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Contents

Abstract

In this thesis we discuss the Pauli equation which models the semi-relativistic evolution of electron states in an electromagnetic field. An introduction is given on the physics and mathematics of quantum mechanics and electromagnetism including core concepts such as the Schrödinger equation, potential couplings to Maxwell's equations and the Lorentz force of classical electromagnetism and the relativistic Klein-Gordon and Dirac equations. From these, one finds two different approaches to arrive at the Pauli equation: A bottom-up approach which adds spin to conform to empirical results and a top-down approach which shows the Pauli equation to be the semi-relativistic limit of the fully relativistic Dirac equation.

Once the Pauli equation's modeling and relevance to modern physics is established, we move to discussing potential numerical approaches to finding solutions. We will present one sensible way to scale the Pauli equation for use in numerical procedures and present a coupled four operator-splitting approach to numerically solving the Pauli equation based on previous results for the magnetic Schrödinger equation in [1]. Most discussions are applied to both the magnetic Schrödinger equation and the Pauli equation. We conclude by presenting a handful of numerical experiments done in a Julia language implementation of this four operator-splitting method and by discussing potential applications and an outlook on potential future research.

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1 Introductory remarks

Schrödinger-type equations lie at the heart of quantum mechanics and enjoy the same status within quantum mechanical theories as Newton's equations of motion do in classical physics. Given an initial state of a physical system, Schrödinger-type equations determine its time evolution and tell us about the presence or absence of various conservation laws and can be used to predict experimental outcomes with excellent precision. It is no surprise then that finding solutions to particular Schrödinger-type equations has been of significant interest to the mathematics, physics and chemistry research communities and as a result the number of papers published on this topic is vast.

Of similar importance to theoretical physics as well as any experimental setups or engineering implementations are descriptions of electromagnetism, one of the four fundamental forces described as part of the standard model of particle physics. The behavior of electrons, present as the negatively charged component particles of atoms as well as on their own as part of so-called beta radiation, is of particular interest since most of the phenomena intuitively connected to electricity emerge in systems dominated by electrons. Being fundamental quantum objects themselves, the behavior of electrons in an electromagnetic field needs to be described by a system of equations on the intersection of electromagnetic theory and quantum theory but as it turns out a naive approach which couples Maxwell's equations to the Schrödinger equation fails to explain and predict experimentally well-established results which are due to an intrinsic property of quantum objects known as spin. To account for this, the so-called magnetic Schrödinger equation has to be expanded by a spin term in order to obtain the Pauli equation, which provides an adequate semi-relativistic quantum model for the behavior of electrons.

The Pauli equation and numerical approaches to solving it are the main subject of this paper. To this end we will first introduce the mathematics of quantum physics and electromagnetism in section 2 and from there explain the motivation and modeling behind the magnetic Schrödinger equation. We will then motivate the Pauli equation starting from the experimental bottom-up approach as well as from a top-down approach beginning with the fully relativistic Dirac equation which describes the behavior of fermions. Once the context for the Pauli equation has been established, we will summarize and present multiple general preparatory steps for dealing with the Pauli and magnetic Schrödinger system numerically in section 3. Section 4 sketches a three operator-splitting method due to [1] which presents an attractive numerical approach to solving the magnetic Schrödinger equation and in section 5 we show how one can sensibly expand their methodology to the Pauli equation system in a four operator-splitting approach. Section 6 presents numerical results obtained from a Julia language [2] implementation of this four operator-splitting algorithm. We conclude by discussing potential future research projects on the numerics of the Pauli equation and by contextualizing the results presented in this paper.

For a full list of the notation and conventions used in this paper, see table 1 in the appendix.

2 Theoretical background

2.1 Spin and the Stern-Gerlach experiment

In this section we will qualitatively motivate quantum mechanical spin based on the seminal Stern-Gerlach experiment [3]. Beyond the introduction of spin which is crucial for understanding the form of the Pauli equation later in section 2.4, we will also use this experiment as an empirical argument for why the quantum mechanical formalism developed in the following sections is sensible and experimentally justified. The important realizations will be that several naturally occurring quantities are in fact discrete ('quantized') quantities, that the classical point particle picture does not match experimental reality and that there is a fundamentally non-classical measurable quantity called 'spin' with various important properties. This section is primarily based on [4, 5]. For a historical understanding of the Stern-Gerlach experiment we refer to Friedrich and Herschbach's extensive and excellent overview of the experiment in its historical context [6].

Towards the second quarter of the 20th century, the quantized nature of the natural world had already been noticed and studied in a multitude of ways, such as blackbody radiation, the photoelectric and Compton effects and others (for historical overviews of the early development of quantum physics, see for example [7, 8]). We have selected the Stern-Gerlach experiment among these as the most relevant of these seminal experiments for the present purpose of studying the Pauli equation since it relates to particles, or more precisely said quantum objects, moving through a magnetic field and showing manifestly non-classical behavior in the process. We will first sketch the experimental setup, then briefly indicate what classical physics would predict to occur given said setup and then argue how this prediction is violated by the experimental results of the Stern-Gerlach experiment. The necessary formalisms to rectify the situation provide a natural entry point into the mathematics of quantum physics from which we will build the theoretical framework required to study and understand the Pauli equation.

For the Stern-Gerlach experiment one first realizes a strongly inhomogeneous magnetic field and sends a highly collimated beam of uncharged paramagnetic particles through it (historically, the choice was neutral silver atoms), see Figure 1. The reason we choose neutral particles is that for charged particles, the Lorentz force would overshadow the effect we wish to observe here, which is about a particle's "intrinsic" coupling to the magnetic field. In classical mechanics, a neutral particle can still couple to the magnetic field if it possesses a so-called magnet moment μ. The force caused on a particle of magnetic moment μ moving through a magnetic field $\mathbf{B}$ is simply

$$\mathbf{F} = \nabla(\mu \cdot \mathbf{B}). \tag{2.1}$$

Since in the Stern-Gerlach setup as seen in Figure 1 a direction of the magnetic field $\mathbf{B}$ is far larger than the others, we have that

$$\mu \cdot \mathbf{B} = \mu_x B_x + \mu_y B_y + \mu_z B_z \approx \mu_z B_z, \tag{2.2}$$

where we have chosen our coordinate system to consider the z-direction to be the direction with the dominant field by convention ($B_z \gg B_x$, $B_z \gg B_y$). For the force on a neutral particle with magnetic moment μ this means that we should expect the

force on the particle to be dominated by a contribution of the following form:

$$\mathbf{F} = \mu_z \frac{\partial B_z}{\partial z} \mathbf{e}_z, \tag{2.3}$$

where $\mathbf{e}_z$ is the standard basis unit vector in z-direction (compare [5]). Since classically the value of μ_z can vary continuously we would also expect that the particle beam would likewise experience a continuous deflection depending on the particular value of the atom passing through, resulting in an image of deflection akin to (4) in Figure 1. The actual outcome of the experiment, however, are two discrete modes of deflection associated with two discrete images as seen in (5) in Figure 1.

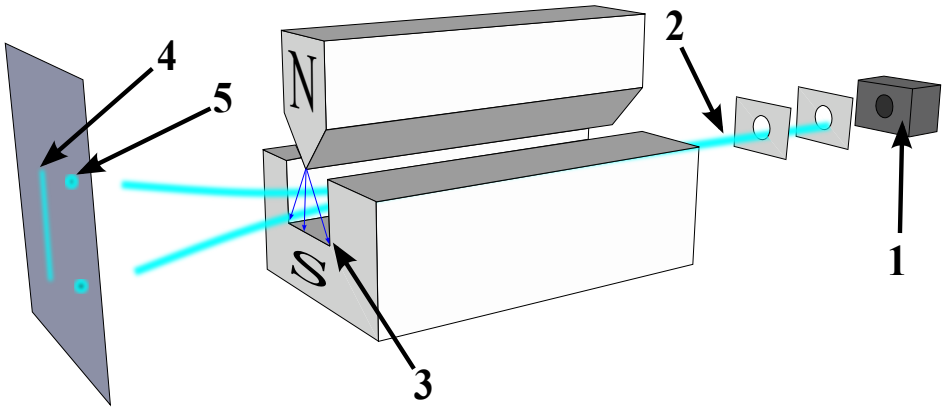

Figure 1: Visualization of Stern-Gerlach experiment including incorrect classical prediction and actual observation, image attribution in [9]. (1) furnace emitting charged particles. (2) particle beam. (3) inhomogeneous magnetic field caused by magnet setup. (4) classically expected outcome. (5) actual experimental observations.

The discrepancy between the classical prediction and the experimental outcome is due to the the classical assumption that an atom's internal magnetic moment μ can vary continuously rather than only a particular set of 'quantized' states being allowed. This experiment hints very strongly at the existence of some sort of intrinsic quantized contribution to an atom's magnetic moment and this particular intrinsic quantized property of particles is called 'spin'. To properly explain how quantum mechanics solves the experimental problems that classical mechanics faced the following sections will introduce the core mathematical aspects of quantum physics including spin and explain how these relate to the intersection with the theory of electromagnetism.

2.2 The mathematics of quantum physics

The core aspects of this section are loosely based on material covered in [4, 10, 11]. A more thorough and in-depth mathematical treatment of quantum mechanics can be found in [12]. We specify further sources that provide supplementary proofs or derivations to the presented material where appropriate.

2.2.1 The Schrödinger equation

Let us start by a brief motivation and derivation of Schrödinger's equation. Clasically, we conceive of energy as consisting of a kinetic term and a potential term as follows:

$$E = \frac{\mathbf{p}^2}{2m} + V, \tag{2.4}$$

where $\mathbf{p}$ is the particle's momentum vector and V is a not further specified potential function. The kinetic term might be more familiar in the form $\frac{m\mathbf{v}^2}{2}$ but with the classic momentum relation $\mathbf{p} = m\mathbf{v}$ it is easy to see that these are equivalent.
One of the fundamental concepts of quantum mechanics is that classically observable (also: measurable) quantities in fact in some sense correspond to operators and their eigenvalues. The operators identified with energy and momentum are as follows:

$$\mathbf{p} \to -i\hbar\nabla, \tag{2.5}$$

$$E \to i\hbar\frac{\partial}{\partial t}. \tag{2.6}$$

Here i is the imaginary unit and $\hbar$ is a fundamental physical constant known as the reduced Planck constant. At this point it is necessary to explain the meaning of what is generally called a *wave function*, denoted with the letter ψ. Quantum mechanics is a fundamentally statistical theory in that physical phenomena are described using a function ψ where the equations of motion give the development of this 'wave function' in time. Generally, this wave function is assumed to be normalizable with

$$\int_{-\infty}^{+\infty} |\psi(x,t)|^2 dx = 1. \tag{2.7}$$

All this condition basically imposes is that the particle described by the wave function ψ has to be *somewhere*, i.e. the probability to find it when looking everywhere is 1 (it turns out there are cases where this does not hold but those are beyond the scope of the present paper). This of course assumes that the square of the absolute value of the wave function is to be interpreted as a probability (this interpretation of ψ is known as Born's rule and there are many subtleties involved with it that we will not further delve into).
Under the most common physical interpretations, the complex-valued and spacetime dependent wavefunction ψ is assumed to give a complete description of the quantum states of a given system, which means that an equation that describes the time-evolution of ψ has similar importance as Newton's equations of motion for a particle in classical mechanics. So what we are looking for, then, to obtain a theory that is apt to be called a quantum theory is an equation that describes the evolution of a particle's wavefunction ψ.

Returning to the energy and momentum operators in Equation (2.5) and (2.6), we can plug these into the energy-momentum relation of classical physics found in Equation (2.4) to obtain an operator. Using this operator to act on the wavefunction ψ, we arrive at the following equation:

$$\left(-\frac{\hbar}{2m}\nabla^2 + V\right)\psi = i\hbar\frac{\partial}{\partial t}\psi. \tag{2.8}$$

This is already the so-called time-dependent Schrödinger equation for a single, non-relativistic particle. It is fundamentally non-relativistic, since the energy-momentum relation we started out with only holds in classical physics and falls apart when one approaches the speed of light. Beyond that, as it turns out, the equation is not covariant with regards to a Lorentz transformation which further rules it out for a relativistic quantum theory. More generally speaking, the Schrödinger equation can be thought to simply be

$$\hat{H}\psi = i\hbar\frac{\partial}{\partial t}\psi, \tag{2.9}$$

where $\hat{H}$ is the Hamilton operator that describes a particle's energy-momentum relation. In this more general form, Schrödinger's equation is actually Lorentz covariant and also holds in the special theory of relativity but it is exactly the shape of $\hat{H}$ which is the problem of unifying special relativity with quantum theory and since all of the physics of a theory is contained in its Lagrangian function or equivalently its Hamiltonian function the equation in this form has no predictive power. Equation (2.8), however, works phenomenally well for describing single quantum objects moving at non-relativistic speeds.

2.2.2 Elementary mathematics of spin

Many properties of quantum objects have classical analogues either directly or via the Ehrenfest theorem such as charge, energy, momentum and many others but there are some phenomena of quantum physics which are without a true classical counterpart. Among the latter is spin, an intrinsic property of quantum objects which plays a role not only in defining entirely different classes of fundamental particles but also has an extremely important relationship to electromagnetism as in addition to a particle's charge, a particle's spin also contributes to how it couples to an electromagnetic field. We have already seen an experimental motivation of spin in section 2.1. In this section we will provide a rough sketch of the mathematical treatment of spin as it pertains to the goal of this paper. For a far more complete mathematical treatment we refer to [12] and [13].

Quantum mechanical observables are mathematically associated with a Hermitian operator whose eigenvalues allow an interpretation as the possible values of measurement. For spin the associated operators are:

$$\hat{S}_{x_i} = \frac{\hbar}{2}\sigma_i. \tag{2.10}$$

There are three of these operators in three dimensional space, representing spin with regards to a particular direction. Conventionally the chosen basis of spin is the z-basis and this will be assumed for the remainder of this paper as well. The σ_i in

this definition are the so-called Pauli matrices which can be written in a short-hand vector-esque form that will be useful in the coming sections:

$$\sigma = \begin{pmatrix} \sigma_1 \\ \sigma_2 \\ \sigma_3 \end{pmatrix} = \begin{pmatrix} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \\ \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \\ \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \end{pmatrix}. \tag{2.11}$$

The spin operators can then be written as:

$$\hat{S} = \frac{\hbar}{2}\sigma = \frac{\hbar}{2}\begin{pmatrix} \sigma_1 \\ \sigma_2 \\ \sigma_3 \end{pmatrix} \tag{2.12}$$

The total spin operator is defined to be

$$\hat{S}^2 = \hat{S}_x^2 + \hat{S}_y^2 + \hat{S}_z^2. \tag{2.13}$$

These spin operators also inherit a defining commutation relation from their relationship to the Pauli matrices:

$$[\hat{S}_{x_i}, \hat{S}_{x_j}] = \sum_l i\hbar\epsilon_{jkl}\hat{S}_{x_l}, \tag{2.14}$$

where ϵ_{jkl} is the antisymmetric Levi-Civita symbol.

2.2.3 The Klein-Gordon equation

Having seen the derivation of the time-dependant Schödinger equation for a non-relativistic particle, one might wonder why one does not simply start with the relativistic energy-momentum relation instead of the classical one, following the same procedure. It turns out that Schrödinger did this even before he arrived at the equation that is now named after him but he discarded the resulting equation for reasons that will be discussed in this section (compare [10]). The equation he arrived at is what we nowadays call the Klein-Gordon Equation, named after Oskar Klein and Walter Gordon, who independently published their findings in 1926 and 1927.
We begin with the relativistic energy relation:

$$E = \sqrt{\mathbf{p}^2c^2 + m^2c^4}. \tag{2.15}$$

This energy-momentum relation only describes free particles, where the potential V vanishes. It turns out that the quantum mechanical operator substitutions were already Lorentz covariant, so the substitution found in Equations (2.5) and (2.6) still hold, although they can be rewritten more elegantly in relativistic index notation as follows:

$$p_\mu \to i\hbar\partial_\mu = i\hbar\frac{\partial}{\partial x^\mu}. \tag{2.16}$$

Under these substitutions then, the equation one ends up with is:

$$\left(\sqrt{(-i\hbar\nabla)^2c^2 + m^2c^4}\right)\psi = i\hbar\frac{\partial}{\partial t}\psi. \tag{2.17}$$

We won't pursue this equation any further since due to the square root it is not really useful to work with. To actually obtain the Klein-Gordon Equation, we have to start with the squared relativistic energy-momentum relation:

$$E^2 = \mathbf{p}^2 c^2 + m^2 c^4, \tag{2.18}$$

which reads as follows using Einstein notation:

$$p^\mu p_\mu - m^2 c^2 = 0. \tag{2.19}$$

Using the appropriate correspondence substitutions on this relation, we obtain:

$$(-\hbar^2 \partial^\mu \partial_\mu - m^2 c^2)\psi = 0. \tag{2.20}$$

We can also state this equation without the use of Einstein notation:

$$-\frac{1}{c^2}\frac{\partial^2 \psi}{\partial t^2} + \nabla^2 \psi = \frac{m^2 c^2}{\hbar^2}\psi, \tag{2.21}$$

or alternatively in its canonical highly compressed form as

$$(\Box + \frac{m^2 c^2}{\hbar^2})\psi = 0, \tag{2.22}$$

where $\Box = \frac{1}{c^2}\frac{\partial^2}{\partial t^2} - \nabla^2$ is the so-called d'Alembert operator. This is known as the *Klein-Gordon equation* and it was originally proposed as an equation describing relativistic electrons. As it turns out, however, this equation fails to reproduce the known Bohr levels in the Hydrogen atom (this is also among the reasons Schrödinger had originally discarded the equation, compare [10]). The reason this equation failed to describe the energy levels of the Hydrogen atom correctly is that it does not actually describe electrons, which are spin-$\frac{1}{2}$ particles, but in fact only describes spin-0 particles.
It might be interesting to note that with the recent discovery of the Higgs boson [14, 15] there is now a known elementary particle with spin-0, which should be described by the Klein-Gordon equation whereas only composite particles of spin-0 were known before.

2.2.4 The Dirac equation

Dirac's idea was to linearize the relativistic energy-momentum relation before moving to quantum mechanics. We can sketch the idea in an abbreviated way compared to how he did it, by attempting to factor the equation:

$$0 = p^\mu p_\mu - m^2 c^2 = (\beta^\kappa p_\kappa + mc)(\gamma^\lambda p_\lambda - mc). \tag{2.23}$$

When we actually do the multiplication on the right, we obtain:

$$p^\mu p_\mu - m^2 c^2 = \beta^\kappa \gamma^\lambda p_\kappa p_\lambda - mc(\beta^\kappa - \gamma^\kappa)p_\kappa - m^2 c^2. \tag{2.24}$$

Comparing the two sides, we obviously require $\beta^\kappa = \gamma^\kappa$, since otherwise we would have linear terms in p. We are left with:

$$p^\mu p_\mu - m^2 c^2 = \gamma^\kappa \gamma^\lambda p_\kappa p_\lambda - m^2 c^2, \tag{2.25}$$

which means the requirement we have to satisfy with γ is:

$$p^\mu p_\mu = \gamma^\kappa \gamma^\lambda p_\kappa p_\lambda. \tag{2.26}$$

It is not difficult but a bit tedious to check what follows from this for the γ:

$$\begin{aligned}(p^0)^2 - (p^1)^2 - (p^2)^2 - (p^3)^2 = (\gamma^0)^2(p^0)^2 + (\gamma^1)^2(p^1)^2 + (\gamma^2)^2(p^2)^2 + (\gamma^3)^2(p^3)^2 \\ +(\gamma^0\gamma^1 + \gamma^1\gamma^0)p_0p_1 + (\gamma^0\gamma^2 + \gamma^2\gamma^0)p_0p_2 + (\gamma^0\gamma^3 + \gamma^3\gamma^0)p_0p_3 \\ +(\gamma^1\gamma^2 + \gamma^2\gamma^1)p_1p_2 + (\gamma^1\gamma^3 + \gamma^3\gamma^1)p_1p_3 + (\gamma^2\gamma^3 + \gamma^3\gamma^2)p_2p_3.\end{aligned}$$

So by comparison of coefficients it turns out that we require:

$$(\gamma^0)^2 = 1, \tag{2.27}$$

$$(\gamma^1)^2 = (\gamma^2)^2 = (\gamma^3)^2 = -1, \tag{2.28}$$

$$\gamma^\mu\gamma^\nu + \gamma^\nu\gamma^\mu = 0 \ \ , \mu \neq \nu. \tag{2.29}$$

The first two equations could be fulfilled by setting $\gamma^0 = 1$ and $\gamma^1 = \gamma^2 = \gamma^3 = i$ but the anti-commutator terms cannot be made to vanish in the way required using scalars. Dirac's achievement was to then postulate that the γ must be matrices with a certain anti-commutation relation:

$$\{\gamma^\mu, \gamma^\nu\} = 2\eta^{\mu\nu}\mathbb{1}. \tag{2.30}$$

It turns out the smallest dimension for which the equations above can be fulfilled is 4×4 matrices, for which one standard notation is:

$$\gamma^0 = \begin{pmatrix} \mathbb{1} & 0 \\ 0 & -\mathbb{1} \end{pmatrix}, \tag{2.31}$$

$$\gamma^i = \begin{pmatrix} 0 & \sigma^i \\ -\sigma^i & 0 \end{pmatrix}, \tag{2.32}$$

The σ^i are the standard Pauli matrices:

$$\sigma = \begin{pmatrix} \sigma_1 \\ \sigma_2 \\ \sigma_3 \end{pmatrix} = \begin{pmatrix} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \\ \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \\ \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \end{pmatrix}. \tag{2.33}$$

and $\mathbb{1}$ is the 4-dimensional identity matrix. All the work so far has been done with the goal of factoring the energy-momentum relation:

$$0 = p^\mu p_\mu - m^2c^2 = (\gamma^\kappa p_\kappa + mc)(\gamma^\lambda p_\lambda - mc). \tag{2.34}$$

By using only one of the factors on the left (it's standard to pick the one with the negative sign), we obtain:

$$\gamma^\mu p_\mu - mc = 0, \tag{2.35}$$

which using $p_\mu \to i\hbar\partial_\mu$ turns into:

$$(i\hbar\gamma^\mu\partial_\mu - mc)\psi = 0. \tag{2.36}$$

This is the Dirac equation which finally gives us a relativistic quantum mechanical equation describing the behavior of spin-$\frac{1}{2}$ particles like electrons. Due to the necessity of moving to 4×4 matrices to factor the energy relation the ψ can no longer be a scalar function. Instead it has to be considered as a 4 dimensional Dirac spinor:

$$\psi = \begin{pmatrix} \psi_1 \\ \psi_2 \\ \psi_3 \\ \psi_4 \end{pmatrix}. \tag{2.37}$$

This very concise motivation of the Dirac equation can be found in many places in the modern literature, e.g. [10]. Furthermore, it turns out that each of the components of the Dirac Spinor has to satisfy the Klein-Gordon equation. Given that the Dirac equation necessitates that we obtain solutions with four components and that the first two components of these solutions would correspond to an electron with spin up and down respectively it is natural to ask what if anything the other two components of the solution physically represent.
Dirac proposed that infinitely many electrons ubiquitously fill up all the negative energy states in a "infinite electron sea". Due to the Pauli exclusion principle and the electron sea's uniformity and omnipresence, no other electrons could thus enter negative energy states and the electron sea would not exhibit any forces on anything. This immediately raises the question of what would happen if we knock an electron out of the electron sea. Such a "hole" would then suddenly be perceived as a positively charged particle and initially one might hope for it to be the proton. The particle has to have the same mass as the electron, however, so it turns out it would appear as an entirely separate positively charged particle with the mass of the electron. Such a particle was indeed observed in 1931, dubbed the positron. The prediction of such particles was a massive success for Dirac's equation but the omnipresent infinite Dirac sea of electrons still did not sit right with many physicists given its metaphysical implications. For there to be no net force or field that is noticeable we would require the vacuum of space has a charge density that cancels the Dirac sea's charge density. On top of this, it is not clear if the Pauli exclusion principle would truly prevent more electrons to take up such negative energy states, since we know from famous mathematical thought experiments like Hilbert's Hotel, that an infinite well can still make room for further particles even if it is already filled.
Under the interpretation of the Dirac sea, what in modern physics we would call a positron would not in fact be a particle but instead a pseudo-particle caused by the absence of an electron in the infinite Dirac sea. Instead, Stückelberg and Feynman proposed viewing the negative energy states of a spin up electron as a positive energy state of a spin down positron instead. Essentially, we introduce the new particle of the positron, which is on an equal footing with the electron and has positive energy states. The currently most wide-spread view in the physics community is viewing the positron as an actual particle according to the proposal of Stückelberg and Feynman and Dirac's idea of the sea of electrons has largely been discarded in favor of this metaphysically simpler interpretation. For further discussions on this topic, see [10].

