$.

5 Conclusion

We have constructed perfectly matched layers for the Dirac equation, which are shown to be stable and to induce no reflections at the continuous level. The equations were discretized appropriately, leading to a stable numerical scheme based on the work of Hammer et al [19]. The PML performance was evaluated in comparison to the absorbing potential technique and transport-like boundary conditions. PML presented superior
Figure 2: Comparison absorbing potential (AP)-PML-transport-like. Same configuration as figure 1, with the difference that the incidence angle is now $\theta = \frac{5\pi}{8}$.

Figure 3: Comparison absorbing potential (AP)-PML-transport-like. Same configuration as figure 1, with the difference that the incidence angle is now $\theta = \frac{6\pi}{8}$.

absorption capabilities at a low implementation cost in configurations with low, medium and high frequencies, as well as with normal and grazing incidence angles.

A natural continuation of this work is to use the derived absorbing layers for concrete applications such as the simulation of electron transport in nanostructures or of the scattering of high energy particles.
Figure 4: Comparison Absorbing potential (AP)-PML-transport-like. Same configuration as figure 1, with the difference that the initial condition is now centered at $[2.8, 2.8]$, $T = 8$, and the incidence angle is $\theta = 7\pi/8$.

Figure 5: Comparison absorbing potential (AP)-PML-transport-like. Purely Gaussian initial condition centered at $(0,0)$ and $T = 10$.

6 Appendix: Proof of lemma 2.1.

We suppose for simplicity that $\hbar = c = m = 1$, $V = 0$, and that there is only one absorbing layer in the $x_1$ direction in the domain $x_1 \geq 0$. The generalization to the setting of the lemma is straightforward. We assume in addition that all functions are smooth and decay sufficiently fast at infinity in order to justify the calculations. We start by differentiating the Dirac equation (5) with respect to the time variable and
obtain a modified Klein-Gordon equation of the form

\[
(\partial^2_t - \Delta + \mathbb{I}_4)\Psi = \sum_{j=1}^{3} \alpha_j \alpha_1 \partial_{x_j} \xi - \alpha_1 \partial_t \xi
\]  

(19)

where \( \xi = (\xi_j)_{j=1,\ldots,4} \) and

\[
\partial_t \xi_j + \sigma_1(x_1) \xi_j = -\sigma_1(x_1) \partial_{x_1} \Psi_j, \quad \xi_j(t = 0, x) = 0.
\]  

(20)

Multiplying (19) by \( \Psi^\dagger \) (the transpose conjugate of \( \Psi \)) on the right, integrating both in \( x \) and \( t \), and then multiplying (20) by \( \xi_j \) and integrating in \((t, x)\) yield, after summation of all equations and taking the real part,

\[
E(t) + \int_0^t \int_{\mathbb{R}^3} \sigma_1(x_1) |\xi(s, x)|^2 ds dx = E(0) + \Re \sum_{j=1}^{3} \int_{\mathbb{R}^3} \partial_t \Psi^\dagger \alpha_j \alpha_1 \partial_{x_j} \xi ds dx - \Re \int_0^t \int_{\mathbb{R}^3} \partial_t \Psi^\dagger \xi ds dx - \lambda \Re \int_0^t \int_{\mathbb{R}^3} \sigma_1(x_1) \xi^\dagger \partial_{x_1} \Psi ds dx
\]

:= \sum_{k=1}^{3} I_k(t).

Above, we have introduced, for some \( \lambda > 0 \) to be defined later on,

\[
E(t) = \frac{1}{2} \| \partial_t \Psi(t, \cdot) \|_{L^2}^2 + \frac{1}{2} \| \Psi(t, \cdot) \|_{H^1}^2 + \frac{\lambda}{2} \| \xi(t, \cdot) \|_{L^2}^2,
\]

where all absolute values in the norm definitions have to be understood as the Euclidean norm in \( \mathbb{C}^4 \). Let us start with the term \( I_1 \): we have

\[
I_1(t) = -\Re \sum_{j=1}^{3} \int_0^t \int_{\mathbb{R}^3} \partial_t \Psi^\dagger \alpha_j \alpha_1 \xi ds dx + \Re \sum_{j=1}^{3} \int_0^t \int_{\mathbb{R}^3} \partial_{x_j} \Psi^\dagger \alpha_j \alpha_1 \partial_t \xi ds dx
\]

\[
= -\Re \sum_{j=1}^{3} \int_{\mathbb{R}^3} (\partial_{x_j} \Psi^\dagger \alpha_j \alpha_1 \xi)(t, x) dx + \Re \sum_{j=1}^{3} \int_{\mathbb{R}^3} (\partial_{x_j} \Psi^\dagger \alpha_j \alpha_1 \xi)(0, x) dx
\]

\[
- \Re \sum_{j=1}^{3} \int_0^t \int_{\mathbb{R}^3} \sigma_1 \partial_{x_j} \Psi^\dagger \alpha_j \alpha_1 \xi ds dx - \Re \sum_{j=1}^{3} \int_0^t \int_{\mathbb{R}^3} \sigma_1 \partial_{x_j} \Psi^\dagger \alpha_j \alpha_1 \partial_{x_j} \Psi ds dx.
\]
Above, we used an integration by parts for the first line, and replaced $\partial_t \xi$ by (20) in the second. With the Cauchy-Schwarz inequality, this gives, since $\xi(0) = 0$,

$$|I_1(t)| \leq C_1 \left( \|\nabla \Psi(t)\|_{L^2} \|\xi(t)\|_{L^2} + \int_0^t \|\nabla \Psi(s)\|_{L^2} \|\xi(s)\|_{L^2} ds + \int_0^t \|\nabla \Psi(s)\|_{L^2}^2 ds \right),$$

where the constant $C_1$ only depends on $\|\sigma_1\|_{L^\infty}$. Regarding $I_2$, we find in the same way,

$$|I_2(t)| \leq C_2 \left( \int_0^t \|\partial_t \Psi(s)\|_{L^2} \|\xi(s)\|_{L^2} ds + \int_0^t \|\partial_t \Psi(s)\|_{L^2} \|\nabla \Psi(s)\|_{L^2} ds \right).$$

The term $I_3$ is straightforward and yields

$$|I_3(t)| \leq \lambda C_3 \int_0^t \|\nabla \Psi(s)\|_{L^2} \|\xi(s)\|_{L^2} ds.$$

Gathering the previous estimates leads to, after using the Young inequality,

$$\left| \sum_{k=1}^3 I_k(t) \right| \leq \frac{1}{4} \|\nabla \Psi(t)\|_{L^2}^2 + C_1^2 \|\xi(t)\|_{L^2}^2 + C \int_0^t E(s) ds.$$

Setting for instance $\lambda = 2 + 2C_1^2$, the estimate of the lemma follows from the Gronwall lemma and the fact that, using the Dirac equation (5),

$$\|\partial_t \Psi(t = 0, \cdot)\| \leq C' \|\Psi(t = 0, \cdot)\|_{H^1}.$$

References