2.3 The mathematics of classical electromagnetism

This section provides a sketch of the relevant pieces of classical electromagnetism needed to understand and work with the Pauli equation as it pertains to this paper. For a more in-depth introduction to the mathematical treatment of electromagnetism, we refer to [16, 17].

2.3.1 Maxwell's equations and the Lorentz force

At a fundamental level electromagnetism is mathematically described by the Maxwell equations and the Lorentz force, either of which can be used as in fact being the *definitions* of the electric vector field $\mathbf{E}$ and the magnetic vector field $\mathbf{B}$. A classical point-particle moving at velocity $\mathbf{v}$ with charge q moving through electromagnetic fields experiences a force acting on it called the Lorentz force:

$$\mathbf{F} = q(\mathbf{E} + \mathbf{v} \times \mathbf{B}). \tag{2.38}$$

While the Lorentz force relates to forces the electromagnetic field causes on particles, Maxwell's equations define how the electric and magnetic fields themselves behave:

$$\nabla \cdot \mathbf{E} = \frac{\rho}{\epsilon_0}, \tag{2.39}$$

$$\nabla \cdot \mathbf{B} = 0, \tag{2.40}$$

$$\nabla \times \mathbf{E} = -\frac{\partial \mathbf{B}}{\partial t}, \tag{2.41}$$

$$\nabla \times \mathbf{B} = \mu_0 \left(\mathbf{J} + \epsilon_0 \frac{\partial \mathbf{E}}{\partial t} \right), \tag{2.42}$$

where ρ represents charge density and $\mathbf{J}$ the current. μ_0 and ϵ_0 are constants satisfying $\frac{1}{\mu_0 \epsilon_0} = c^2$ with c being c-velocity of special relativity, often colloquially dubbed the 'speed of light'. For simplicity, we will primarily work with Maxwell's equations in the form they take in a vacuum with neither charge density nor currents present, i.e. $\rho = 0$ and $\mathbf{J} = 0$:

$$\nabla \cdot \mathbf{E} = 0, \tag{2.43}$$

$$\nabla \cdot \mathbf{B} = 0, \tag{2.44}$$

$$\nabla \times \mathbf{E} = -\frac{\partial \mathbf{B}}{\partial t}, \tag{2.45}$$

$$\nabla \times \mathbf{B} = \frac{1}{c^2} \frac{\partial \mathbf{E}}{\partial t}. \tag{2.46}$$

2.3.2 Electromagnetic wave equations

The classical electromagnetic wave formalism is one of the most important contributions of Maxwell's theory to the development of physics and studying this classical behavior of the $\mathbf{E}$ and $\mathbf{B}$ fields is important for gaining not only a physical intuition about the behavior of these fields but also to understand some of the underlying mathematical structure. We will remain in the vacuum throughout this section for simplicity but similar equations can be shown to hold in more general cases as well, see for example [16, 18].

To see how electromagnetic waves arise from the above-introduced Maxwell equations one first computes $\nabla \times (\nabla \times \mathbf{E})$ and $\nabla \times (\nabla \times \mathbf{B})$ using the corresponding Maxwell equations:

$$\nabla \times (\nabla \times \mathbf{E}) = -\frac{\partial}{\partial t}(\nabla \times \mathbf{B}), \tag{2.47}$$

$$\nabla \times (\nabla \times \mathbf{B}) = \frac{1}{c^2}\frac{\partial}{\partial t}(\nabla \times \mathbf{E}). \tag{2.48}$$

A well-known cross product identity tells us that for the curl of the curl of any given vector field $\mathbf{v}$ we have

$$\nabla \times (\nabla \times \mathbf{v}) = \nabla(\nabla \cdot \mathbf{v}) - \nabla^2\mathbf{v}. \tag{2.49}$$

Using this on the above equations yields:

$$\nabla(\nabla \cdot \mathbf{E}) - \nabla^2\mathbf{E} = -\frac{\partial}{\partial t}(\nabla \times \mathbf{B}), \tag{2.50}$$

$$\nabla(\nabla \cdot \mathbf{B}) - \nabla^2\mathbf{B} = \frac{1}{c^2}\frac{\partial}{\partial t}(\nabla \times \mathbf{E}). \tag{2.51}$$

Remembering the Maxwell equations which tell us that $\nabla \cdot \mathbf{E} = 0$ and $\nabla \cdot \mathbf{B} = 0$ we obtain:

$$-\nabla^2\mathbf{E} = -\frac{\partial}{\partial t}(\nabla \times \mathbf{B}), \tag{2.52}$$

$$-\nabla^2\mathbf{B} = \frac{1}{c^2}\frac{\partial}{\partial t}(\nabla \times \mathbf{E}). \tag{2.53}$$

Now we plug in the Maxwell equations for $\nabla \times \mathbf{E}$ and $\nabla \times \mathbf{B}$ to obtain:

$$-\nabla^2\mathbf{E} = -\frac{1}{c^2}\frac{\partial^2\mathbf{E}}{\partial t^2}, \tag{2.54}$$

$$-\nabla^2\mathbf{B} = -\frac{1}{c^2}\frac{\partial^2\mathbf{B}}{\partial t^2}. \tag{2.55}$$

Rearranging this shows that these are proper mathematical wave equations for the $\mathbf{E}$ and $\mathbf{B}$ fields with propagation speed c:

$$-\frac{1}{c^2}\frac{\partial^2\mathbf{E}}{\partial t^2} + \nabla^2\mathbf{E} = 0, \tag{2.56}$$

$$-\frac{1}{c^2}\frac{\partial^2\mathbf{B}}{\partial t^2} + \nabla^2\mathbf{B} = 0. \tag{2.57}$$

In classical electrodynamics, the propagation of light is described by such electromagnetic wave equations and light is characterized as an electromagnetic wave.

2.3.3 The electromagnetic potential formalism

Treatment of electromagnetism in physics typically moves from the proper fields $\mathbf{E}$ and $\mathbf{B}$ to an electromagnetic potential formalism which retains the same relatively simple structure but in addition offers certain amounts of gauge freedom in the choices of the potential to adapt to a particular situation. In the case of the magnetic field

$\mathbf{B}$ the equation $\nabla \cdot \mathbf{B} = 0$ naturally leads to the introduction of a magnetic potential $\mathbf{A}$ defined by the constituting relation

$$\mathbf{B} = \nabla \times \mathbf{A}, \tag{2.58}$$

since the divergence of any curl is always zero and thus automatically satisfies the relevant Maxwell equation no matter the choice of $\mathbf{A}$ as long as all of the expressions remain well-defined. The introduction of this magnetic potential raises the question of how one can relate it to the electric field. Maxwell's equations straightforwardly imply that using such a magnetic potential, one needs to introduce a scalar electric potential ϕ as follows:

$$\mathbf{E} = -\nabla\phi - \frac{\partial \mathbf{A}}{\partial t}. \tag{2.59}$$

This equation in fact defines the electric potential ϕ. Owing to the mathematical structure of Maxwell's equations one has a certain amount gauge freedom in the selection of $\mathbf{A}$ and ϕ which can prove very useful in the simplification of various equations when used well. Common gauge choices in physics involve the Coulomb gauge which demands that $\nabla \cdot \mathbf{A} = 0$ or the Lorenz gauge which demands that $\nabla \cdot \mathbf{A} = -\frac{1}{c^2}\frac{\partial \phi}{\partial t}$. The abstract form of the gauge freedom allows any transformation of ϕ and $\mathbf{A}$ which satisfy:

$$\bar{\phi} \to \phi - \frac{\partial \lambda}{\partial t}, \tag{2.60}$$

$$\bar{\mathbf{A}} \to \mathbf{A} + \nabla\lambda, \tag{2.61}$$

for an arbitrary function of space and time $\lambda(t, \mathbf{x})$ which is twice differentiable in all coordinates. The Coulomb and Lorenz gauge can be shown to indeed be of this form. Naturally we can now translate Maxwell's equations into this electromagnetic potential formalism, yielding:

$$\nabla^2\phi + \frac{\partial}{\partial t}\left(\nabla \cdot \mathbf{A}\right) = 0, \tag{2.62}$$

$$\left(\nabla^2\mathbf{A} - \frac{1}{c^2}\frac{\partial^2 \mathbf{A}}{\partial t^2}\right) - \nabla\left(\nabla \cdot \mathbf{A} + \frac{1}{c^2}\frac{\partial \phi}{\partial t}\right) = 0. \tag{2.63}$$

However, the above equations only hold in the vacuum. The full potential-based Maxwell equations are:

$$\nabla^2\varphi + \frac{\partial}{\partial t}\left(\nabla \cdot \mathbf{A}\right) = -\frac{\rho}{\epsilon_0}, \tag{2.64}$$

$$\left(\nabla^2\mathbf{A} - \frac{1}{c^2}\frac{\partial^2 \mathbf{A}}{\partial t^2}\right) - \nabla\left(\nabla \cdot \mathbf{A} + \frac{1}{c^2}\frac{\partial \phi}{\partial t}\right) = -\mu_0\mathbf{J}. \tag{2.65}$$

The Lorentz force can also be written in terms of the potentials as follows:

$$\mathbf{F} = q\left[-\nabla\phi - \frac{\partial \mathbf{A}}{\partial t} + \mathbf{v} \times (\nabla \times \mathbf{A})\right] \tag{2.66}$$

Consequently, the electromagnetic potential formalism can fully substitute the previously introduced electromagnetic formalism while providing gauge freedom to simplify many problems.

2.3.4 The Lagrangian and Hamiltonian formalisms

In order to be able to work within the fields of modern physics, a good grasp of the Lagrangian formalism is required. For the sake of completion we give a very brief overview of it here, a much more extensive treatment can be found in all textbooks covering classical mechanics at a rigorous mathematical level. A specific treatment for the case of electromagnetism can be found in [17].
The so-called Lagrangian density function $\mathcal{L}$ contains all the relevant information about a given physical theory and thus constitutes a first principle approach. The specific Lagrangian density that is appropriate for a certain framework can not be analytically derived and is thus generally only constructed once one already has an idea of what it should describe.
Given a certain Lagrangian $\mathcal{L}$, which depends on a given number of so-called fields φ_i and their derivatives, one defines the so-called *action* S as:

$$\mathcal{S}[\varphi] := \int \mathcal{L} \mathrm{d}^n x. \tag{2.67}$$

The equations of motion for the given fields are then derived by utilizing the so-called Hamiltonian principle of least action:

$$\frac{\delta \mathcal{S}}{\delta \varphi_i} = 0, \tag{2.68}$$

which leads to the Euler-Lagrange Equations:

$$\partial_\mu \left(\frac{\partial \mathcal{L}}{\partial(\partial_\mu \varphi_i)} \right) - \frac{\partial \mathcal{L}}{\partial \varphi_i} = 0. \tag{2.69}$$

The treatment of physical theories in this framework is generally referred to as the Lagrangian formalism. There exists a generally equivalent formulation of physical theories called Hamiltonian formalism which relies on the use of a function H called the Hamiltonian (this is the same Hamiltonian function discussed in section 2.2.1). The Hamiltonian of a given theory can be obtained directly from the Lagrangian via a method called the *Legendre transformation*, which for the case of classical mechanics is given by:

$$H = \dot{\mathbf{x}} \cdot \mathbf{p} - \mathcal{L}. \tag{2.70}$$

A suitable Lagrangian density function for the theory of classical mechanics with electromagnetism sketched in section 2.3.3 is (compare [17]):

$$\mathcal{L} = \frac{1}{2} m \dot{\mathbf{x}}^2 + \frac{q}{c} \left(\dot{\mathbf{x}} \cdot \mathbf{A} \right) - q\phi. \tag{2.71}$$

That this is indeed a suitable Lagrangian can easily be verified by plugging it into the Euler-Lagrange equations and computing the equations of motion from it and comparing the result to the theory of classical electromagnetism discussed in section 2.3.3. From this Lagrangian we can derive the so-called *generalized momenta* by taking the following derivative

$$p_i := \frac{\partial \mathcal{L}}{\partial \dot{x}_i} = m\dot{x}_i + \frac{q}{c} A_i, \tag{2.72}$$

which of course translates into vector notation as

$$\mathbf{p} = m\dot{\mathbf{x}} + \frac{q}{c}\mathbf{A}. \tag{2.73}$$

Rewriting this as an equation for $\dot{\mathbf{x}}$ gives

$$\dot{\mathbf{x}} = \frac{1}{m}\left(\mathbf{p} - \frac{q}{c}\mathbf{A}\right). \tag{2.74}$$

Since the Hamiltonian is easier to work with when it comes to the Schrödinger Equation, we use this information of $\dot{\mathbf{x}}$ to perform the Legendre transform as in Equation 2.70 to obtain

$$H = \frac{1}{2m}\left(\mathbf{p} - \frac{q}{c}\mathbf{A}\right)^2 + q\phi. \tag{2.75}$$

This is the Hamiltonian function of classical electromagnetism in the potential formalism.

2.4 Motivation of the Pauli equation

The goal of this section is to motivate the following equation as an appropriate model for semi-relativistic quantum objects moving through an electromagnetic field:

$$\left[\frac{1}{2m}\left(\sigma \cdot \left(-i\hbar\nabla - \frac{q}{c}\mathbf{A}\right)\right)^2 + q\phi\right]\psi = i\hbar\frac{\partial}{\partial t}\psi. \tag{2.76}$$

This equation is called the *Pauli equation*. As in the section motivating the Schrödinger Equation, one should keep in mind that equations of physics are generally not derived in a rigorous mathematical sense but rather motivated or 'modeled'. Nevertheless, given a particular set of initial assumptions the motivation can be seen as a derivation from that specific set of premises. This also means that there may and in fact should be mutually complementing ways to arrive at the same equations from different physical starting points. We will thus be arguing for the Pauli equation as the sensible equation modeling the above-stated phenomena in two different ways: First, we will show for a bottom-up approach which uses experimental information to modify a naive magnetic Schrödinger equation with a spin term to arrive at the Pauli equation and then we will show that in a top-down approach one can also arrive at the Pauli equation as the semi-classical limit of the fully relativistic Dirac equation discussed above.

2.4.1 The magnetic Schrödinger equation

One of the premises in any 'derivation' of the Pauli equation is that the general form of the Schrödinger Equation seen in Equation (2.9) holds. It may be useful for present purposes to restate said general equation here:

$$\hat{H}\psi = i\hbar\frac{\partial}{\partial t}\psi. \tag{2.77}$$

The starting point is thus the same as for many physics problems: the search for the proper Hamiltonian for the system we intend to model. Since the goal is to obtain an equation of motion for quantum objects in an electromagnetic field, the

natural place for a first attempt might be to revisit the classical understanding of electromagnetism and see if it can be coupled to the Schrödinger equation. In classical mechanics, the Lorentz force describes how a classical point particle of charge q moves under the influence of both an electric field $\mathbf{E}$ and a magnetic field $\mathbf{B}$, respectively instantiated by their potentials ϕ and $\mathbf{A}$ (see section 2.3). Let us now also restate the corresponding *classical* Hamiltonian found in Equation (2.75):

$$H(\mathbf{x}, \mathbf{p}, t) = \frac{1}{2m}\left(\mathbf{p} - \frac{q}{c}\mathbf{A}(\mathbf{x}, t)\right)^2 + q\phi(\mathbf{x}, t). \tag{2.78}$$

The next step is a direct attempt to translate this Hamiltonian into the language of quantum mechanics. We recall the canonical identity $\mathbf{p} \to -i\hbar\nabla$ and we rewrite the potentials to correspond to operators $\mathbf{A} \to \hat{A}$ and $\phi \to \hat{\phi}$ but for these operators we make the stronger assumptions $\mathbf{A} = \hat{A}$ and $\phi = \hat{\phi}$ (this corresponds to assuming that the electromagnetic field itself is not actually quantized, an approach that can only ever be approximately correct). This leaves us with almost exactly what we started with but now in an approximately quantum mechanical form:

$$\hat{H}(\hat{x}, \hat{p}, t) = \frac{1}{2m}\left(-i\hbar\nabla - \frac{q}{c}\mathbf{A}(\hat{x}, t)\right)^2 + q\phi(\hat{x}, t). \tag{2.79}$$

Expanding the quadratic term yields:

$$\hat{H}(\hat{x}, \hat{p}, t) = -\frac{\hbar^2}{2m}\nabla^2 + \frac{i\hbar q}{2mc}\left(\mathbf{A}\cdot\nabla + \nabla\cdot\mathbf{A}\right) + \frac{q^2}{2mc^2}\mathbf{A}^2 + q\phi. \tag{2.80}$$

which leads to the following, so-called *magnetic Schrödinger equation* which is a first candidate for a quantum theory that incorporates the electromagnetic field:

$$\left[-\frac{\hbar^2}{2m}\nabla^2 + \frac{i\hbar q}{2mc}\left(\mathbf{A}\cdot\nabla + \nabla\cdot\mathbf{A}\right) + \frac{q^2}{2mc^2}\mathbf{A}^2 + q\phi\right]\psi = i\hbar\frac{\partial}{\partial t}\psi, \tag{2.81}$$

which we could also more compactly write as

$$\left[\frac{1}{2m}\left(-i\hbar\nabla - \frac{q}{c}\mathbf{A}\right)^2 + q\phi\right]\psi = i\hbar\frac{\partial}{\partial t}\psi. \tag{2.82}$$

On top of this, we can utilize the aforementioned gauge freedom of electromagnetism to set $\nabla\cdot\mathbf{A} = 0$. This gauge choice is called Coulomb Gauge and eliminates a term in the equation, which leads to the following magnetic Schrödinger Equation:

$$\left[-\frac{\hbar^2}{2m}\nabla^2 + \frac{i\hbar q}{mc}\mathbf{A}\cdot\nabla + \frac{q^2}{2mc^2}\mathbf{A}^2 + q\phi\right]\psi = i\hbar\frac{\partial}{\partial t}\psi. \tag{2.83}$$

Note that the factor $\frac{1}{2}$ drops from the $\mathbf{A}\cdot\nabla$ term due to the product rule having to be applied to $\nabla\cdot(\mathbf{A}\psi)$. We observe that as one should expect of a sensible physical theory of electromagnetism, removing the electromagnetic fields by letting the relevant terms vanish leaves us with the original Schrödinger Equation found in Equation (2.8).

This motivation has led to a first candidate equation for electromagnetic quantum mechanics - the magnetic Schrödinger equation - which unfortunately does *not* experimentally agree with the observed behavior of electrons in an electromagnetic field.

The reason is that we have thus far completely ignored quantum mechanical *spin*, a property of quantum objects that intimately couples to their electromagnetic properties that was experimentally established in the Stern-Gerlach experiment and has had countless further experimental observations since. It is the goal of the following sections to rectify this omission, leading to the formulation of the Pauli equation which shares many similarities but also striking differences to the magnetic Schrödinger equation.

2.4.2 Bottom-up: Adding spin

The intrinsic property of particles called spin which couples to the magnetic field is responsible for the empirical inadequacy of the magnetic Schrödinger equation even when the process we aim to describe would fit well within the Newtonian regime, i.e. when the expected errors from ignoring special relativity are negligible. Spin was already mentioned and introduced in sections 2.1 and 2.2.2 and can generally be thought of as sort of an intrinsic additional angular momentum term inherent to all quantum objects. Experimental results such as those of the Stern-Gerlach experiment confirm that particles, moving through an electromagnetic field have angular momentum terms that are not accounted for by the magnetic Schrödinger Equation motivated in the previous section.
In order to introduce spin into our formalism and in light of what was discussed about the mathematics of spin in section 2.2.2, we move from a scalar wavefunction ψ to a 2-spinor u to incorporate the possibilities of scalar spin-up u_1 and spin-down u_2 states. Recall that the total spin operator is given by:

$$\hat{S}^2 = \hat{S}_x^2 + \hat{S}_y^2 + \hat{S}_z^2, \tag{2.84}$$

where $\hat{S}_{x_i} = \frac{\hbar}{2}\sigma_i$. The addition of a coupling term between spin and the magnetic field with the introduction of a vector-like object $\sigma = (\hat{\sigma}_1, \hat{\sigma}_2, \hat{\sigma}_3)$ and the move to the 2-spinor yields the Pauli Equation:

$$\left[-\frac{\hbar^2}{2m}\nabla^2 + \frac{i\hbar q}{2mc}\left(\mathbf{A}\cdot\nabla + \nabla\cdot\mathbf{A}\right) - \frac{\hbar q}{2mc}\sigma\cdot(\nabla\times\mathbf{A}) + q\phi(\hat{x},t)\right]u = i\hbar\frac{\partial}{\partial t}u, \tag{2.85}$$

or more compactly and using $\mathbf{B} = \nabla\times\mathbf{A}$

$$\left[\frac{1}{2m}\left(-i\hbar\nabla - \frac{q}{c}\mathbf{A}\right)^2 - \frac{\hbar q}{2mc}\sigma\cdot\mathbf{B} + q\phi\right]u = i\hbar\frac{\partial}{\partial t}u. \tag{2.86}$$

where a 2×2 identity matrix is implied to be multiplied with the scalar potential term. In fact, an attentive reader will find that many objects in this equation must have implicit redefinitions attached to them in order for this equation to still be well-defined. Since u is now obligatorily a 2-spinor with two components it is no longer obvious how to apply the operator terms involving gradients to it. For the sake of remaining explicit and avoiding notational obfuscation we state how all of these are

defined here:

$$\mathbf{A} = \begin{pmatrix} A_1 \\ A_2 \\ A_3 \end{pmatrix}, \quad u = \begin{pmatrix} u_1 \\ u_2 \end{pmatrix},$$

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

$$\nabla u = \nabla \begin{pmatrix} u_1 \\ u_2 \end{pmatrix} = \begin{pmatrix} \partial_x u_1 & \partial_y u_1 & \partial_z u_1 \\ \partial_x u_2 & \partial_y u_2 & \partial_z u_2 \end{pmatrix},$$

$$\nabla^2 u = \begin{pmatrix} \partial_x^2 u_1 + \partial_y^2 u_1 + \partial_z^2 u_1 \\ \partial_x^2 u_2 + \partial_y^2 u_2 + \partial_z^2 u_2 \end{pmatrix} = \begin{pmatrix} \nabla^2 u_1 \\ \nabla^2 u_2 \end{pmatrix},$$

$$(\mathbf{A} \cdot \nabla) u = \begin{pmatrix} \partial_x u_1 & \partial_y u_1 & \partial_z u_1 \\ \partial_x u_2 & \partial_y u_2 & \partial_z u_2 \end{pmatrix} \begin{pmatrix} A_1 \\ A_2 \\ A_3 \end{pmatrix} = \begin{pmatrix} A_1 \partial_x u_1 + A_2 \partial_y u_1 + A_3 \partial_z u_1 \\ A_1 \partial_x u_2 + A_2 \partial_y u_2 + A_3 \partial_z u_2 \end{pmatrix}.$$

The spin-coupling term $-\frac{\hbar q}{2mc}\sigma \cdot \mathbf{B}$ which we added to the magnetic Schrödinger equation is sometimes referred to as the Stern-Gerlach term in light of its experimental history and as it was introduced here is ad-hoc to match experimental deviations from the magnetic Schrödinger equation - it is the most simple way in which spin can mathematically be coupled to the magnetic field $\mathbf{B}$. The resulting equation is called the *Pauli equation*. This equation can then be written in a slightly more elegant and compact (but arguably less transparent) form by using the so-called Pauli vector identity:

$$(\sigma \cdot a)(\sigma \cdot b) = a \cdot b + i\sigma(a \times b). \tag{2.87}$$

which yields the Pauli Equation in the following more commonly stated form:

$$\left[\frac{1}{2m}\left(\sigma \cdot \left(-i\hbar\nabla - \frac{q}{c}\mathbf{A}\right)\right)^2 + q\phi\right] u = i\hbar\frac{\partial}{\partial t}u. \tag{2.88}$$

We will go into a lot more detail on how equation 2.86 and equation 2.88 are related and present the explicit derivations in section 3.2 in preparation of the numerical treatment of the Pauli equation. Just as in the case of the magnetic Schrödinger equation, the Pauli equation retains all of the gauge freedom of electromagnetism and the choice of the Coulomb gauge $\nabla \cdot \mathbf{A} = 0$ in particular simplifies the equation significantly.

2.4.3 Top-down: The semi-relativistic limit of the Dirac equation

Since both the Dirac equation and the Pauli Equation describe spin-$\frac{1}{2}$ particles, the Dirac Equation is expected to reduce to the Pauli equation in the non-relativistic limit and this is indeed the case as we will sketch in this section. For a more in-depth treatment of this semi-relativistic limit, see for example [19, 20] and [21]. We first re-state the Dirac Equation in one of its more elegant forms, where natural units

are used (meaning $c = \hbar = 1$ all throughout this section; see [22] for an in-depth discussion of the Dirac equation and [23] for its original derivation):

$$(\gamma^\mu p_\mu + m)\psi = 0, \tag{2.89}$$

where γ^μ are the so-called gamma matrices

$$\gamma^0 = \begin{pmatrix} \mathbb{1} & 0 \\ 0 & -\mathbb{1} \end{pmatrix}, \quad \gamma^i = \begin{pmatrix} 0 & \sigma^i \\ -\sigma^i & 0 \end{pmatrix} . \tag{2.90}$$

and ψ is a 4 dimensional Dirac spinor (*not* a 4-vector):

$$\psi = \begin{pmatrix} \psi_1 \\ \psi_2 \\ \psi_3 \\ \psi_4 \end{pmatrix} . \tag{2.91}$$

Recalling that $p_\mu = (E, -p_x, -p_y, -p_z)$ we note that we can write $\gamma^\mu p_\mu$ as:

$$\gamma^\mu p_\mu = \gamma^0 p_0 + \gamma^i p_i = \begin{pmatrix} p_0 & 0 \\ 0 & -p_0 \end{pmatrix} + \begin{pmatrix} 0 & \sigma^i p_i \\ -\sigma^i p_i & 0 \end{pmatrix} = \begin{pmatrix} E & -\sigma \cdot \mathbf{p} \\ \sigma \cdot \mathbf{p} & -E \end{pmatrix} .$$

The Dirac Equation in (2.89) does not contain a term for the electromagnetic field, but this can be fixed by a method known as minimal coupling, where we replace

$$p^\mu \to p^\mu - qA^\mu. \tag{2.92}$$

This can be motivated by taking a close look at the Hamiltonian in (2.75). Using this substitution, the Dirac equation takes the following form:

$$\left(\gamma^\mu \left(p_\mu - qA_\mu\right) - m\right) \psi = 0, \tag{2.93}$$

which, when plugging in the gamma matrices like demonstrated above gives:

$$\begin{pmatrix} (m - E + q\phi) & \sigma \cdot (\mathbf{p} - q\mathbf{A}) \\ -\sigma \cdot (\mathbf{p} - q\mathbf{A}) & (m + E - q\phi) \end{pmatrix} \begin{pmatrix} \psi_+ \\ \psi_- \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix} . \tag{2.94}$$

The notation ψ_+ and ψ_- simply denotes a decomposition of the original 4-spinor into two 2-spinors. This system gives us two coupled equations in ψ_+ and ψ_-. In the non-relativistic limit, we want the electron energy to approach its rest mass and the relativistic gamma factor in the momentum to become 1. Thus, we have the following rules:

$$E - q\phi \to m \tag{2.95}$$

$$\mathbf{p} \to m\mathbf{v} \tag{2.96}$$

Now we examine the coupled equations one by one:

$$(E - q\phi)\psi_+ - \sigma \cdot (\mathbf{p} - q\mathbf{A})\, \psi_- = m\psi_+ \tag{2.97}$$

$$(E - q\phi)\psi_- - \sigma \cdot (\mathbf{p} - q\mathbf{A})\, \psi_+ = -m\psi_- \tag{2.98}$$

Plugging the above approximations into these equations first of all yields:

$$m\psi_- - \sigma \cdot (\mathbf{p} - q\mathbf{A})\,\psi_+ = -m\psi_- \tag{2.99}$$

$$\sigma \cdot (\mathbf{p} - q\mathbf{A})\,\psi_+ = 2m\psi_- \tag{2.100}$$

$$\frac{1}{2m}\sigma \cdot (\mathbf{p} - q\mathbf{A})\,\psi_+ = \psi_- \tag{2.101}$$

So in the non-relativistic limit, we get

$$\psi_- \to \frac{1}{2m}\sigma \cdot (\mathbf{p} - q\mathbf{A})\,\psi_+ \tag{2.102}$$

Plugging this relation into the first of the two coupled equations above, we obtain:

$$(E - q\phi)\,\psi_+ - \sigma \cdot (\mathbf{p} - q\mathbf{A})\left(\frac{1}{2m}\sigma \cdot (\mathbf{p} - q\mathbf{A})\,\psi_+\right) = m\psi_+ \tag{2.103}$$

$$(E - m)\psi_+ = q\phi\psi_+ + \frac{(\sigma \cdot (\mathbf{p} - q\mathbf{A}))^2}{2m}\psi_+ \tag{2.104}$$

The term $(E - m)$ is the particles' energy reduced by its rest mass, which is just what the classical energy term is. In quantum mechanics, the appropriate operator form for the energy is $i\partial_t$. Substituting this in, we get:

$$i\frac{\partial}{\partial t}\psi_+ = q\phi\psi_+ + \frac{(\sigma \cdot (\mathbf{p} - q\mathbf{A}))^2}{2m}\psi_+ \tag{2.105}$$

which is the Pauli equation. Thus, the Dirac equation's top two entries satisfy the Pauli Equation in the non-relativistic limit as would be expected of sensible physics. An equivalent derivation can easily be made for the lower two entries, i.e. ψ_-, but we omit this since the objects of interest in quantum electromagnetic settings are generally electrons and not positrons.

3 Preparing the Pauli equation for numerical approaches

3.1 Nondimensionalization

When treating differential equations numerically one often requires them to be in a particular dimensionless form in order to elegantly implement them on a computer. The process of translating a differential equation into its dimensionless form by means of various variable transforms is called "scaling" or "nondimensionalization". For a good general treatment of such subject matters, see for example [24] and for a more in-depth treatment see for example [25].

3.1.1 Scaling the generic Schrödinger equation

In this section we will present one quite canonical way of scaling the generic as well as magnetic Schrödinger equation and an analogous extension of this scaling will then be used in the following section to also scale the Pauli equation. No claim is made with regards to the compatibility of this particular scaling method with asymptotic analysis methods but finding such a scaling might be a worthwhile endeavor in a future project by itself.
To find one possible scaling to the Schrödinger equation which can naturally be extended to the Pauli equation, we begin with the Schrödinger equation in canonical form:

$$\left[-\frac{\hbar^2}{2m}\nabla^2 + V\right]\psi = i\hbar\frac{\partial\psi}{\partial t}. \tag{3.1}$$

Using some length and time scale inherent to the system labeled L and T we transform the coordinates as follows:

$$\bar{x} = \frac{x}{L_0}, \quad \bar{t} = \frac{t}{T_0}. \tag{3.2}$$

In the particular case of a numerical implementation one could use the size of the spatial box and the duration of time or the stepsize in space and time respectively for L_0 and T_0. Furthermore, we introduce a reference value V_0 which transforms the potential V to be dimensionless:

$$\bar{V} = \frac{V}{V_0}. \tag{3.3}$$

The nature of this V_0 is in need of further specification which we will deal with momentarily. First, note that using these three definitions to transform the Schrödinger equation we obtain:

$$\left[-\frac{\hbar^2}{mL_0^2V_0}\bar{\nabla}^2 + \bar{V}\right]\bar{\psi} = i\frac{\hbar}{T_0V_0}\frac{\partial\bar{\psi}}{\partial\bar{t}}. \tag{3.4}$$

To allow consistency of the addition in the Schrödinger equation it is a given that the dimensions of V_0 must equal those of the kinetic term $-\frac{\hbar^2}{2m}\nabla^2$. The SI units of the reduced Planck length $\hbar$ are $\frac{kgm^2}{s}$ and its general dimensions are $\frac{ML^2}{T}$. This means by extension that the dimensions of V_0 as well as the kinetic term are $\frac{M^2L^4}{MT^2L^2} = \frac{ML^2}{T^2}$.

There are multiple ways to realize this dimensionality for V_0 with potentially very different asymptotic properties. For example, the choice

$$V_0 = \frac{\hbar}{T_0} \tag{3.5}$$

has the correct dimensions for V_0 and thus leads to the dimensionless equation

$$\left[-\epsilon\bar{\nabla}^2 + \bar{V}\right]\bar{\psi} = i\frac{\partial\bar{\psi}}{\partial\bar{t}}. \tag{3.6}$$

where

$$\epsilon = \frac{\hbar T_0}{L_0^2}. \tag{3.7}$$

However as noted before there are many other choices that could be made for V_0 and we will not be using this particular option. Instead, we will utilize the following value based on the intrinsic length and distance scales introduced above:

$$V_0 = \frac{M_0 L_0^2}{T_0^2}, \tag{3.8}$$

where the reference mass M_0 is chosen to be the one from the kinetic term of the original equation. This yields the scaled Schrödinger equation as it is typically found in the literature:

$$\left[-\epsilon^2\bar{\nabla}^2 + \bar{V}\right]\bar{\psi} = i\epsilon\frac{\partial\bar{\psi}}{\partial\bar{t}}, \tag{3.9}$$

where the scaling parameter is now

$$\epsilon = \frac{\hbar T_0}{M_0 L_0^2}. \tag{3.10}$$

What does this mean for the physical meaning of the ϵ parameter? For one, if a limit is taken with regards to ϵ, such as for example $\epsilon \to 0$, then since the parameter only contains reference quantities and $\hbar$ it would physically correspond to taking the same limit with regards to $\hbar$. This means that $\epsilon \to 0$ physically corresponds to $\hbar \to 0$, i.e. the classical limit. Since V_0 is made up entirely of reference quantities nothing physically relevant is lost in the scaled equation when considering its ϵ limits - this will not be the case for the magnetic Schrödinger and Pauli equation.

3.1.2 Scaling the magnetic Schrödinger equation

To extend the scaling in the previous section to the magnetic Schrödinger equation in particular we begin with the magnetic Schrödinger equation in the following form:

$$\left[-\frac{\hbar^2}{2m}\nabla^2 + \frac{i\hbar q}{mc}\mathbf{A}\cdot\nabla + \frac{q^2}{2mc^2}\mathbf{A}^2 + q\phi\right]\psi = i\hbar\frac{\partial}{\partial t}\psi. \tag{3.11}$$

This is the form that already has eliminated one term using the Coulomb gauge $\nabla\cdot\mathbf{A}$ for the sake of visual simplicity but as the constant in front of that term is the same as the one in front of the $\mathbf{A}\cdot\nabla$ term the scaling works equivalently for the case with full gauge freedom. The role of the generic potential V is now being played by three separate terms containing the magnetic and electric potentials.

As before, the first step is to transform the equation to depend on $\bar{x} = \frac{x}{L_0}$ and $\bar{t} = \frac{t}{T_0}$, yielding:

$$\left[-\frac{\hbar^2}{2mL_0^2}\bar{\nabla}^2 + \frac{i\hbar q}{mcL_0}\mathbf{A}\cdot\bar{\nabla} + \frac{q^2}{2mc^2}\mathbf{A}^2 + q\phi\right]\bar{\psi} = i\frac{\hbar}{T_0}\frac{\partial}{\partial\bar{t}}\bar{\psi}. \tag{3.12}$$

At this stage we need to consider the intrinsic dimensionality of the potentials $\mathbf{A}$ and ϕ. We state them here (in addition to their base SI unit form):

$$[\mathbf{A}] = \frac{ML}{T^2I} \rightarrow^{SI} \frac{kgm}{As^2}, \tag{3.13}$$

$$[\phi] = \frac{ML^2}{T^3I} \rightarrow^{SI} \frac{kgm^2}{As^3}. \tag{3.14}$$

Since q in the magnetic Schrödinger equation reflects a constant charge, its dimensions are TI corresponding to the SI base units Coulomb $C = As$. This means that we could for example use the system-intrinsic value q_0T_0 as our scaling factor for the dimension of electric current I. As before, we introduce as of now generic scaling quantities for the potentials:

$$\bar{\mathbf{A}} = \frac{\mathbf{A}}{A_0}, \quad \bar{\phi} = \frac{\phi}{\phi_0}, \tag{3.15}$$

which will be used to determine a sensible scaling option. Note that A_0 is a scalar quantity, not a vector. Applying this transformation and leads to the following version of the magnetic Schrödinger equation:

$$\left[-\frac{\hbar^2}{2M_0L_0^2\phi_0}\bar{\nabla}^2 + \frac{iA_0\hbar q_0}{M_0cL_0\phi_0}\bar{\mathbf{A}}\cdot\bar{\nabla} + \frac{A_0^2q_0^2}{2M_0c^2\phi_0}\bar{\mathbf{A}}^2 + q_0\bar{\phi}\right]\bar{\psi} = i\frac{\hbar}{T_0\phi_0}\frac{\partial}{\partial\bar{t}}\bar{\psi}. \tag{3.16}$$

Once again there are a multitude of possibilities for consistent choices of A_0 and ϕ_0. The one which produces an equation which appears as the most natural extension of the scaling shown for the generic equation and the one often used in the literature will be obtained from this approach by setting

$$A_0 = \frac{L_0M_0c}{T_0q_0}, \tag{3.17}$$

$$\phi_0 = \frac{L_0^2M_0}{T_0^2q_0}, \tag{3.18}$$

which results in the following scaled equation (after cancellation and division by q_0):

$$\left[-\frac{\hbar^2T_0^2}{2M_0^2L_0^4}\bar{\nabla}^2 + \frac{i\hbar T_0}{M_0L_0^2}\bar{\mathbf{A}}\cdot\bar{\nabla} + \frac{1}{2}\bar{\mathbf{A}}^2 + \bar{\phi}\right]\bar{\psi} = i\frac{\hbar T_0}{M_0L_0^2}\frac{\partial}{\partial\bar{t}}\bar{\psi}. \tag{3.19}$$

Introducing the scaling parameter

$$\epsilon = \frac{\hbar T_0}{M_0L_0^2}, \tag{3.20}$$

this can be cast in the following from:

$$\left[-\frac{\epsilon^2}{2}\bar{\nabla}^2 + i\epsilon\bar{\mathbf{A}}\cdot\bar{\nabla} + \frac{1}{2}\bar{\mathbf{A}}^2 + \bar{\phi}\right]\bar{\psi} = i\epsilon\frac{\partial}{\partial\bar{t}}\bar{\psi}. \tag{3.21}$$

Note how this and the previously discussed scaling for the generic Schrödinger equation have the same scaling parameter, marking that this scaling is a natural extension of the former to the magnetic Schrödinger equation case. In the coming section we will show that a corresponding scaling parameter also works for the Pauli equation.

As before for the generic Schrödinger equation we can ask what physical meaning can be assigned to this scaling and the corresponding limits. At first glance it might appear to be the same as for the generic Schrödinger equation, as indeed taking $\epsilon \to 0$ once again corresponds to $\hbar \to 0$. The crucial difference here however comes from the inclusion of the c velocity in the scaling of the magnetic vector potential: Since A_0 effectively scales c out of the magnetic Schrödinger equation entirely, this new scaled magnetic Schrödinger equation is not capable of performing the $c \to \infty$ limit, which is an important limit that corresponds to moving from relativistic to non-relativistic physics. This can partially be remedied by noting that the $c \to \infty$ limit in this case would thus correspond to $\bar{\mathbf{A}} = 0$ but nevertheless it is of note that the equation as-is in this scaled formulation more naturally lends itself to the non-QM limit $\hbar \to 0$ via $\epsilon \to 0$ rather than the non-relativistic limit.

3.1.3 Scaling the Pauli equation

The scaling method for the magnetic Schrödinger equation discussed in the previous section can be extended to the full Pauli equation in a natural way. We begin with the Pauli equation in the following form:

$$\left[\frac{1}{2M_0}\left(\sigma \cdot \left(-i\hbar\nabla - \frac{q_0}{c}\mathbf{A}\right)\right)^2 + q_0\phi\right] u = i\hbar\frac{\partial}{\partial t}u. \tag{3.22}$$

and apply the same nondimensionalization as before by setting

$$\bar{x} = \frac{x}{L_0}, \quad \bar{t} = \frac{t}{T_0}, \tag{3.23}$$

$$\bar{\mathbf{A}} = \frac{A}{A_0}, \quad \bar{\phi} = \frac{\phi}{\phi_0}, \tag{3.24}$$

which in a first step yields:

$$\left[\frac{1}{2}\left(\sigma \cdot \left(-i\frac{\hbar}{L_0\sqrt{M_0\phi_0}}\bar{\nabla} - \frac{q_0 A_0}{c\sqrt{M_0\phi_0}}\bar{\mathbf{A}}\right)\right)^2 + q_0\bar{\phi}\right] \bar{u} = i\frac{\hbar}{T_0\phi_0}\frac{\partial}{\partial\bar{t}}\bar{u}. \tag{3.25}$$

Once again there are a multitude of options to use here to scale the Pauli equation but pursuing the approach outlined in the previous sections and aiming to obtain a form of the equation that is consistent with the form of the Schrödinger equation often present in literature, we again choose

$$A_0 = \frac{L_0 M_0 c}{T_0 q_0}, \tag{3.26}$$

$$\phi_0 = \frac{L_0^2 M_0}{T_0^2 q_0}, \tag{3.27}$$

which yields

$$\left[\frac{1}{2}\left(\sigma \cdot \left(-i\epsilon\bar{\nabla} - \bar{\mathbf{A}}\right)\right)^2 + \bar{\phi}\right] \bar{u} = i\epsilon\frac{\partial}{\partial\bar{t}}\bar{u}, \tag{3.28}$$

where the scaling parameter ϵ is defined by

$$\epsilon = \frac{\hbar T_0}{M_0 L_0^2}. \tag{3.29}$$

Regarding the physical meaning of this scaling, the situation is essentially analogous to the magnetic Schrödinger equation case. The $\epsilon \to 0$ limit simply corresponds to $\hbar \to 0$ and the speed of light c is scaled out of the equation via its inclusion in the scaling of the magnetic vector potential. The statements made for the magnetic Schrödinger equation in this regard hold for this scaling of the Pauli equation scaling as well.

3.2 Rewriting the Pauli equation to remove spin from the kinetic term

The scaled Pauli equation derived in the previous section, i.e.

$$\left[\frac{1}{2}\left(\sigma \cdot (p - \mathbf{A})\right)^2 + \phi\right] u = i\epsilon\partial_t u, \tag{3.30}$$

is a nice and compact way to write the Pauli equation but the very deep involvement of the σ term is an unnecessary complication for numerical implementations of the equation. Fortunately there are ways to remove the σ term from the kinetic part of the equation entirely, not only making the $\mathbf{A} = 0$ limit to the Schrödinger equation much more clear but also providing a more approachable Pauli equation. This section will give a step-by-step derivation of how to rewrite the Pauli equation in that way. The natural way to begin such an endeavor is to expand the square and distribute the Pauli matrix vector σ across the various terms. This yields:

$$\left[\frac{1}{2}\left((\sigma \cdot p)^2 - (\sigma \cdot p)(\sigma \cdot \mathbf{A}) - (\sigma \cdot \mathbf{A})(\sigma \cdot p) + (\sigma \cdot \mathbf{A}^2)\right) + \phi\right] u = i\epsilon\partial_t u. \tag{3.31}$$

Before we can further simplify this equation, we need two secondary results. The first is a multiplicative identity that is known to hold for σ:

$$(\sigma \cdot a)(\sigma \cdot b) = a \cdot b + i\sigma(a \times b). \tag{3.32}$$

This is a well-known result sometimes known as the Pauli vector identity.
The second result we need to simplify the above equation is significantly more subtle and related to the operator and wave function images in quantum mechanics. Not adequately accounting for the switch between the operator image and the wave function image in this step can lead to a wrong result, so it is crucial to do this carefully and correctly. The subtlety involves the often claimed equivalence between p and $-i\hbar\nabla$ or in this case $-i\epsilon\nabla$. However, it is very important to realize that these are not 'equal' in the literal mathematical sense but that one goes over into the other when moving from the operator image to the wave function formalism.
If one were to be careless, one might use the previous multiplicative identity to obtain terms which contain $(p \times \mathbf{A})$ and then claim that this equals $(-i\epsilon\nabla \times \mathbf{A}) = -i\epsilon\mathbf{B}$. This is *incorrect*! In the notational conventions of quantum mechanics, one always needs to think of operators acting on states and wave functions, they cannot be

treated in such a standalone fashion. The correct interpretation of $(p \times \mathbf{A})$ goes as follows, using Einstein summation convention (sums are implied over repeated up and down indices) to simplify the calculation. First we recall that for any two vectors $\mathbf{v}$ and $\mathbf{w}$

$$(\mathbf{v} \times \mathbf{w})_i = \epsilon_{ijk} v^j w^k, \tag{3.33}$$

where ϵ_{ijk} is the fully anti-symmetric Levi-Civita symbol and we write $\hbar$ to avoid confusion with ϵ_{ijk}. Then, we look at the following expression acting on the wave function u:

$$(p \times \mathbf{A})_i u = -i\hbar \epsilon_{ijk} \partial^j (A^k u), \tag{3.34}$$

which using the product rule yields

$$-i\hbar \epsilon_{ijk} \partial^j (A^k u) = -i\hbar \epsilon_{ijk} (u \partial^j A^k + A^k \partial^j u). \tag{3.35}$$

We rewrite this equation by making use of the anti-symmetry of the Levi-Civita symbol $\epsilon_{ijk} = -\epsilon_{ikj}$ to obtain:

$$-i\hbar \epsilon_{ijk} \partial^j (A^k u) = (-i\hbar \epsilon_{ijk} \partial^j A^k) u + (i\hbar \epsilon_{ikj} A^k \partial^j) u. \tag{3.36}$$

At this point we can safely use the correspondence of $-i\hbar\partial^j$ and p^j because we have written the equation acting on wave functions, properly accounting for the conversion. We obtain:

$$\epsilon_{ijk} p^j (A^k u) = (-i\hbar \epsilon_{ijk} \partial^j A^k) u - (\epsilon_{ikj} A^k p^j) u, \tag{3.37}$$

which we rearrange to yield

$$\epsilon_{ijk} p^j (A^k u) + (\epsilon_{ikj} A^k p^j) u = (-i\hbar \epsilon_{ijk} \partial^j A^k) u. \tag{3.38}$$

Translating this back into vector notation from the Einstein notation, we find that:

$$[(\mathbf{p} \times \mathbf{A}) + (\mathbf{A} \times \mathbf{p})] = (-i\hbar \nabla \times \mathbf{A}) = -i\hbar \mathbf{B}. \tag{3.39}$$

Due to the notational subtleties this is in stark contrast to what one might naively expect as discussed above due to the additional term on the left-hand side. We thus find that $(p \times \mathbf{A})$ does not equal $-i\hbar\mathbf{B}$ but that instead $(\mathbf{p} \times \mathbf{A}) + (\mathbf{A} \times \mathbf{p}) = -i\hbar\mathbf{B}$ holds.
Returning now to Equation 3.31, we utilize the identity in Equation 3.32 to obtain:

$$\left[\frac{1}{2}\left(\mathbf{p}^2 + i\sigma(\mathbf{p} \times \mathbf{p}) - (\mathbf{A} \cdot \mathbf{p} + \mathbf{p} \cdot \mathbf{A}) - i\sigma(\mathbf{p} \times \mathbf{A} + \mathbf{A} \times \mathbf{p}) + (\mathbf{A}^2 + i\sigma \mathbf{A} \times \mathbf{A}\right) + \phi\right] u = i\epsilon \partial_t u. \tag{3.40}$$

Since for any given vector $\mathbf{v}$ we have that $\mathbf{v} \times \mathbf{v} = 0$, this reduces to:

$$\left[\frac{1}{2}\left(\mathbf{p}^2 - (\mathbf{A} \cdot \mathbf{p} + \mathbf{p} \cdot \mathbf{A}) - i\sigma(p \times \mathbf{A} + \mathbf{A} \times \mathbf{p}) + \mathbf{A}^2\right) + \phi\right] u = i\epsilon \partial_t u. \tag{3.41}$$

Using identity 3.39 we can replace the complexity of the third term with the comparably simple magnetic field $\mathbf{B}$ to obtain

$$\left[\frac{1}{2}\left(\mathbf{p}^2 - A \cdot \mathbf{p} - \mathbf{p} \cdot A - \epsilon\sigma \cdot \mathbf{B} + \mathbf{A}^2\right) + \phi\right] u = i\epsilon \partial_t u. \tag{3.42}$$

If desired, this can be written in the following way which is the canonical result of removing spin from the kinetic term of the Pauli equation:

$$\left[\frac{1}{2}\left((\mathbf{p}-A)^2-\epsilon\sigma\cdot\mathbf{B}\right)+\phi\right]u=i\epsilon\partial_t u. \tag{3.43}$$

For the present purpose, a more important way to write this equation is to use the Coulomb gauge $\nabla\cdot\mathbf{A}=0$ and thus eliminate one of the terms (note again that the factor $\frac{1}{2}$ cancels out because of an application of the chain rule), finally yielding:

$$\left[\frac{1}{2}\left(\mathbf{p}^2-2\mathbf{A}\cdot\mathbf{p}-\epsilon\sigma\cdot\mathbf{B}+\mathbf{A}^2\right)+\phi\right]u=i\epsilon\partial_t u. \tag{3.44}$$

Using the correspondence between $\mathbf{p}$ and $-i\epsilon\nabla$ we can now safely write this as

$$\left[\frac{1}{2}\left(-\epsilon^2\nabla+2i\epsilon\mathbf{A}\cdot\nabla+\mathbf{A}^2-\epsilon\sigma\cdot\mathbf{B}\right)+\phi\right]u=i\epsilon\partial_t u, \tag{3.45}$$

which matches the form of the Pauli equation obtained by simply adding the simplest possible non-trivial spin coupling to the magnetic field to the magnetic Schrödinger equation as discussed in section 2.4.2.

3.3 The explicit form of the Pauli equation system

So far we have seen a number of different forms of the Pauli equation, such as the original form which one often encounters in physics textbooks:

$$\left[\frac{1}{2m}\left(\sigma\cdot\left(-i\hbar\nabla-\frac{q}{c}\mathbf{A}\right)\right)^2+q\phi\right]u=i\hbar\frac{\partial}{\partial t}u. \tag{3.46}$$

In section 3.1.3 we derived a scaled version of this equation where the Pauli equation is expressed in dimensionless form:

$$\left[\frac{1}{2}\left(\sigma\cdot(-i\epsilon\nabla-\mathbf{A})\right)^2+\phi\right]u=i\epsilon\partial_t u, \tag{3.47}$$

from which we derived the following alternative version with spin removed from the kinetic term in section 3.2:

$$\left[\frac{1}{2}\left((-i\epsilon\nabla-\mathbf{A})^2-\epsilon\sigma\cdot\mathbf{B}\right)+\phi\right]u=i\epsilon\partial_t u. \tag{3.48}$$

All three of these forms presented here retain full gauge freedom and can for example be further simplified using the Coulomb Gauge $\nabla\cdot\mathbf{A}=0$. Furthermore, all of these forms of the Pauli equation use various forms of short-hand notation to make the physicist's and mathematician's life easier when reading the equation. When it comes to implementing the equation numerically, however, a fully explicit form of the equation is needed where we cannot rely on elegant notation to hide complicated terms. Thus, the purpose of this section is to write down the fully explicit Pauli equation which will prove useful for the numerical work done in coming sections.
We will base this fully explicit form off of the scaled Pauli equation where the spin has been removed form the kinetic term. We begin with a reminder of what all of

the short-hand notation in the Pauli equation means. The magnetic vector potential $\mathbf{A}$ is a vector with three components, u is a spinor with two components and σ is a vector-like shorthand for an object with the Pauli matrices σ_i as its components:

$$\mathbf{A} = \begin{pmatrix} A_1 \\ A_2 \\ A_3 \end{pmatrix}, \quad u = \begin{pmatrix} u_1 \\ u_2 \end{pmatrix},$$

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

Additionally, ϕ is a scalar field, ϵ is a scaling parameter and $\mathbf{B} = \nabla \times \mathbf{A}$. We also restate the adapted definitions of the shorthands involving ∇ present in the Pauli equation since under the common meaning of those objects the equation would not even be well-defined:

$$\nabla u = \nabla \begin{pmatrix} u_1 \\ u_2 \end{pmatrix} = \begin{pmatrix} \partial_x u_1 & \partial_y u_1 & \partial_z u_1 \\ \partial_x u_2 & \partial_y u_2 & \partial_z u_2 \end{pmatrix}, \quad (3.49)$$

$$\nabla^2 u = \begin{pmatrix} \partial_x^2 u_1 + \partial_y^2 u_1 + \partial_z^2 u_1 \\ \partial_x^2 u_2 + \partial_y^2 u_2 + \partial_z^2 u_2 \end{pmatrix} = \begin{pmatrix} \nabla^2 u_1 \\ \nabla^2 u_2 \end{pmatrix}, \quad (3.50)$$

$$(\mathbf{A} \cdot \nabla) u = \begin{pmatrix} \partial_x u_1 & \partial_y u_1 & \partial_z u_1 \\ \partial_x u_2 & \partial_y u_2 & \partial_z u_2 \end{pmatrix} \begin{pmatrix} A_1 \\ A_2 \\ A_3 \end{pmatrix} = \begin{pmatrix} A_1 \partial_x u_1 + A_2 \partial_y u_1 + A_3 \partial_z u_1 \\ A_1 \partial_x u_2 + A_2 \partial_y u_2 + A_3 \partial_z u_2 \end{pmatrix}, \quad (3.51)$$

The Pauli equation should yield the normal Schrödinger equation in the limit where $\mathbf{A} = 0$, so it serves as a suitable warm-up for writing the full Pauli equation explicitly to attempt to see this Schrödinger-limit in an explicit way. Setting $\mathbf{A} = 0$ we see that we obtain:

$$\frac{1}{2}(-\epsilon^2 \nabla^2 + \phi) u = i\epsilon \partial_t u, \quad (3.52)$$

where u is still the Pauli 2-spinor. Plugging in the explicit form of $\nabla^2 u$, this equation reads:

$$-\frac{\epsilon^2}{2} \begin{pmatrix} \partial_x^2 u_1 + \partial_y^2 u_1 + \partial_z^2 u_1 \\ \partial_x^2 u_2 + \partial_y^2 u_2 + \partial_z^2 u_2 \end{pmatrix} + \begin{pmatrix} \phi u_1 \\ \phi u_2 \end{pmatrix} = i\epsilon \begin{pmatrix} \partial_t u_1 \\ \partial_t u_2 \end{pmatrix}. \quad (3.53)$$

The two rows of this equation are the non-magnetic Schrödinger equations for u_1 and u_2 respectively, with no coupling between the two Schrödinger equations:

$$-\frac{\epsilon^2}{2}(\partial_x^2 u_1 + \partial_y^2 u_1 + \partial_z^2 u_1) + \phi u_1 = i\epsilon \partial_t u_1, \quad (3.54)$$

$$-\frac{\epsilon^2}{2}(\partial_x^2 u_2 + \partial_y^2 u_2 + \partial_z^2 u_2) + \phi u_2 = i\epsilon \partial_t u_2, \quad (3.55)$$

which can once again be put in their more common compressed notation:

$$(-\frac{\epsilon^2}{2}\nabla^2 + \phi) u_1 = i\epsilon \partial_t u_1, \quad (3.56)$$

$$(-\frac{\epsilon^2}{2}\nabla^2 + \phi) u_2 = i\epsilon \partial_t u_2. \quad (3.57)$$

In this way one can see the Schrödinger limit of the Pauli equation's rows explicitly. Moving on to the full Pauli equation (with Coulomb gauge), we first plug in all of the relevant definitions to obtain the rather lengthy expression:

$$-\frac{\epsilon^2}{2}\begin{pmatrix}\partial_x^2 u_1+\partial_y^2 u_1+\partial_z^2 u_1\\ \partial_x^2 u_2+\partial_y^2 u_2+\partial_z^2 u_2\end{pmatrix}+i\epsilon\begin{pmatrix}A_1\partial_x u_1+A_2\partial_y u_1+A_3\partial_z u_1\\ A_1\partial_x u_2+A_2\partial_y u_2+A_3\partial_z u_2\end{pmatrix}$$
$$+\frac{1}{2}\begin{pmatrix}\mathbf{A}^2 u_1\\ \mathbf{A}^2 u_2\end{pmatrix}-(B_1\sigma_1+B_2\sigma_2+B_3\sigma_3)\begin{pmatrix}u_1\\ u_2\end{pmatrix}+\begin{pmatrix}\phi u_1\\ \phi u_2\end{pmatrix}=i\epsilon\begin{pmatrix}\partial_t u_1\\ \partial_t u_2\end{pmatrix}.$$

Of specific interest is the explicit form of the coupling term containing the Pauli matrices and the **B** field. We take a look at this coupling term on its own:

$$(B_1\sigma_1+B_2\sigma_2+B_3\sigma_3)\begin{pmatrix}u_1\\ u_2\end{pmatrix}=\left(\begin{pmatrix}0 & B_1\\ B_1 & 0\end{pmatrix}+\begin{pmatrix}0 & -iB_2\\ iB_2 & 0\end{pmatrix}+\begin{pmatrix}B_3 & 0\\ 0 & -B_3\end{pmatrix}\right)\begin{pmatrix}u_1\\ u_2\end{pmatrix}$$
$$=B_1\begin{pmatrix}u_2\\ u_1\end{pmatrix}+iB_2\begin{pmatrix}-u_2\\ u_1\end{pmatrix}+B_3\begin{pmatrix}u_1\\ -u_2\end{pmatrix}.$$

Plugging this expression for the coupling term into the above full equation, we obtain two rows representing two coupled equations, together constituting the Pauli equation:

$$\left[-\frac{\epsilon^2}{2}\nabla^2+i\epsilon\mathbf{A}\cdot\nabla+\left(\frac{1}{2}\mathbf{A}^2+\phi\right)\right]u_1-\frac{\epsilon}{2}B_1u_2+\frac{i\epsilon}{2}B_2u_2-\frac{\epsilon}{2}B_3u_1=i\epsilon\partial_t u_1, \quad (3.58)$$
$$\left[-\frac{\epsilon^2}{2}\nabla^2+i\epsilon\mathbf{A}\cdot\nabla+\left(\frac{1}{2}\mathbf{A}^2+\phi\right)\right]u_2-\frac{\epsilon}{2}B_1u_1-\frac{i\epsilon}{2}B_2u_1+\frac{\epsilon}{2}B_3u_2=i\epsilon\partial_t u_2. \quad (3.59)$$

One of the B-terms can respectively be written inside of the brackets to result in slightly more compact form if desired:

$$\left[-\frac{\epsilon^2}{2}\nabla^2+i\epsilon\mathbf{A}\cdot\nabla+\left(\frac{1}{2}\mathbf{A}^2+\phi-\frac{\epsilon}{2}B_3\right)\right]u_1+\left[-\frac{\epsilon}{2}B_1+\frac{i\epsilon}{2}B_2\right]u_2=i\epsilon\partial_t u_1, \quad (3.60)$$
$$\left[-\frac{\epsilon^2}{2}\nabla^2+i\epsilon\mathbf{A}\cdot\nabla+\left(\frac{1}{2}\mathbf{A}^2+\phi+\frac{\epsilon}{2}B_3\right)\right]u_2+\left[-\frac{\epsilon}{2}B_1-\frac{i\epsilon}{2}B_2\right]u_1=i\epsilon\partial_t u_2. \quad (3.61)$$

Without using the Coulomb gauge there would simply be one additional straightforward term involving $\nabla\cdot\mathbf{A}$.

3.4 Notes on conservation laws

In general we say that a conservation law holds for a physical quantity if its value remains constant in time. The importance of conservation laws for theoretical and mathematical physics, in part due to the important relationship to dynamical symmetries via the famous Noether theorem, can hardly be overstated. They are also often subject of experimental physics research, often with the intent of verifying or falsifying whether certain quantities in fact are conserved in a given system. It turns out that conservation laws are also very useful for numerical methods and implementations for two different reasons: First and perhaps more immediately conceivable, they provide a means to check if a particular computer implementation is sensible. If, for example, the energy of a physical system continuously rises in a system of

which we would expect conservation of energy then something about the algorithm or method could be wrong or errors could be compiling in an unfortunate way. The second and more sophisticated use of conservation laws for the purposes of numerics is using them to come up with particular methods specialized to the given problem in the first place and which have the conservation laws built in (compare for example [26–28]).

Local conservation of 'mass' is often expressed as a continuity equation. A generic continuity equation looks something like this:

$$\frac{\partial \rho}{\partial t} + \nabla \cdot \mathbf{j} = k \tag{3.62}$$

and intuitively states that the change in density of a given quantity at any given location is associated with a flowing current $\mathbf{j}$. The k in this case reflects that so-called sources or sinks, in which an amount of the quantity of interest can be locally generated or removed from the system, can mathematically be described using the same formalism. A continuity equation thus becomes a conservation law when $k = 0$ and we have

$$\frac{\partial \rho}{\partial t} + \nabla \cdot \mathbf{j} = 0. \tag{3.63}$$

The situation is non-trivially complicated in quantum mechanics compared to classical physics because one has to take a lot of care with concepts such as densities given that in many cases we are no longer dealing with classical continuous quantities. However, one density that is well defined in quantum physics is the probability density given by the state of a quantum system $\rho = |\psi(x,t)|^2$ which satisfies $\int_{-\infty}^{+\infty} |\psi(x,t)|^2 dx = 1$ (compare Born's rule in section 2.2.1). Given that the quantum state $\psi(x,t)$ is a complex scalar field we can write this probability density as

$$\rho := |\psi|^2 = \bar{\psi}\psi, \tag{3.64}$$

where we have introduced the so-called adjoint wave function $\bar{\psi}(x,t)$. To show that a normalized wave function, i.e. a state which is set up to satisfy $\int_{-\infty}^{+\infty} |\psi(x,t)|^2 dx = 1$, remains in this normalized state as it evolves in time we show that a continuity equation holds for this probability. The density of the probability being precisely $\bar{\psi}\psi$, we need to find a sensible expression for the current corresponding to this probability. For the sake of simplicity, we begin with the Schrödinger equation case. We recall the Schrödinger equation:

$$\hat{H}\psi = i\hbar \frac{\partial}{\partial t}\psi. \tag{3.65}$$

Any physically sensible Hamiltonian $\hat{H}$ is by definition Hermitian, from which one immediately obtains the two expressions

$$\frac{\partial}{\partial t}\psi = -\frac{i\hat{H}\psi}{\hbar}, \tag{3.66}$$

$$\frac{\partial}{\partial t}\bar{\psi} = \frac{i\hat{H}\bar{\psi}}{\hbar}, \tag{3.67}$$

A left multiplication with $\bar{\psi}$ and ψ respectively then yields

$$\bar{\psi}\frac{\partial}{\partial t}\psi = -\frac{i\bar{\psi}\hat{H}\psi}{\hbar}, \tag{3.68}$$

$$\psi\frac{\partial}{\partial t}\bar{\psi} = \frac{i\psi\hat{H}\bar{\psi}}{\hbar}, \tag{3.69}$$

which upon adding the two equations together and recognizing the product rule of derivation on the left hand side leaves us with

$$\frac{\partial}{\partial t}\bar{\psi}\psi = \frac{i}{\hbar}\left(\psi\hat{H}\bar{\psi} - \bar{\psi}\hat{H}\psi\right). \tag{3.70}$$

Recognizing the first term as the time derivative of the probability density, we can see that this can be rearranged into the form of a continuity equation with

$$\nabla\cdot\mathbf{j} = -\frac{i}{\hbar}\left(\psi\hat{H}\bar{\psi} - \bar{\psi}\hat{H}\psi\right). \tag{3.71}$$

All that is left now is to plug in the actual Hamiltonian $\hat{H} = \frac{-\hbar^2}{2m}\nabla^2 + V$ where the V term cancels out of the equation:

$$\frac{\partial}{\partial t}\bar{\psi}\psi - \frac{i\hbar}{2m}\left(\psi\nabla^2\bar{\psi} - \bar{\psi}\nabla^2\psi\right) = 0. \tag{3.72}$$

Since the term in the continuity equation is $\nabla\cdot\mathbf{j}$ and we are looking for an expression for $\mathbf{j}$ it makes sense to pull out a ∇ to rewrite this as follows:

$$\frac{\partial}{\partial t}\bar{\psi}\psi - \frac{i\hbar}{2m}\nabla\cdot\left(\psi\nabla\bar{\psi} - \bar{\psi}\nabla\psi\right) = 0, \tag{3.73}$$

Thus we have derived a continuity equation for the particle probability density $\rho = |\psi|^2$. This has the important consequence for the internal consistency of quantum mechanics that the time evolution of a normalized state is again a normalized state and comes with the added numerical approach bonuses discussed above.
Having seen how to derive the continuity equation for the Schrödinger equation, the extension of this procedure to the Pauli equation is straightforward. It is easiest to derive from the version of the Pauli equation which has the spin term removed from its kinetic term (see section 3.2):

$$\left[\frac{1}{2}\left((-i\epsilon\nabla - A)^2 - \epsilon\sigma\cdot\mathbf{B}\right) + \phi\right]u = i\epsilon\partial_t u. \tag{3.74}$$

We will discuss the scaled version of this equation here but every step works equivalently for the non-scaled version. Once again one begins by writing down the following relations for the Pauli equation and its adjoint. Noting that the electromagnetic fields and their corresponding potentials are real (scalar or vector respectively) valued fields and that the Pauli matrices representing spin are all Hermitian, the resulting two equations look as follows:

$$\partial_t u = -\frac{i}{\epsilon}\left[\frac{1}{2}\left((-i\epsilon\nabla - \mathbf{A})^2 - \epsilon\sigma\cdot\mathbf{B}\right) + \phi\right]u, \tag{3.75}$$

$$\partial_t \bar{u} = \frac{i}{\epsilon}\left[\frac{1}{2}\left((i\epsilon\nabla - \mathbf{A})^2 - \epsilon\sigma\cdot\mathbf{B}\right) + \phi\right]\bar{u}, \tag{3.76}$$

where to remain well-defined the adjoint 2-spinor has to be defined as

$$\bar{u} = \begin{pmatrix} \bar{u}_1 & \bar{u}_2 \end{pmatrix}. \tag{3.77}$$

As before, multiplication from the appropriate side with u or $\bar{u}$ respectively yields:

$$\bar{u}\partial_t u = -\frac{i}{2\epsilon}\bar{u}\left((-i\epsilon\nabla - \mathbf{A})^2 - \bar{u}\epsilon\sigma\cdot\mathbf{B}\right)u - \frac{i}{\epsilon}\bar{u}\phi u, \tag{3.78}$$

$$(\partial_t\bar{u})\,u = \frac{i}{2\epsilon}\left((i\epsilon\nabla - \mathbf{A})^2 - \epsilon\sigma\cdot\mathbf{B}\right)\bar{u}u + \frac{i}{\epsilon}\phi\bar{u}u, \tag{3.79}$$

Moving on from this point we add these two equations together and cancel equal terms to obtain:

$$\bar{u}\partial_t u + (\partial_t\bar{u})\,u = -\frac{i}{2\epsilon}\bar{u}(-i\epsilon\nabla - \mathbf{A})^2 u + \frac{i}{2\epsilon}(i\epsilon\nabla - \mathbf{A})^2\bar{u}u. \tag{3.80}$$

The quadratic terms are expanded as follows:

$$\bar{u}(-i\epsilon\nabla - \mathbf{A})^2 u = -\epsilon^2\bar{u}\nabla^2 u + i\epsilon\bar{u}(\nabla\cdot\mathbf{A}u) + i\epsilon\bar{u}(\mathbf{A}\cdot\nabla)u + \bar{u}\mathbf{A}^2 u, \tag{3.81}$$

$$(i\epsilon\nabla - \mathbf{A})^2\bar{u}u = -\epsilon^2(\nabla^2\bar{u})u - i\epsilon(\nabla\cdot\mathbf{A}\bar{u})u - i\epsilon(\mathbf{A}\cdot\nabla\bar{u})u + \mathbf{A}^2\bar{u}u. \tag{3.82}$$

Plugging this expansion into the above equation, recognizing and inverting the product rule on the left-hand side as well as simplifying finally yields:

$$\partial_t\bar{u}u = i\epsilon\left((\bar{u}\nabla^2 u)^T - (\nabla^2\bar{u})u\right) + \nabla(\mathbf{A}\bar{u}u). \tag{3.83}$$

Once again, comparison with the continuity equation gives us the expression for $\nabla\cdot\mathbf{j}$, which suggests the following rewriting of the equation:

$$\partial_t\bar{u}u + \nabla\left(-i\epsilon\left((\bar{u}\nabla u)^T - (\nabla\bar{u})u\right) - \mathbf{A}\bar{u}u\right) = 0, \tag{3.84}$$

suggesting the current

$$\tilde{\mathbf{j}} = -i\epsilon\left((\bar{u}\nabla u)^T - (\nabla\bar{u})u\right) - \mathbf{A}\bar{u}u \tag{3.85}$$

for the Pauli equation system. However, since the expression we obtained is only for $\nabla\cdot\mathbf{j}$ and not $\mathbf{j}$ itself, any divergence free terms potentially contained in $\mathbf{j}$ might not show in the result of this motivation. Indeed it turns out that for full consistency of the associated concepts the Pauli current requires the addition of a spin coupling term for the current as follows:

$$\mathbf{j} = -\epsilon\left((\bar{u}\nabla u)^T - (\nabla\bar{u})u\right) - \mathbf{A}\bar{u}u - \epsilon\nabla\times(\bar{u}\sigma u). \tag{3.86}$$

This term is irrelevant for the truth of the derived continuity equation and the corresponding conservation law for the Pauli equation's probability density since its divergence vanishes, so we will not go into any further detail about it here. For further discussion of this current and the spin term whose motivation we omit in particular, see the original argument for this term in [29]. For the sake of completion we also reproduce the non-scaled current here:

$$\mathbf{j} = -\frac{i\hbar}{2m}\left((\bar{u}\nabla u)^T - (\nabla\bar{u})u\right) - \frac{q}{mc}\mathbf{A}\bar{u}u - \frac{|q|\hbar}{2m}\nabla\times(\bar{u}\sigma u). \tag{3.87}$$

Given certain additional assumptions global conservation laws are weaker statements than local ones. In the case of the Schrödinger and Pauli equation the particular assumption that is required is that all the relevant quantities vanish sufficiently fast when approaching infinity, e.g. by demanding all the relevant functions to be in L^2 or for the case of the conservation of energy an appropriate Sobolev space. If this is the case the argument from the local conservation to the global one is a mere application of integration and the Gauss theorem yielding:

$$\frac{d}{dt}\int \rho d\mathbf{x} = 0, \tag{3.88}$$

where ρ is the probability density of either the Schrödinger or Pauli system. This is sometimes referred to as charge conservation (compare [30]).
A consistent physical theory also conserves energy, more or less by definition of how modern physical theories are formulated (see section 2.3.4). Energy must thus be conserved by the Schrödinger and Pauli systems and this is indeed the case. For the generic linear Schrödinger case with $V(x,t) \in \mathbb{R}$ it takes the following form:

$$\frac{d}{dt}\int \left(\frac{1}{2}|\nabla\psi|^2 + V|\psi|^2\right) d\mathbf{x} = 0. \tag{3.89}$$

A straightforward analogous equation can also be shown to hold for the Pauli system where the Schrödinger Hamiltonian is replaced by the Pauli Hamiltonian. In fact, the conservation of energy is a direct result of the time symmetry of the Schrödinger and Pauli systems via Noether's famous theorem.

4 Numerics for the the magnetic Schrödinger equation

The numerical side of Schrödinger-type equations has received a vast amount of treatment and discussion in the recent scientific literature due in part to its importance in physics but also for the unique mathematical problems both linear and non-linear variants of the Schrödinger equation pose for various potentials. We will not discuss all of the aspects of this active field of research here nor even a significant portion of it as doing so would require a full monograph as opposed to a paper. Instead, we will focus in particular on methods proposed for the magnetic Schrödinger equation and the Pauli equation, for which the numerical literature is significantly more sparsely populated. For introductions and discussions of the numerical treatment of Schrödinger-type equations using operator splitting among other methods see for example [31–33].

4.1 A three operator-splitting method by Caliari et al.

In this section we review a result by [1], where they presented a numerical approach to solving the magnetic Schrödinger equation using a three operator splitting method. Their work is respectively to some degree based on previous work done by [31–33], which are also references for this section. We will focus on presenting and summarizing these results, omitting the proofs and only mentioning what is necessary. See the original paper [1] for the full details. This method is important for the present work, as extending this numerical procedure to the Pauli equation as opposed to the magnetic Schrödinger equation is the primary goal of this thesis. The extension of this method to the Pauli equation will be discussed in section 5.

4.1.1 Introducing the method

Caliari et al. [1] look for a numerical approach to the following equation, called the magnetic Schrödinger equation:

$$i\epsilon\partial_t\psi = \left(\frac{1}{2}(i\epsilon\nabla + \mathbf{A})^2 + \phi\right)\psi, \tag{4.1}$$

$$t \geq 0, x \in \mathbb{R}^d, \tag{4.2}$$

$$\psi(x,0) = \psi_0, \tag{4.3}$$

$$\lim_{|x|\to\infty} \psi(x,t) = 0. \tag{4.4}$$

Here the unknown $\psi(x,t)$ is a *scalar* complex quantum mechanical wave function, $\phi(x,t)$ is a scalar potential field and $\mathbf{A}(x,t) \in \mathbb{R}^d$ is the magnetic vector potential (while we have been and will continue to work in three spatial dimensions in this paper due to this being natural for the Pauli equation, many of these methods are valid for arbitrary dimensions d). The small parameter ϵ is the scaled Planck constant and we have vanishing boundary conditions.
To solve this system, they propose a three operator splitting method consisting of

the abstracted PDE:

$$\partial_t \psi = (\mathcal{A} + \mathcal{B} + \mathcal{C})\psi, \tag{4.5}$$

$$0 \leq t \leq T, \tag{4.6}$$

$$\psi(x, 0) = \psi_0(x). \tag{4.7}$$

They consider this problem in a Banach space X with norm $||\cdot||$. The setting for this three operator splitting is general enough to include the magnetic Schrödinger equation. To see this, we first expand the square parentheses in the magnetic Schrödinger equation from Equation 4.1 to obtain:

$$i\epsilon\partial_t\psi = -\frac{\epsilon^2}{2}\nabla^2\psi + i\epsilon\mathbf{A}\cdot\nabla\psi + i\epsilon\nabla\cdot\mathbf{A}\psi + \frac{1}{2}|\mathbf{A}|^2\psi + \phi\psi, \tag{4.8}$$

which as we have seen in previous sections simplifies significantly when using gauge freedom to set $\nabla \cdot \mathbf{A} = 0$ (the Coulomb gauge):

$$i\epsilon\partial_t\psi = -\frac{\epsilon^2}{2}\nabla^2\psi + i\epsilon\mathbf{A}\cdot\nabla\psi + \frac{1}{2}|A|^2\psi + \phi\psi. \tag{4.9}$$

This way a translation into the above three operator scheme is straightforward:

$$\mathcal{A}\psi = \frac{i\epsilon}{2}\nabla^2\psi, \tag{4.10}$$

$$\mathcal{B}\psi = -\frac{i}{\epsilon}(\frac{1}{2}|\mathbf{A}|^2 + \phi)\psi, \tag{4.11}$$

$$\mathcal{C}\psi = \mathbf{A}\cdot\nabla\psi. \tag{4.12}$$

Following Caliari et al. and common notational convention, we write $e^{\Delta t\mathcal{L}}\psi_0$ for the exact solution at time Δt of the differential equation $\partial_t\psi = \mathcal{L}\psi$ with initial values $\psi(x, 0) = \psi_0(x)$. They prove stability, convergence and provide local and global error bounds for the following first order Lie splitting scheme:

$$\psi_{n+1} = e^{\Delta t\mathcal{C}}e^{\Delta t\mathcal{A}}e^{\Delta t\mathcal{B}}\psi_n \tag{4.13}$$

Here, Δt is the step size in time and ψ_n is the first order numerical approximation of the true solution $\psi(t) = e^{t\mathcal{A}+t\mathcal{B}+t\mathcal{C}}\psi_0$ in the n-th step. The error bounds to such an approximation are essentially determined by the Baker-Campbell-Hausdorff formula (for a discussion of this with respect to the Schrödinger equation see for example [34]). The results they prove naturally only hold within certain bounds for $\mathcal{A}, \mathcal{B}$ and $\mathcal{C}$ which of course translates to certain conditions for the electromagnetic potentials. We now list the assumptions they use:

Assumption 1 (see [1]): Let $\mathcal{B}$ be a bounded operator and let $\mathcal{A}$, $\mathcal{C}$ and $\mathcal{A} + \mathcal{C}$ generate the strongly continuous semigroups $e^{t\mathcal{A}}$, $e^{t\mathcal{C}}$ and $e^{t\mathcal{A}+\mathcal{C}}$ on the Banach space X with norm $||\cdot||$. We assume that along the exact solution $\psi(t)$, the

following bounds hold for $0 \leq t \leq T$:

$$||[\mathcal{A}, \mathcal{C}]e^{s\mathcal{A}}\psi(t)|| \leq c_1, \tag{4.14}$$
$$||\mathcal{C}e^{s\mathcal{A}}\mathcal{B}\psi(t)|| \leq c_2, \tag{4.15}$$
$$||\mathcal{C}^2e^{s\mathcal{A}}\psi(t)|| \leq c_3, \tag{4.16}$$
$$||\mathcal{C}e^{\sigma\mathcal{A}}e^{s(\mathcal{A}+\mathcal{C})}\psi(t)|| \leq c_4, \tag{4.17}$$
$$||[\mathcal{A}+\mathcal{C}, \mathcal{B}]e^{s(\mathcal{A}+\mathcal{C})}\psi(t)|| \leq c_5, \tag{4.18}$$

where all the c_i are constants independent of $0 \leq \sigma$ and $s \leq T$.

For the proofs of stability and global error bounds they also need:

Assumption 2 (see [1]): There is a constant $\omega_{\mathcal{C}}$ such that $||e^{t\mathcal{C}}||_* \leq e^{t\omega_{\mathcal{C}}}$ for $0 \leq t \leq T$.

An equivalent statement actually holds for $\mathcal{A}$ and $\mathcal{B}$ under Assumption 1 already and thus Assumption 2 only concerns $\mathcal{C}$. It is crucial to check if these assumptions make sense for the magnetic Schrödinger equation, since otherwise stability, convergence and error bounds cannot be guaranteed. For the argument that the magnetic Schrödinger equation in fact does satisfy these assumptions we refer to the full Caliari et al. paper [1], as reproducing the full argument here would stray too far from the goal of discussing the Pauli equation.
Omitting proofs for the sake of brevity, we give an overview of the important results Caliari et al. prove about the first order three operator splitting method introduced above, given the there mentioned assumptions about $\mathcal{A}, \mathcal{B}$ and $\mathcal{C}$.

Theorem 4.1.1. (Local error bounds) *Under Assumption 1, the following error bound holds:*

$$||e^{\Delta t\mathcal{C}}e^{\Delta t\mathcal{A}}e^{\Delta t\mathcal{B}}u(t) - u(t+\Delta t)|| \leq C\Delta t^2, \tag{4.19}$$

where $t \in [0, T-\Delta t]$ and C is a constant independent of t and Δt.

Theorem 4.1.2. (Stability) *Under Assumption 1* and *Assumption 2, the proposed Lie splitting is stable, meaning that there exists a constant C such that*

$$||e^{\Delta t\mathcal{C}}e^{\Delta t\mathcal{A}}e^{\Delta t\mathcal{B}}||^j \leq C, \tag{4.20}$$

for all $j \in \mathbb{N}$ and Δt satisfying $0 \leq j\Delta t \leq T$.

From consistency and stability they can conclude convergence:

Theorem 4.1.3. (Global error bounds) *Under Assumptions 1 and 2, this Lie splitting method for the initial value problem 4.5 is convergent of order 1, meaning there exists a constant C such that*

$$||\psi_n - \psi(t_n)|| \leq C\Delta t. \tag{4.21}$$

for all $n \in \mathbb{N}$ and Δt satisfying $0 \leq n\Delta t = t_n \leq T$.

As stated above, we do not reproduce the relevant proofs here and refer to the original paper for the detailed treatment [1]. This section is merely intended to provide an overview of significant previous results.

4.1.2 Notes on the implementation of the different steps

Up until now we have omitted discussion of how the individual solutions for the $\mathcal{A}$,$\mathcal{B}$ and $\mathcal{C}$ steps are found. Based on the physical background and the form of the parts, Caliari et al. call the $\mathcal{A}$ step the 'kinetic step', the $\mathcal{B}$ step the 'potential step' and the $\mathcal{C}$ step the 'advection step'. In the Coulomb gauge they are able to show that such a scheme respects the conservation of probability density property $\partial_t ||\psi(t,\cdot)||_{L^2}^2 = 0$ of the magnetic Schrödinger equation in each of the above steps. Furthermore, without reproducing their mathematical arguments here, they prove that under assumptions on the sufficient smoothness of $\mathbf{A}$ and ϕ the Assumptions 1 and 2 hold for this problem with $X = L^2$ and thus the three operator splitting method can be used.
The potential step with the $\mathcal{B}$ operator is an easy to solve ODE, while the kinetic step with the $\mathcal{A}$ operator can be done in Fourier space utilizing FFTs. The primary question they address is how to approach solving the advection step with $\mathcal{C}$ using a method of characteristics.
They discuss three different approaches to the solution of this advection step problem with different computational efficiency: A direct Fourier series method with $O(\prod_i N_i^2)$, a polynomial interpolation method which has a step with $O(N_1 \cdot N_2 \cdot ... \cdot N_d \cdot (logN_1 + ... + logN_d))$ and a step with $O(p^i \prod_i N_i)$ and a non-equispaced FFT variant method which results in $O(N_1 \cdot N_2 \cdot ... \cdot N_d \cdot (logN_1 + ... + logN_d + |log\epsilon|^d))$ where ϵ is the desired precision. The cited numbers are for the d dimensional equation but note that we will only consider the three dimensional case for the Pauli equation as it naturally lives in three dimensional space.
We will discuss each of these steps in detail and give explicit characterizations of each solution step when applying a similar operator splitting approach to the Pauli equation in the following sections.
Lastly, it should be noted that Caliari et al. [1] also compare their first order Lie splitting error in numerical experiments to the error of a three operator second order convergent Strang splitting, i.e.

$$\psi_{n+1} = e^{\frac{\Delta t}{2}\mathcal{B}} e^{\frac{\Delta t}{2}\mathcal{A}} e^{\Delta t\mathcal{C}} e^{\frac{\Delta t}{2}\mathcal{A}} e^{\frac{\Delta t}{2}\mathcal{B}} \psi_n \tag{4.22}$$

but they only provide the above-mentioned proofs for the three operator first order Lie splitting.

5 Numerics for the Pauli equation

In this section we will discuss a possible operator splitting method extension to the Pauli equation system adapted from previous work done on the magnetic Schrödinger equation ([1] and [33]) as discussed above. A different numerical approach to the Pauli equation based on a leapfrog approach has previously been discussed in [35] but will not be detailed here. Other than the references used in this paper, the Pauli system has received relatively little attention so far in the numerics literature despite its rather important placement in physics and potential use for experiments.

5.1 Adapting the operator-splitting method to the Pauli equation

5.1.1 Comparison with the magnetic Schrödinger equation case

Many of the computational aspects of the operator splitting method discussed in section 4.1 can be applied to the Pauli equation system with only the need for straightforward modifications. The generalization to the Pauli system is not unique since there are some choices for the placement of certain fields within operators that may or may not affect the ease for doing the analysis for the problem. Computationally, however, we find that the chosen four operator splitting method preserves the intuitiveness of the method while still maintaining a very reasonable level of efficiency. For convenience, we restate the Pauli system of equations here:

$$\left[-\frac{\epsilon^2}{2}\nabla^2 + i\epsilon\mathbf{A}\cdot\nabla + \left(\frac{1}{2}\mathbf{A}^2 + \phi - \frac{\epsilon}{2}B_3\right)\right]u_1 + \left[-\frac{\epsilon}{2}B_1 + \frac{i\epsilon}{2}B_2\right]u_2 = i\epsilon\partial_t u_1, \quad (5.1)$$

$$\left[-\frac{\epsilon^2}{2}\nabla^2 + i\epsilon\mathbf{A}\cdot\nabla + \left(\frac{1}{2}\mathbf{A}^2 + \phi + \frac{\epsilon}{2}B_3\right)\right]u_2 + \left[-\frac{\epsilon}{2}B_1 - \frac{i\epsilon}{2}B_2\right]u_1 = i\epsilon\partial_t u_2. \quad (5.2)$$

The first difference of note is that, as expanded upon in the previous sections, the Pauli equation is actually a system of two coupled equations which decouple in the absence of electromagnetic fields. This means that instead of one equation, we now need to solve two equations and one approach to do so in particular is to separate out the coupling aspect of the system as its own operation and move from the three operator splitting for the magnetic Schrödinger equation to a four operator splitting for the Pauli equation. In particular, we can rewrite the Pauli system of equations elegantly in a matrix multiplication form as follows, which lends itself to the operator splitting view. To allow a more concise notation we first define the following

shorthands:

$$\mathcal{A} = \frac{i\epsilon}{2}\nabla^2, \tag{5.3}$$

$$\mathcal{C} = \mathbf{A} \cdot \nabla, \tag{5.4}$$

$$\mathcal{B}_1 = \left(\frac{1}{2}\mathbf{A}^2 + \phi - \frac{\epsilon}{2}B_3\right), \tag{5.5}$$

$$\mathcal{B}_2 = \left(\frac{1}{2}\mathbf{A}^2 + \phi + \frac{\epsilon}{2}B_3\right), \tag{5.6}$$

$$\mathcal{D}_1 = \left[-\frac{\epsilon}{2}B_1 + \frac{i\epsilon}{2}B_2\right], \tag{5.7}$$

$$\mathcal{D}_2 = \left[-\frac{\epsilon}{2}B_1 - \frac{i\epsilon}{2}B_2\right], \tag{5.8}$$

$$\mathfrak{A} = \begin{pmatrix} \mathcal{A} & 0 \\ 0 & \mathcal{A} \end{pmatrix}, \quad \mathfrak{C} = \begin{pmatrix} \mathcal{C} & 0 \\ 0 & \mathcal{C} \end{pmatrix}, \tag{5.9}$$

$$\mathfrak{B} = \begin{pmatrix} \mathcal{B}_1 & 0 \\ 0 & \mathcal{B}_2 \end{pmatrix}, \quad \mathfrak{D} = \begin{pmatrix} 0 & \mathcal{D}_1 \\ \mathcal{D}_2 & 0 \end{pmatrix}. \tag{5.10}$$

$$\tag{5.11}$$

It can then easily be verified that the Pauli system of equations takes the following form when written as a matrix multiplication:

$$\left[\begin{pmatrix} \mathcal{A} & 0 \\ 0 & \mathcal{A} \end{pmatrix} + \begin{pmatrix} \mathcal{C} & 0 \\ 0 & \mathcal{C} \end{pmatrix} + \begin{pmatrix} \mathcal{B}_1 & 0 \\ 0 & \mathcal{B}_2 \end{pmatrix} + \begin{pmatrix} 0 & \mathcal{D}_1 \\ \mathcal{D}_2 & 0 \end{pmatrix}\right] \begin{pmatrix} u_1 \\ u_2 \end{pmatrix} = \partial_t \begin{pmatrix} u_1 \\ u_2 \end{pmatrix} \tag{5.12}$$

The idea is to adapt the previously discussed method and solve this coupled system using a Lie splitting method plus a coupling step, i.e. we take the u_n iteratively defined as follows to be a numerical approximation to the true solution of the system where of course u_n has a spin up and a spin down component:

$$u_{n+1} = e^{\Delta t\mathfrak{D}} e^{\Delta t\mathfrak{C}} e^{\Delta t\mathfrak{A}} e^{\Delta t\mathfrak{B}} u_n. \tag{5.13}$$

In analogy to the magnetic Schrödinger case as discussed in [1], we will refer to the $\mathfrak{A}$ step as the kinetic step, the $\mathfrak{C}$ step as the advection step, the $\mathfrak{B}$ step as the potential step and the $\mathfrak{D}$ step as the coupling step. In contrast to the magnetic Schrödinger equation case the chosen potential step here includes part of the equation's matrix diagonal coupling to the electromagnetic field for computational efficiency. The coupling step performed at the end is thus the only off diagonal matrix multiplication in the loop.
A lot of general efficiency improvements can be gained by solving the individual steps directly as matrix equations instead of solving two separate steps akin to the magnetic Schrödinger equation case. Additionally, for particular use cases of this approach such as for time independent electromagnetic fields the efficiency can be improved drastically since some of the steps allow once and for all solutions of either analytic or numerical kind which can be stored in memory once and repeatedly applied during the solution step loop. We now discuss details on the particular methods used for each individual step.

5.1.2 The potential step

The potential step of the Lie four operator splitting approach to the Pauli equation is the solution to the following equation:

$$\begin{pmatrix} \mathcal{B}_1 & 0 \\ 0 & \mathcal{B}_2 \end{pmatrix} \begin{pmatrix} u_1 \\ u_2 \end{pmatrix} = \partial_t \begin{pmatrix} u_1 \\ u_2 \end{pmatrix}, \tag{5.14}$$

which is

$$\begin{pmatrix} \frac{1}{2}\mathbf{A}^2 + \phi - \frac{\epsilon}{2}B_3 & 0 \\ 0 & \frac{1}{2}\mathbf{A}^2 + \phi + \frac{\epsilon}{2}B_3 \end{pmatrix} \begin{pmatrix} u_1 \\ u_2 \end{pmatrix} = \partial_t \begin{pmatrix} u_1 \\ u_2 \end{pmatrix}. \tag{5.15}$$

As in the case of the magnetic Schrödinger equation, this step allows an analytic once and for all solution for a given system if the EM fields are independent of time. Since the derivative of the matrix exponential is exactly

$$\partial_t e^{t\mathfrak{B}} \begin{pmatrix} u_{1,0} \\ u_{2,0} \end{pmatrix} = \mathfrak{B} e^{t\mathfrak{B}} \begin{pmatrix} u_{1,0} \\ u_{2,0} \end{pmatrix}$$

meaning that

$$u(x,t) = e^{t\mathfrak{B}} \begin{pmatrix} u_{1,0}(x) \\ u_{2,0}(x) \end{pmatrix} \tag{5.16}$$

solves the potential step. More generally:

$$u(x, t+\Delta t) = e^{\Delta t \mathfrak{B}} \begin{pmatrix} u_1(x,t) \\ u_2(x,t) \end{pmatrix}. \tag{5.17}$$

If the fields are constant in time then the matrix exponential $e^{\Delta t\mathfrak{B}}$ is an analytic solution to the potential step and can be pre-computed and stored once before entering the solution step loop in order to save significant amounts of unnecessary re-computation time. If the fields depend on t either directly or via a coupling to something like the Maxwell equations then instead of this analytic solution one simply computes the ODE solution to the potential step equation via any given numerical method of adequate precision. Since this will have to be done anew in every step of the solution loop this will incur significantly higher computation costs for this step.

5.1.3 The kinetic step

The kinetic step of the Lie four operator splitting approach to the Pauli equation is the solution to the following equation:

$$\begin{pmatrix} \mathcal{A} & 0 \\ 0 & \mathcal{A} \end{pmatrix} \begin{pmatrix} u_1 \\ u_2 \end{pmatrix} = \partial_t \begin{pmatrix} u_1 \\ u_2 \end{pmatrix}, \tag{5.18}$$

which is

$$\begin{pmatrix} \frac{i\epsilon}{2}\nabla^2 & 0 \\ 0 & \frac{i\epsilon}{2}\nabla^2 \end{pmatrix} \begin{pmatrix} u_1 \\ u_2 \end{pmatrix} = \partial_t \begin{pmatrix} u_1 \\ u_2 \end{pmatrix}. \tag{5.19}$$

In essence this step is simply the solution to two free Schrödinger equations and any method suitable to solving such equations can be utilized here. In particular, as with the magnetic Schrödinger equation above, it is sensible to solve this equation in Fourier space especially considering that the next step - the advection step - can directly benefit from an already performed FFT. Instead of inverting with an IFFT after this step, one can directly pass on the still Fourier transformed data to the advection step.

5.1.4 The advection step

The advection step of the Lie four operator splitting approach to the Pauli equation is the solution to the following equation:

$$\begin{pmatrix} \mathcal{C} & 0 \\ 0 & \mathcal{C} \end{pmatrix} \begin{pmatrix} u_1 \\ u_2 \end{pmatrix} = \partial_t \begin{pmatrix} u_1 \\ u_2 \end{pmatrix}, \tag{5.20}$$

which is

$$\begin{pmatrix} \mathbf{A} \cdot \nabla & 0 \\ 0 & \mathbf{A} \cdot \nabla \end{pmatrix} \begin{pmatrix} u_1 \\ u_2 \end{pmatrix} = \partial_t \begin{pmatrix} u_1 \\ u_2 \end{pmatrix}. \tag{5.21}$$

As with the kinetic step, the solution to this step is equivalent to performing the advection step solution for the magnetic Schrödinger equation twice - once for the spin up and once for the spin down state. The fundamental idea here remains the same, as each of the two equations is a three dimensional advection equation which can be solved using the method of characteristics. To this end, one first notes that the characteristic equation at a particular grid point x^j here (just as with the magnetic Schrödinger equation, compare [1]) would be:

$$\frac{\partial x_C^j(t)}{\partial t} = -\mathbf{A}(x_C^j(t)), \tag{5.22}$$

$$x_C^j(t_n + \Delta t) = x^j, \tag{5.23}$$

$$t \in [t_n, t_n + \Delta t] \tag{5.24}$$

By $x_C^j(t)$ we denote the characteristic which at time $t_n + \Delta t$ passes through our grid point x^j. The desired solutions to the characteristic equation are the values for $x_C^j(t_n)$, i.e. one time step backwards, which are solutions to the characteristic equation above with respective end points at the known grid points x_j. For a temporally constant magnetic field potential this can be pre-computed and stored once and for all for a given field configuration before entering the solution loop. For time dependent fields the equation changes to a non-autonomous form which increases the computational as well as storage cost. Many different numerical methods can be used to solve this equation as long as the order of accuracy remains consistent with the method used for the other steps and the desired outcome. Essentially what one does here is a backwards time step using an ODE solver. In the case of our implementation we used a simple explicit midpoint method and any sufficiently accurate explicit finite difference method will generally suffice (compare [1]).
Solving the characteristic equation at each point of our spatial grid provides us with another point on the characteristic on which the solution to the advection equation would be constant, meaning we can obtain the desired $u(x^j, t_n + \Delta t)$ simply via $u(x^j, t_n + \Delta t) = u(x_C^j, t_n)$. However, quite naturally it is not reasonable to expect these new points x_C^j on the characteristics to themselves lie on our discretized spatial grid, so while we have $u(x^j, t_n)$ at all grid points x^j, we do not have the values of this function at the desired points x_C^j. This calls for an interpolation: If we can use an interpolation method to approximate $u(x_C^j, t_n)$ based on our knowledge of $u(x^j, t_n)$, then we can use this interpolation to obtain $u(x^j, t_n + \Delta t) = u(x_C^j, t_n)$.
There are several ways to interpolate u in this way and we have already provided the list that Caliari et al. discuss for the case of the magnetic Schrödinger equation in the relevant section on their method. For our Pauli equation case, the Fourier

space interpolation is extremely natural for the implementation, as the FFT of the wave functions was already computed in the kinetic step and can directly be passed on to the advection step. This means that we can simply use a canonical Fourier interpolation of functions to get the values at the points $u(x_C^j, t_n)$ (for a very good and short resource on how this is in general done, see for example [36]).
To summarize: The kinetic step hands an already Fourier transformed dataset to the advection step solver. This advection step solver already has a pre-computed set of points of interest x_C^j . Given the Fourier transformed data $\hat{u}(x^j, t_n)$, we interpolate to $u(x_C^j, t_n)$ using Fourier interpolation. Per the method of characteristics, the value of the functions at these points is the same as those we desire, i.e. $u(x^j, t_n + \Delta t) = u(x_C^j, t_n)$. Since the Fourier interpolation inherently performs an inverse Fourier transform we can pass on the data from this step to the coupling step without having to perform any additional inverse Fourier transforms.

5.1.5 The coupling step

The coupling step of the Lie four operator splitting approach to the Pauli equation is the solution to the following equation:

$$\begin{pmatrix} 0 & \mathcal{D}_1 \\ \mathcal{D}_2 & 0 \end{pmatrix} \begin{pmatrix} u_1 \\ u_2 \end{pmatrix} = \partial_t \begin{pmatrix} u_1 \\ u_2 \end{pmatrix}, \tag{5.25}$$

which is

$$\begin{pmatrix} 0 & -\frac{\epsilon}{2}B_1 + \frac{i\epsilon}{2}B_2 \\ -\frac{\epsilon}{2}B_1 - \frac{i\epsilon}{2}B_2 & 0 \end{pmatrix} \begin{pmatrix} u_1 \\ u_2 \end{pmatrix} = \partial_t \begin{pmatrix} u_1 \\ u_2 \end{pmatrix}. \tag{5.26}$$

Unlike the previous three steps and as the name implies, this is a coupled system of equations with off-diagonal components. In principle this is just another ODE system, which could be combined with the potential step if the conceptional reduction of steps would be the goal. However, for most implementation as well as testing purposes it is easier to handle the coupling aspect of the equations all at once and treat the two parts of the Pauli equation as separate equations for the other three steps. Once again, significant computational costs can be saved if the fields are taken to be temporally constant, as the solution just as for the potential step is then simply given by the matrix exponential:

$$\begin{pmatrix} u_1(x, t + \Delta t) \\ u_2(x, t + \Delta t) \end{pmatrix} = e^{\Delta t \mathfrak{D}} \begin{pmatrix} u_1(x, t) \\ u_2(x, t) \end{pmatrix} \tag{5.27}$$

where care needs to be taken to perform a true matrix exponential operation and not merely an exponentiation of the diagonal components, as that is only a valid way to perform a matrix exponential if the given matrix is diagonal. If the fields indeed are constant in time then this solution can also be pre-computed outside of the solution loop, stored and called whenever it is time to perform the coupling step instead of perpetually re-computing the solution. Just as with the potential step if one were to work with time dependent EM fields, either directly or via something like the Maxwell equations, then the system of equation can instead be solved with any of the many efficient methods to solve such a system of ODEs to desired accuracy. The computational cost this will incur is significant, as this coupled ODE solution would then of course have to be re-computed in every step of the solution loop. In fact, for

time dependent EM fields it is almost certainly necessary to combine the potential and coupling step into a single operator and equation as follows:

$$\begin{pmatrix} \frac{1}{2}\mathbf{A}^2 + \phi - \frac{\epsilon}{2}B_3 & -\frac{\epsilon}{2}B_1 + \frac{i\epsilon}{2}B_2 \\ -\frac{\epsilon}{2}B_1 - \frac{i\epsilon}{2}B_2 & \frac{1}{2}\mathbf{A}^2 + \phi + \frac{\epsilon}{2}B_3 \end{pmatrix} \begin{pmatrix} u_1 \\ u_2 \end{pmatrix} = \partial_t \begin{pmatrix} u_1 \\ u_2 \end{pmatrix} \tag{5.28}$$

because solving this equation instead of the potential and coupling step separately means that during each solution step in the loop we only need to call an ODE system solver once instead of twice.

6 Numerical experiments

A proof of concept of the methodology outlined in section 5 has been implemented in the programming language Julia [2]. This section describes the performed numerical experiments and presents their results.
All listed numerical experiments were performed on a three dimensional $10 \times 10 \times 10$ spacial grid with spatial stepsize 0.5 between the grid points and time stepsize 0.1. The scaling parameter ϵ was set to 1. We present numerical results in terms of selected xy-plane contour plot cuts of the wave function at $z = 0$, showing the absolute values, real parts and imaginary parts of both the spin up and the spin down states at different times during the simulation.

6.1 Set #1: Single peaked initial state

This set was performed using the initial state

$$u_1(x, 0) = \pi^{-3/2} \left(e^{-(x-4)^2-(y-4)^2-(z)^2} \right), \tag{6.1}$$

$$u_2(x, 0) = 0. \tag{6.2}$$

This ensures that the state's initial spin up z-peak lies in the xy-plane and produces one Gaussian wave packet centered around $(4, 4, 0)$. The initial spin down state is zero. This initial state is the same for all the different EM-field setups in this set, so we only print the initial state once in Figure 2.

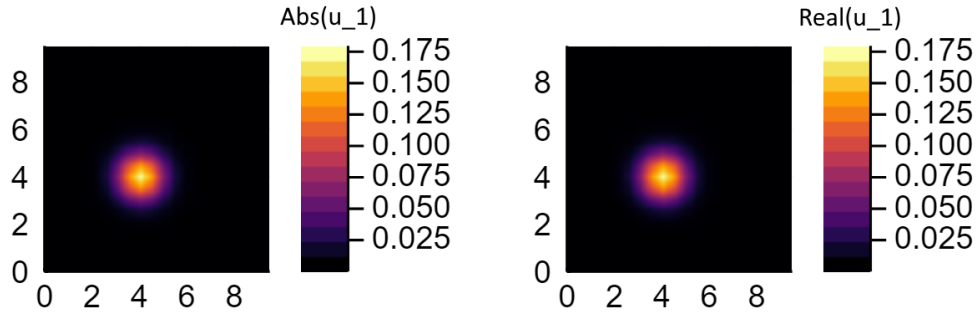

Figure 2: Contour plots of initialized state at $t = 0$ used in set #1. Plots show values indicated in the legend in the xy-plane where $z = 0$. Since the imaginary parts and u_2 are zero they are not shown.

6.1.1 Vanishing EM-fields

Initially we set

$$\mathbf{A} = 0, \quad \phi = 0. \tag{6.3}$$

Under vanishing EM fields there is no coupling or mixing between spin up and spin down states. Figure 3 shows the system at $t = 0.4$ and Figure 4 shows the system at $t = 2.0$.

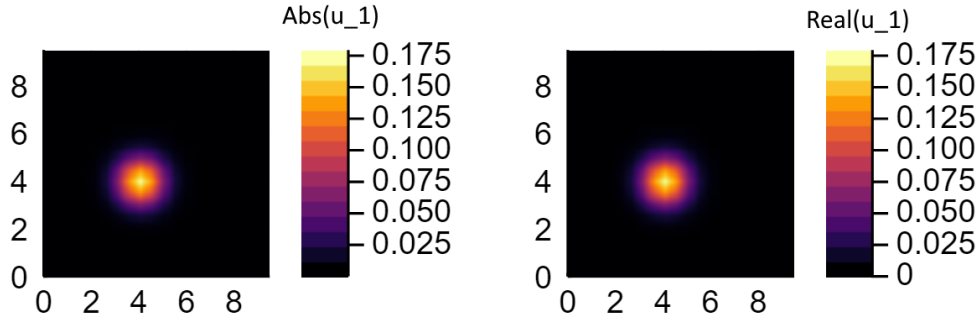

Figure 3: Contour plots of state at $t = 0.4$. Plots show values indicated in the legend in the xy-plane where $z = 0$. Since the imaginary parts and u_2 are zero they are not shown.

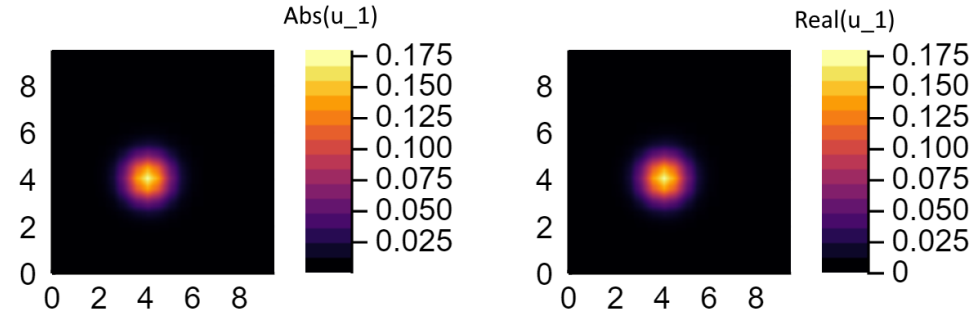

Figure 4: Contour plots of state at $t = 2.0$. Plots show values indicated in the legend in the xy-plane where $z = 0$. Since the imaginary parts and u_2 are zero they are not shown.

6.1.2 Constant magnetic field in z direction

Next we set the magnetic field to be constant in z direction with a still vanishing electric potential, specifically:

$$\mathbf{A} = (y, -x, 0), \tag{6.4}$$

$$\mathbf{B} = (0, 0, -2) \tag{6.5}$$

$$\phi = 0. \tag{6.6}$$

Since the z component of the EM fields does not enter into the coupling term, we again observe no such coupling. Figure 5 shows the system at $t = 0.1$. Figure 6 shows the system at $t = 0.2$. Figure 7 shows the system at $t = 0.3$.

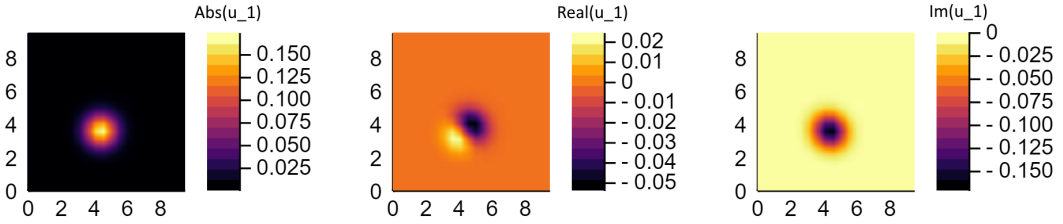

Figure 5: Contour plots of state at $t = 0.1$ in the xy-plane where $z = 0$. Since u_2 remains zero it is not shown.

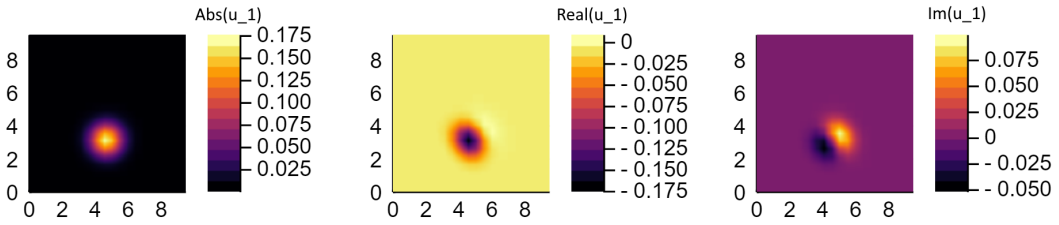

Figure 6: Contour plots of state at $t = 0.2$ in the xy-plane where $z = 0$. Since u_2 remains zero it is not shown.

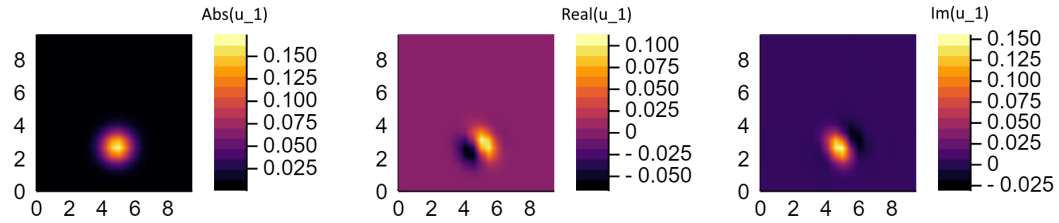

Figure 7: Contour plots of state at $t = 0.3$ in the xy-plane where $z = 0$. Since u_2 remains zero it is not shown.

6.1.3 Constant magnetic field in y direction

Next we set the magnetic field to be constant in y direction, also with a vanishing electric potential, specifically:

$$\mathbf{A} = (0, 0, x), \tag{6.7}$$

$$\mathbf{B} = (0, -1, 0), \tag{6.8}$$

$$\phi = 0. \tag{6.9}$$

With one of the non-z components of $\mathbf{B}$ being non-zero now, we observe coupling between the spin up and spin down state. We also observe that the peak of the state now leaves the xy-plane where $z = 0$ causing a gradual decrease in the height of the peak in that plane. Figure 8 shows the system at $t = 0.1$, Figure 9 shows the system at $t = 0.2$, Figure 10 shows the system at $t = 0.3$ and Figure 11 shows the system at $t = 0.4$.

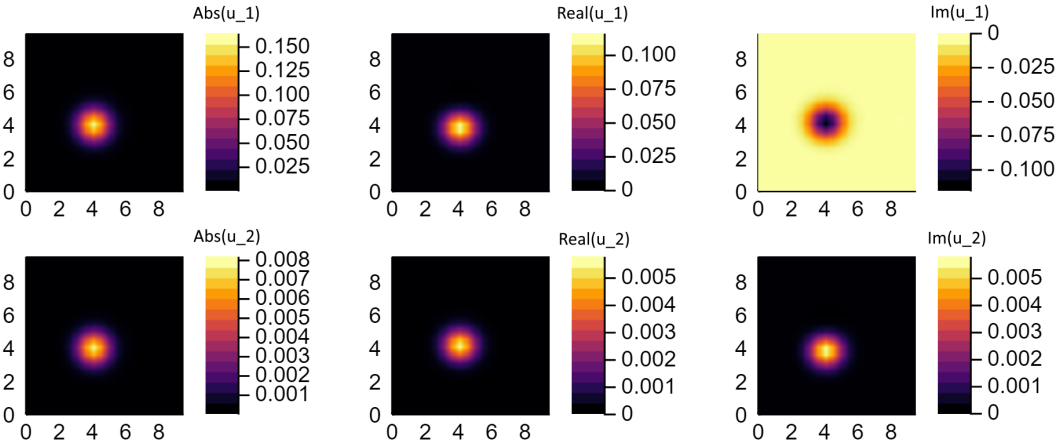

Figure 8: Contour plots of state at $t = 0.1$ in the xy-plane where $z = 0$.

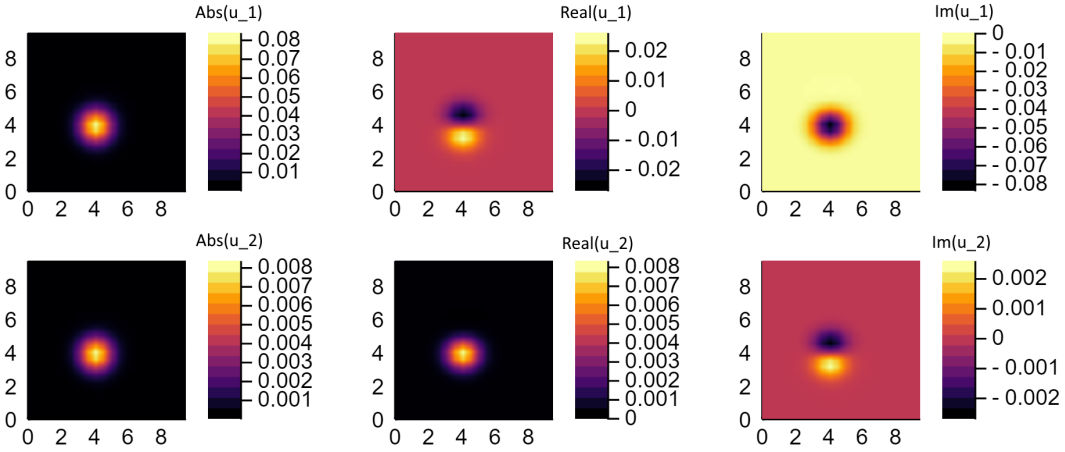

Figure 9: Contour plots of state at $t = 0.2$ in the xy-plane where $z = 0$.

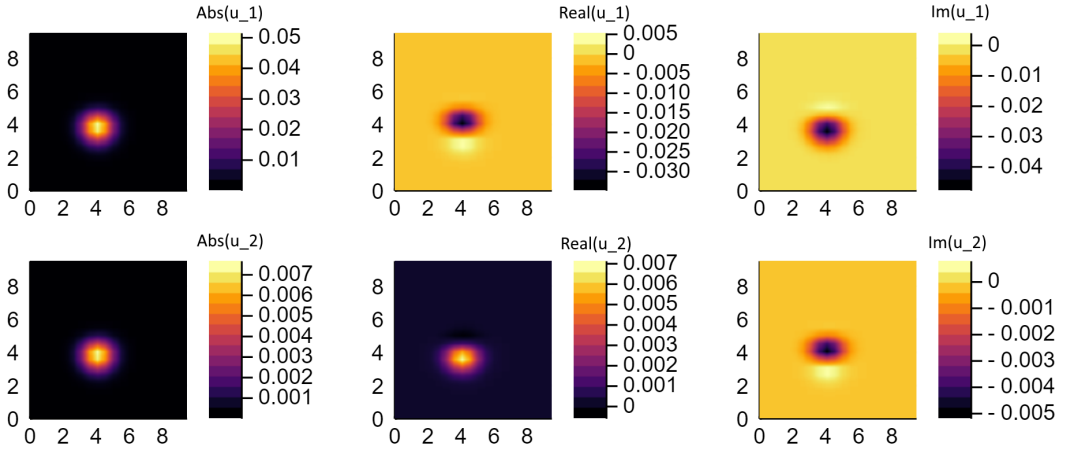

Figure 10: Contour plots of state at $t = 0.3$ in the xy-plane where $z = 0$.

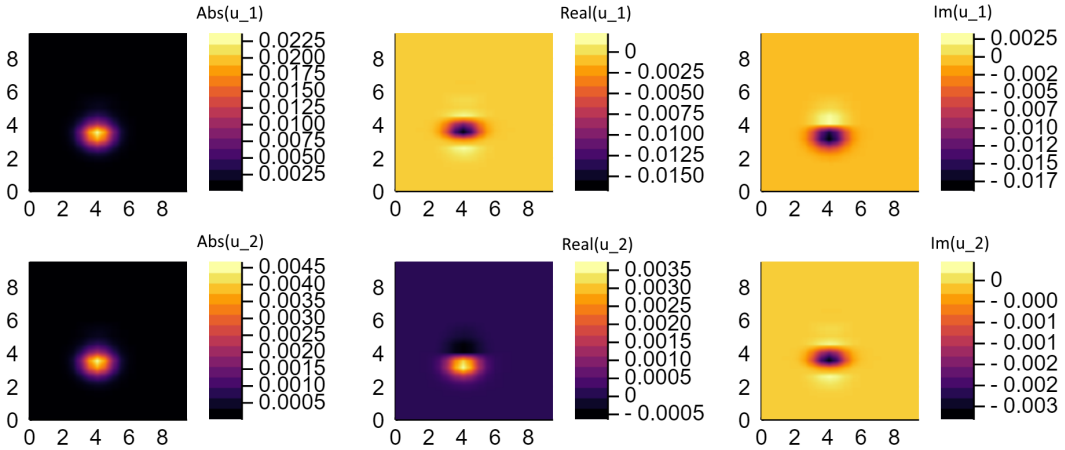

Figure 11: Contour plots of state at $t = 0.4$ in the xy-plane where $z = 0$.

6.1.4 Sinusoidal electromagnetic potentials

The final setup of this set is inspired by the electromagnetic fields used in [1] which have a sinusoidal form:

$$\mathbf{A} = \begin{pmatrix} \sin\left(\frac{\pi}{10}(y+5)\right) + \sin\left(\frac{\pi}{10}(z+5)\right) \\ \sin\left(\frac{\pi}{10}(x+5)\right) + \sin\left(\frac{\pi}{10}(z+5)\right) \\ \sin\left(\frac{\pi}{10}(x+5)\right) + \sin\left(\frac{\pi}{10}(y+5)\right) \end{pmatrix}, \tag{6.10}$$

$$\mathbf{B} = \begin{pmatrix} \frac{\pi}{5}\cos\left(\frac{\pi}{5}(y+5)\right) - \frac{\pi}{5}\cos\left(\frac{\pi}{5}(z+5)\right) \\ -\frac{\pi}{5}\cos\left(\frac{\pi}{5}(x+5)\right) + \frac{\pi}{5}\cos\left(\frac{\pi}{5}(z+5)\right) \\ \frac{\pi}{5}\cos\left(\frac{\pi}{5}(x+5)\right) - \frac{\pi}{5}\cos\left(\frac{\pi}{5}(y+5)\right) \end{pmatrix}, \quad \phi = 0. \tag{6.11}$$

Figures 12 to 16 show excerpts of the system at different times ranging from $t = 0.2$ to $t = 1.0$.

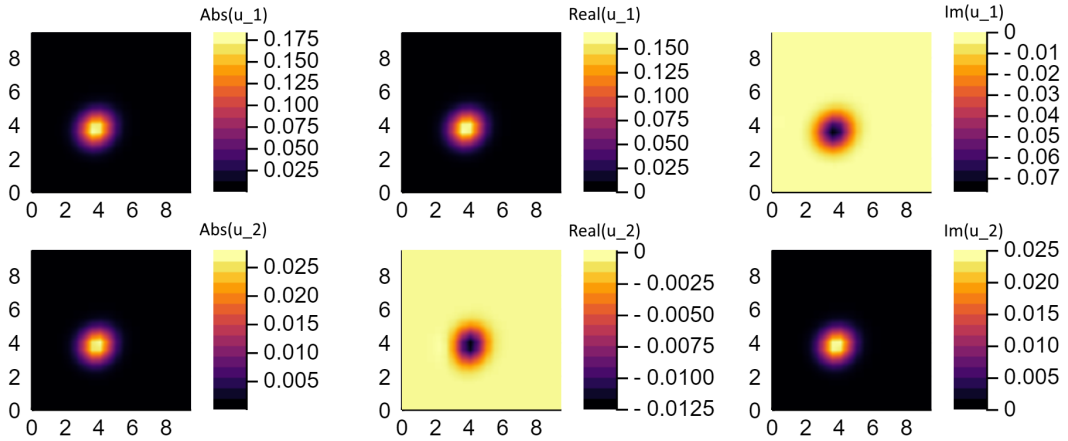

Figure 12: Contour plots of state at $t = 0.2$ in the xy-plane where $z = 0$.

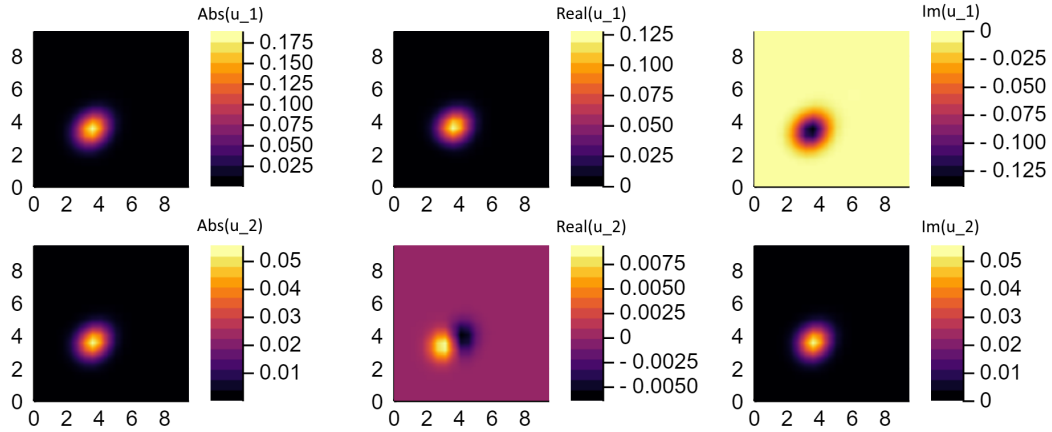

Figure 13: Contour plots of state at $t = 0.4$ in the xy-plane where $z = 0$.

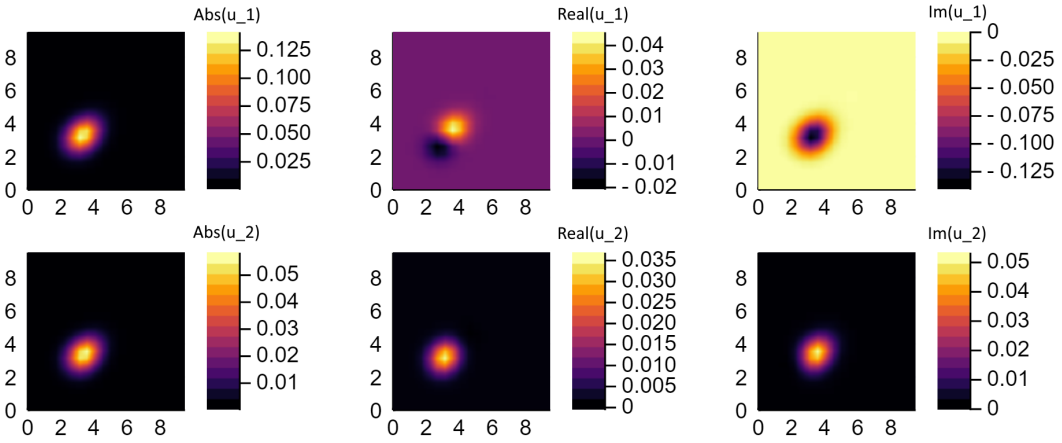

Figure 14: Contour plots of state at $t = 0.6$ in the xy-plane where $z = 0$.

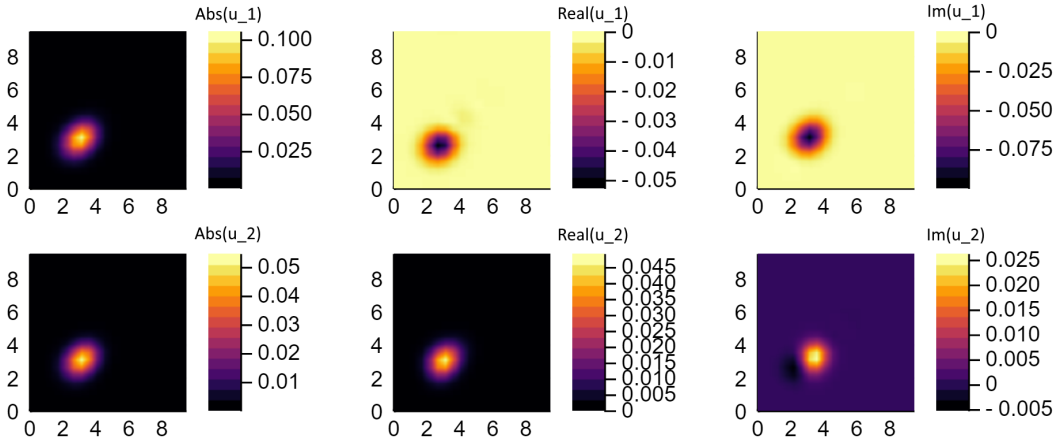

Figure 15: Contour plots of state at $t = 0.8$ in the xy-plane where $z = 0$.

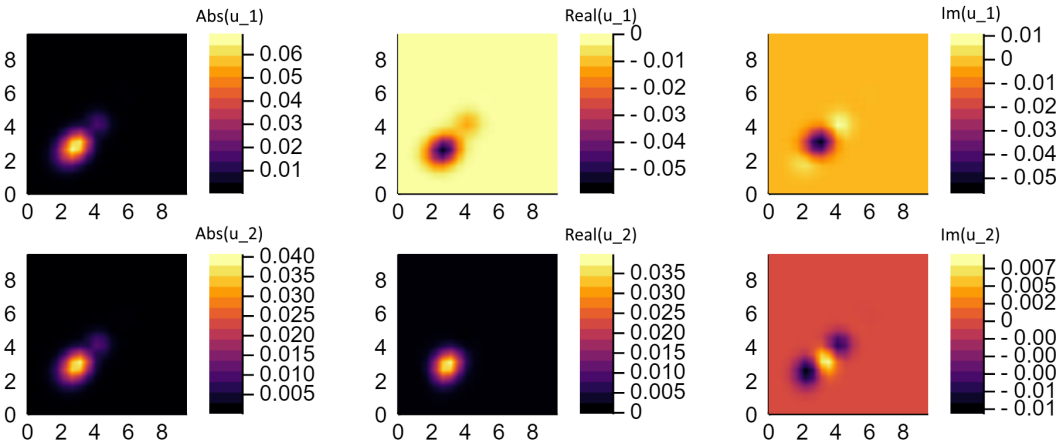

Figure 16: Contour plots of state at $t = 1.0$ in the xy-plane where $z = 0$.

6.2 Set #2: Double peaked initial state

This set was performed using the initial state

$$u_1(x,0) = \pi^{-3/2}\left(e^{-(x-4)^2-(y-4)^2-(z)^2} + e^{-(x-6)^2-(y-6)^2-(z)^2}\right), \tag{6.12}$$

$$u_2(x,0) = 0. \tag{6.13}$$

Figure 17 shows the non-zero parts of the initialized state at $t = 0$.

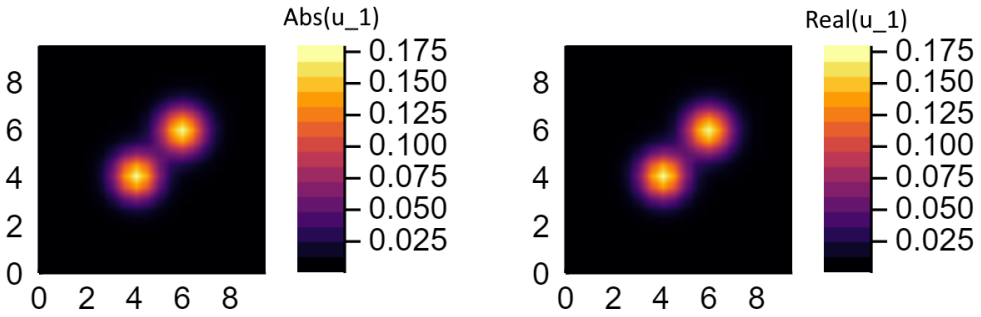

Figure 17: Contour plots of initialized state at $t = 0$ used in set #2. Plots show values indicated in the legend in the xy-plane where $z = 0$. Since the imaginary parts and u_2 are zero they are not shown.

6.2.1 Constant magnetic field in z direction

We test the double peaked system for a constant magnetic field in z direction:

$$\mathbf{A} = (y, -x, 0), \tag{6.14}$$

$$\mathbf{B} = (0, 0, -2) \tag{6.15}$$

$$\phi = 0. \tag{6.16}$$

Since only the z-component of the magnetic field is non vanishing we observe no spin coupling. Figure 18 shows the system at $t = 0.2$ and Figure 19 shows the system at $t = 0.4$.

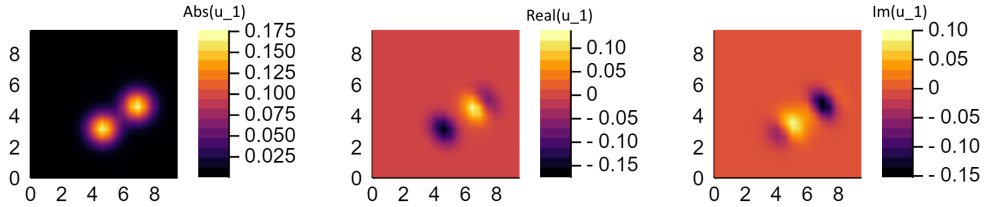

Figure 18: Contour plots of state at $t = 0.2$ in the xy-plane where $z = 0$. Since u_2 and imaginary parts remains zero they are not shown.

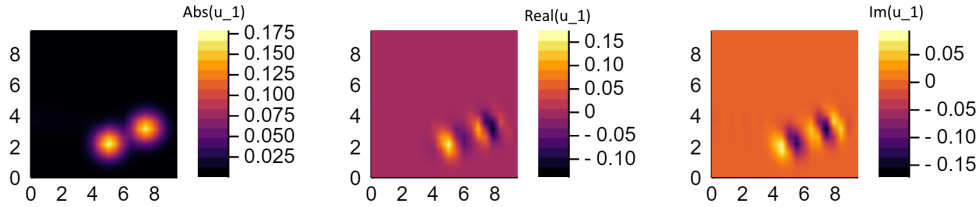

Figure 19: Contour plots of state at $t = 2.0$ in the xy-plane where $z = 0$. Since u_2 and imaginary parts remains zero they are not shown.

6.2.2 Sinusoidal electromagnetic potentials

The final choice of EM fields for set #2 is the sinusoidal fields inspired by [1]:

$$\mathbf{A} = \begin{pmatrix} \sin\left(\frac{\pi}{10}(y+5)\right) + \sin\left(\frac{\pi}{10}(z+5)\right) \\ \sin\left(\frac{\pi}{10}(x+5)\right) + \sin\left(\frac{\pi}{10}(z+5)\right) \\ \sin\left(\frac{\pi}{10}(x+5)\right) + \sin\left(\frac{\pi}{10}(y+5)\right) \end{pmatrix}, \tag{6.17}$$

$$\mathbf{B} = \begin{pmatrix} \frac{\pi}{5}\cos\left(\frac{\pi}{5}(y+5)\right) - \frac{\pi}{5}\cos\left(\frac{\pi}{5}(z+5)\right) \\ -\frac{\pi}{5}\cos\left(\frac{\pi}{5}(x+5)\right) + \frac{\pi}{5}\cos\left(\frac{\pi}{5}(z+5)\right) \\ \frac{\pi}{5}\cos\left(\frac{\pi}{5}(x+5)\right) - \frac{\pi}{5}\cos\left(\frac{\pi}{5}(y+5)\right) \end{pmatrix}, \quad \phi = 0. \tag{6.18}$$

Figure 20 shows the system at $t = 0.2$, Figure 21 shows the system at $t = 0.4$, Figure 22 shows the system at $t = 0.6$ and Figure 23 shows the system at $t = 0.8$.

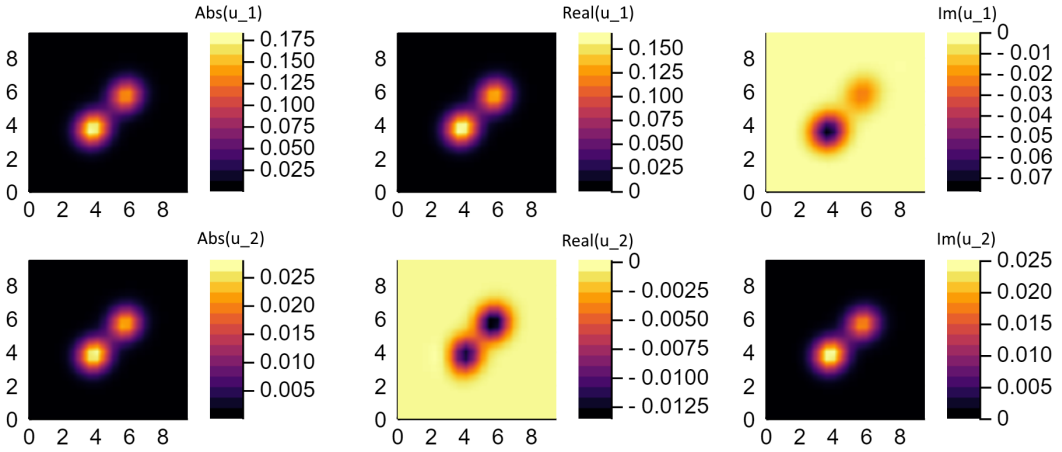

Figure 20: Contour plots of state at $t = 0.2$ in the xy-plane where $z = 0$.

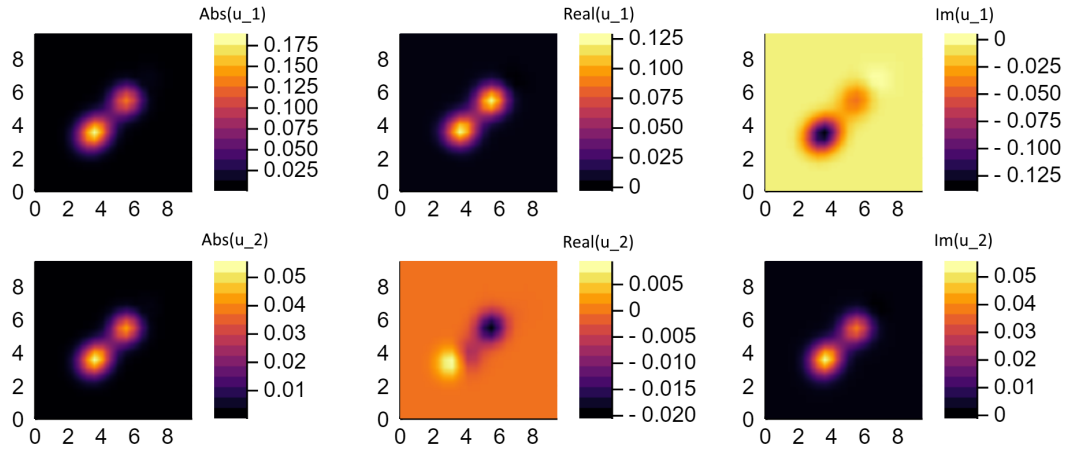

Figure 21: Contour plots of state at $t = 0.4$ in the xy-plane where $z = 0$.

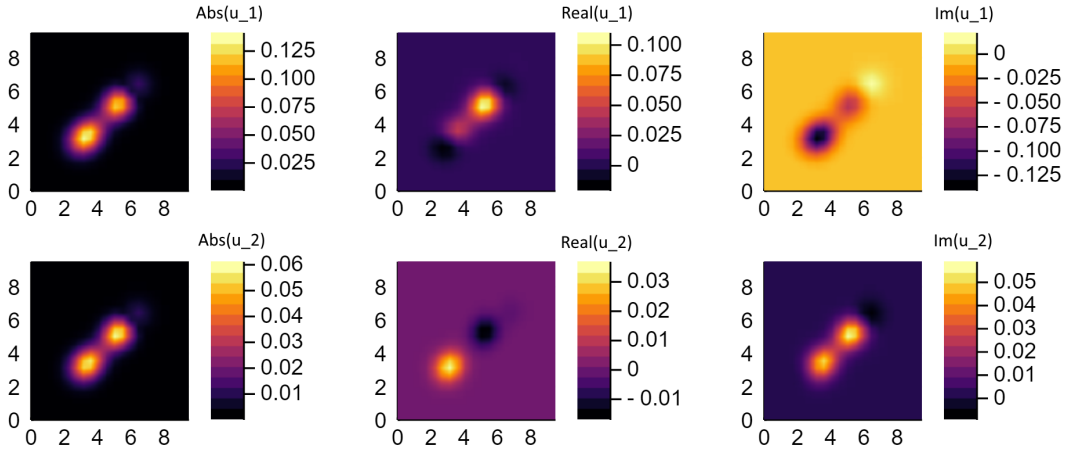

Figure 22: Contour plots of state at $t = 0.6$ in the xy-plane where $z = 0$.

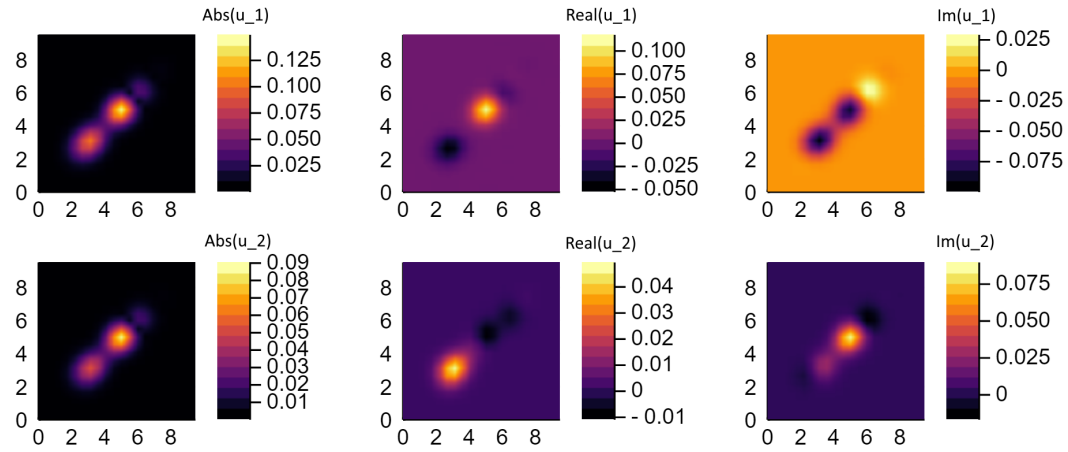

Figure 23: Contour plots of state at $t = 0.8$ in the xy-plane where $z = 0$.

6.3 Set #3: Triple peaked initial state

For the purposes of the third set of numerical experiments we will not only add a third peak to the initial state of the system but initialize said third peak as a spin down state with negative real part. The initial state is then as follows:

$$u_1(x,0) = \pi^{-3/2}\left(e^{-(x-4)^2-(y-4)^2-(z)^2} + e^{-(x-6)^2-(y-6)^2-(z)^2}\right), \tag{6.19}$$

$$u_2(x,0) = -\pi^{-3/2}e^{-(x-4)^2-(y-4)^2-(z)^2}. \tag{6.20}$$

We show a contour plot of the initial state in the xy-plane where $z = 0$ in Figure 24.

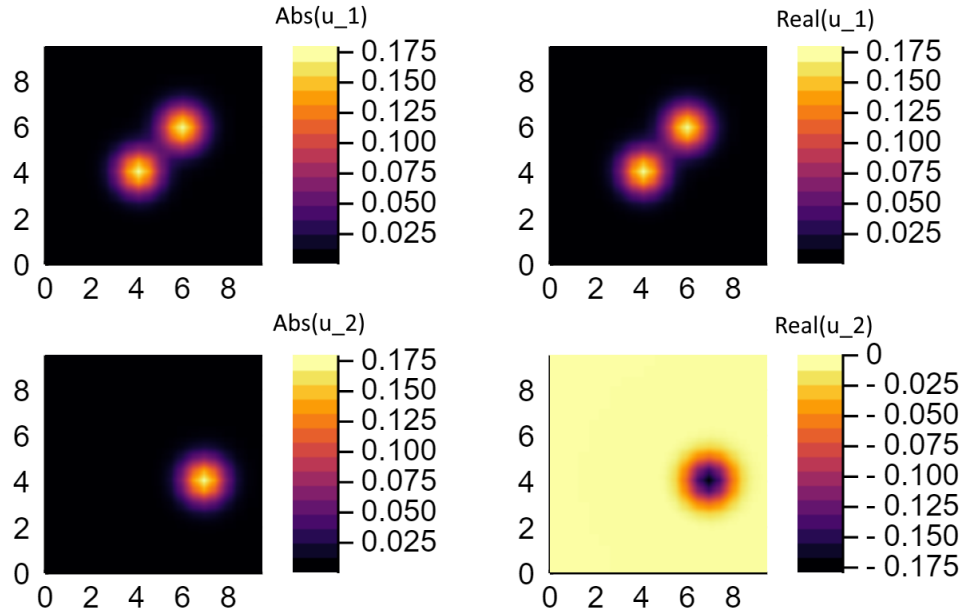

Figure 24: Contour plots of initialized state at $t = 0$ used in set #3. Plots show values indicated in the legend in the xy-plane where $z = 0$. Since the imaginary parts are zero they are not shown.

6.3.1 Sinusoidal electromagnetic potentials

As before this set is inspired by the electromagnetic fields used in [1] which have a sinusoidal form:

$$\mathbf{A} = \begin{pmatrix} \sin\left(\frac{\pi}{10}(y+5)\right) + \sin\left(\frac{\pi}{10}(z+5)\right) \\ \sin\left(\frac{\pi}{10}(x+5)\right) + \sin\left(\frac{\pi}{10}(z+5)\right) \\ \sin\left(\frac{\pi}{10}(x+5)\right) + \sin\left(\frac{\pi}{10}(y+5)\right) \end{pmatrix}, \tag{6.21}$$

$$\mathbf{B} = \begin{pmatrix} \frac{\pi}{5}\cos\left(\frac{\pi}{5}(y+5)\right) - \frac{\pi}{5}\cos\left(\frac{\pi}{5}(z+5)\right) \\ -\frac{\pi}{5}\cos\left(\frac{\pi}{5}(x+5)\right) + \frac{\pi}{5}\cos\left(\frac{\pi}{5}(z+5)\right) \\ \frac{\pi}{5}\cos\left(\frac{\pi}{5}(x+5)\right) - \frac{\pi}{5}\cos\left(\frac{\pi}{5}(y+5)\right) \end{pmatrix}, \quad \phi = 0. \tag{6.22}$$

Figure 25 shows the system at $t = 0.2$, Figure 26 shows the system at $t = 0.4$ and Figure 27 shows the system at $t = 0.6$.

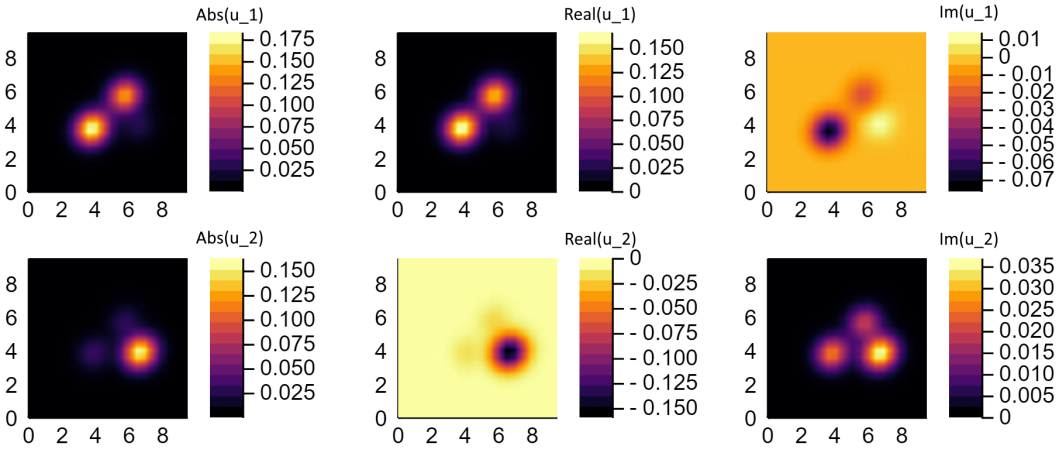

Figure 25: Contour plots of state at $t = 0.2$ in the xy-plane where $z = 0$.

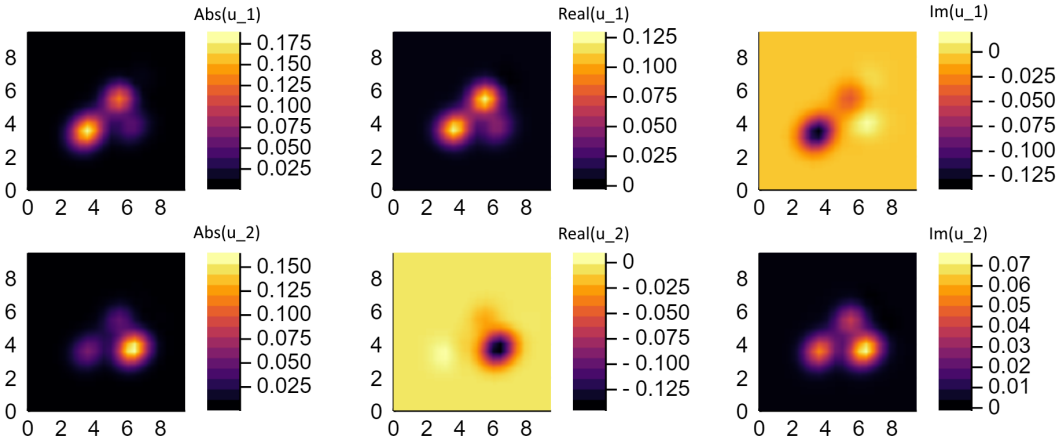

Figure 26: Contour plots of state at $t = 0.4$ in the xy-plane where $z = 0$.

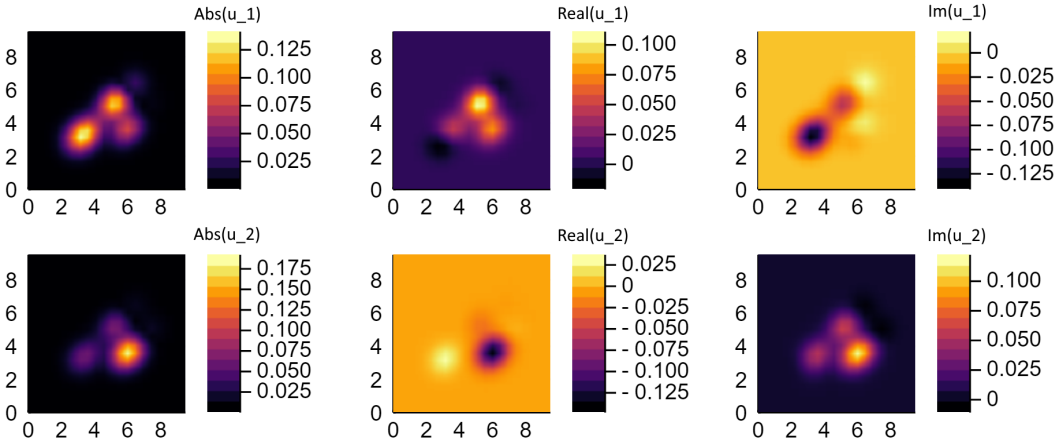

Figure 27: Contour plots of state at $t = 0.6$ in the xy-plane where $z = 0$.

6.4 Set #4: More complex single peaked initial state

The fourth set of numerical experiments performed for this thesis is not a sum of simple Gaussian wave packets as the previous ones were but a slightly more complex state based on a similar numerical experiment performed in [35]. The state is initialized with:

$$u_1(x,0) = \frac{1-((x-6)^2+(y-3)^2+z^2)}{\pi^{3/2}} e^{-(x-6)^2-(y-3)^2-z^2}, \tag{6.23}$$

$$u_2(x,0) = 0. \tag{6.24}$$

We show a contour plot of the initial state in the xy-plane where $z = 0$ in Figure 28.

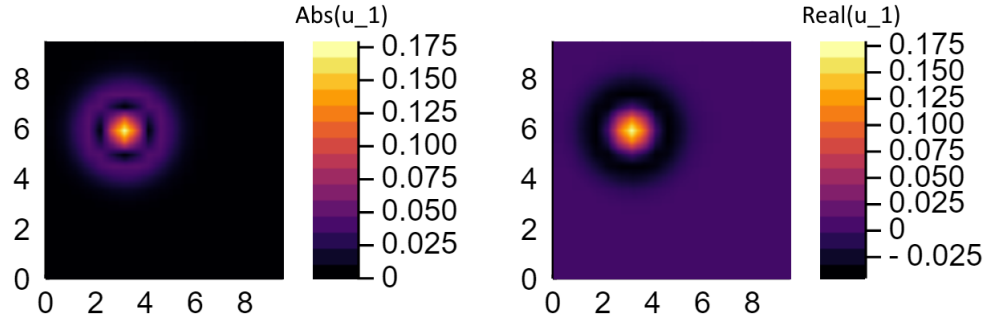

Figure 28: Contour plots of initialized state at $t = 0$ used in set #4. Plots show values indicated in the legend in the xy-plane where $z = 0$. Since the imaginary parts are zero they are not shown.

6.4.1 Confining ϕ and constant B in y direction

We use a confining electric potential and constant magnetic field in y direction, again inspired by a numerical experiment performed in [35]:

$$\mathbf{A} = (y, -x, 0), \tag{6.25}$$

$$\mathbf{B} = (0, 0, -2) \tag{6.26}$$

$$\phi = -2\left((x-4)^2+(y-4)^2+z^2\right). \tag{6.27}$$

Figures 29 to 32 show the system from $t = 0.11$ to $t = 0.44$. To ensure a sensible numerical result in the presence of this ϕ potential, the time step had to be reduced from 0.1 to at least 0.01.

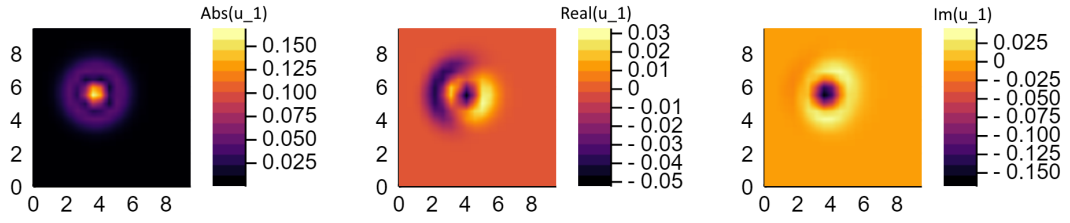

Figure 29: Contour plots of state at $t = 0.11$ in the xy-plane where $z = 0$.

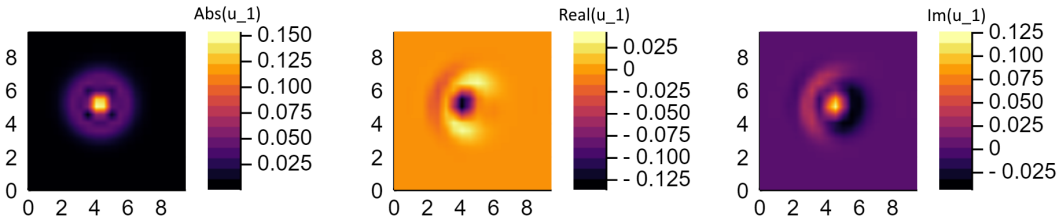

Figure 30: Contour plots of state at $t = 0.22$ in the xy-plane where $z = 0$.

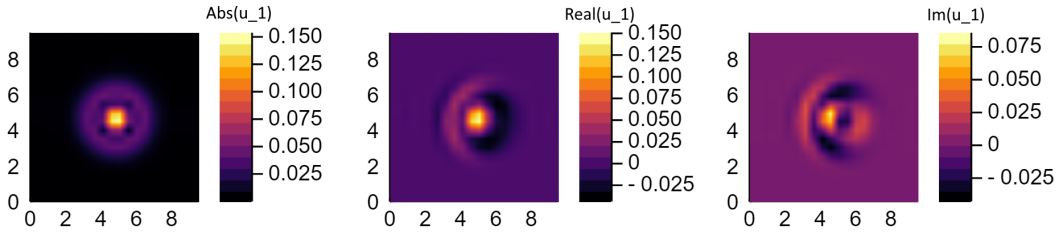

Figure 31: Contour plots of state at $t = 0.33$ in the xy-plane where $z = 0$.

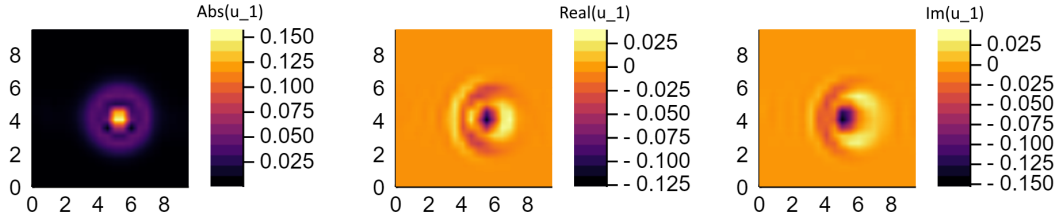

Figure 32: Contour plots of state at $t = 0.44$ in the xy-plane where $z = 0$.

6.5 Set #5: More complex double peaked initial state

For the fifth and final set of numerical experiments, the chosen initial state is a sum of an up state like in set #4 along with an analogous down state:

$$u_1(x,0) = \frac{1-((x-6)^2+(y-3)^2+z^2)}{\pi^{3/2}} e^{-(x-6)^2-(y-3)^2-z^2}, \tag{6.28}$$

$$u_2(x,0) = \frac{1-((x-3)^2+(y-6)^2+z^2)}{\pi^{3/2}} e^{-(x-3)^2-(y-6)^2-z^2}. \tag{6.29}$$

We show a contour plot of the initial state in the xy-plane where $z = 0$ in Figure 33.

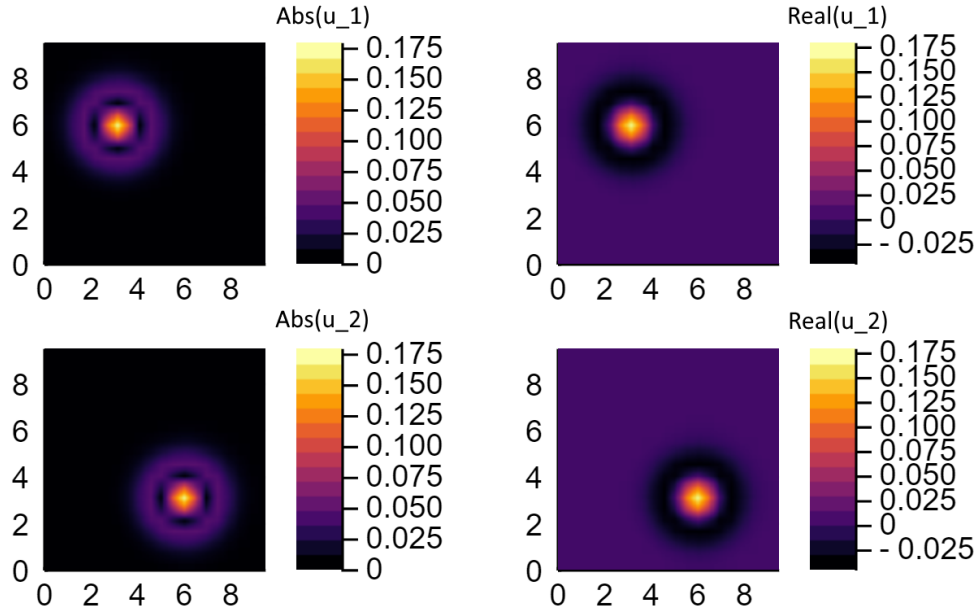

Figure 33: Contour plots of initialized state at $t = 0$ used in set #5. Plots show values indicated in the legend in the xy-plane where $z = 0$. Since the imaginary parts are zero they are not shown.

6.5.1 Sinusoidal electromagnetic potentials

As before this set is inspired by the electromagnetic fields used in [1] which have a sinusoidal form:

$$\mathbf{A} = \begin{pmatrix} \sin\left(\frac{\pi}{10}(y+5)\right) + \sin\left(\frac{\pi}{10}(z+5)\right) \\ \sin\left(\frac{\pi}{10}(x+5)\right) + \sin\left(\frac{\pi}{10}(z+5)\right) \\ \sin\left(\frac{\pi}{10}(x+5)\right) + \sin\left(\frac{\pi}{10}(y+5)\right) \end{pmatrix}, \tag{6.30}$$

$$\mathbf{B} = \begin{pmatrix} \frac{\pi}{5}\cos\left(\frac{\pi}{5}(y+5)\right) - \frac{\pi}{5}\cos\left(\frac{\pi}{5}(z+5)\right) \\ -\frac{\pi}{5}\cos\left(\frac{\pi}{5}(x+5)\right) + \frac{\pi}{5}\cos\left(\frac{\pi}{5}(z+5)\right) \\ \frac{\pi}{5}\cos\left(\frac{\pi}{5}(x+5)\right) - \frac{\pi}{5}\cos\left(\frac{\pi}{5}(y+5)\right) \end{pmatrix}, \quad \phi = 0. \tag{6.31}$$

Figures 34 to 38 show the system from $t = 0.2$ to $t = 1.0$.

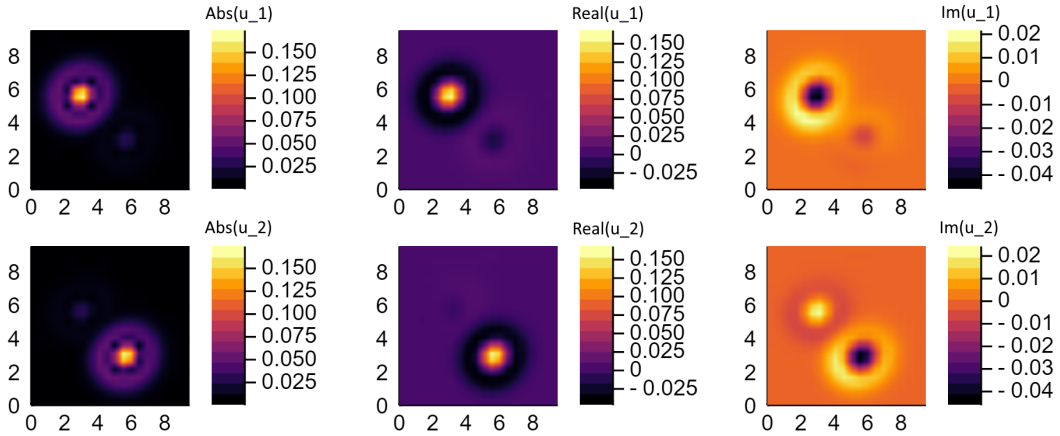

Figure 34: Contour plots of state at $t = 0.2$ in the xy-plane where $z = 0$.

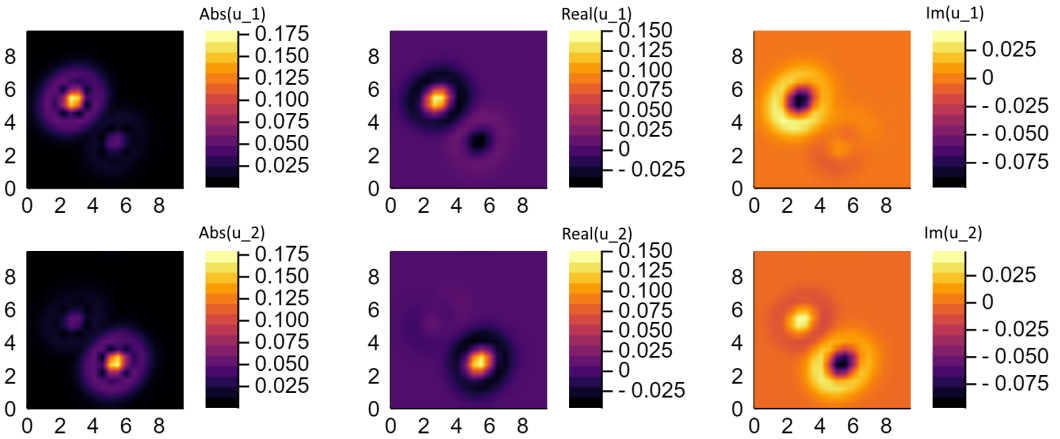

Figure 35: Contour plots of state at $t = 0.4$ in the xy-plane where $z = 0$.

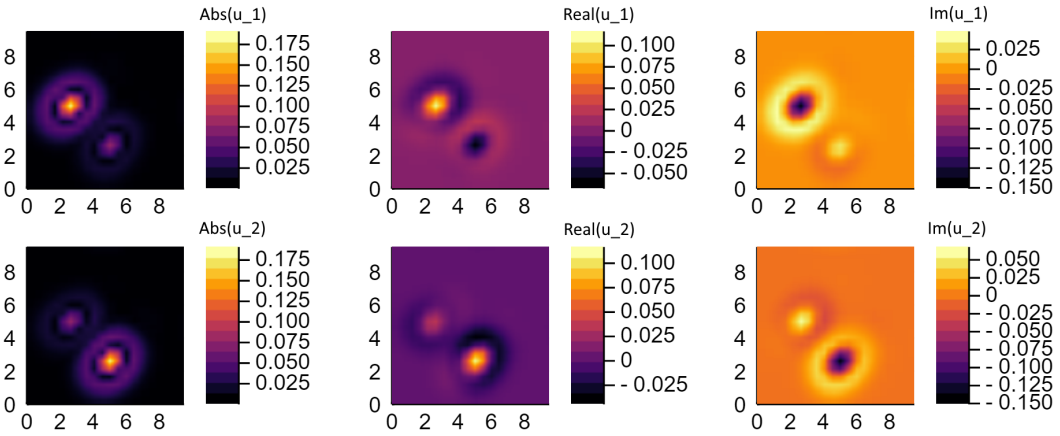

Figure 36: Contour plots of state at $t = 0.6$ in the xy-plane where $z = 0$.

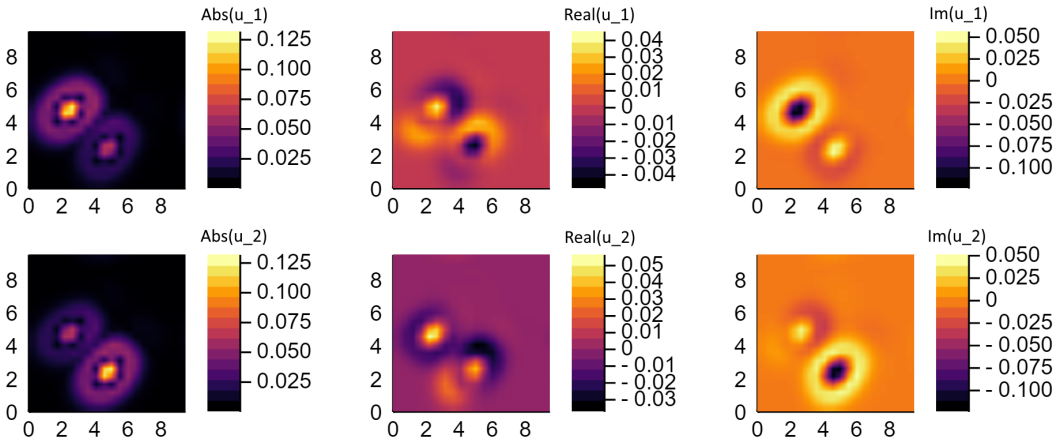

Figure 37: Contour plots of state at $t = 0.8$ in the xy-plane where $z = 0$.

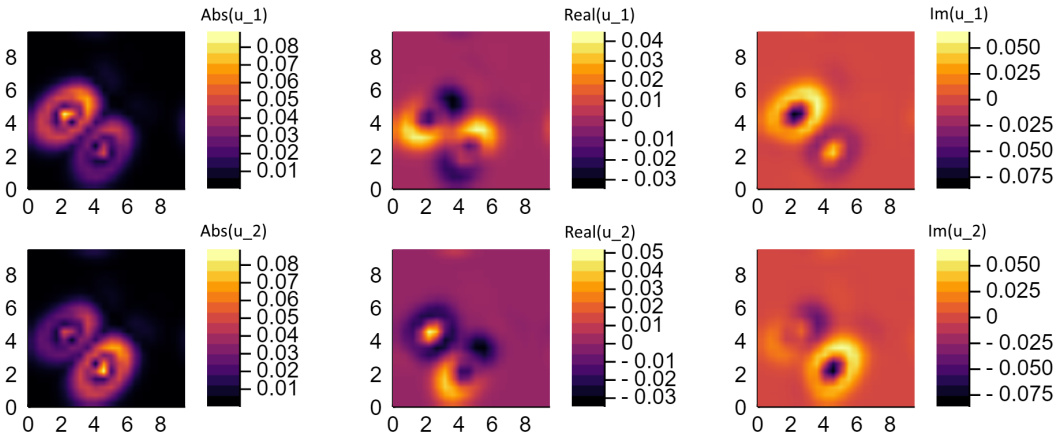

Figure 38: Contour plots of state at $t = 1.0$ in the xy-plane where $z = 0$.

7 Discussion

In this paper we have presented an operator splitting method for the Pauli equation system based on previous work on the magnetic Schrödinger equation due to [1] and [33]. We have also presented numerical experiments generated using a Julia language implementation of this procedure.
A number of open questions remain: Regarding the numerical four operator splitting method, a proof of stability and convergence of the scheme in analogy to [1] is desirable and currently in the works. Furthermore, the numerical implementation at present only covers time independent electromagnetic fields and a more general implementation is needed to observe potentially far more complex phenomena in numerical experiments. Applying this methodology for time dependent fields has already been theoretically covered in this paper and the implementation is straightforward but so far remains to be done. Even more interesting than this would be to directly couple the Pauli system to a system of equations describing the evolution of EM-fields such as the Maxwell or Poiswell system (compare [35]) - once again this should in principle be straightforward given what has been discussed and in this paper but still remains to be done.
With regards to computational efficiency, creating an in-depth comparison with other methods to solve the Pauli equation numerically is difficult given the sparse literature on the subject. Some of the questions raised here are set to be explicitly addressed in upcoming publications.

A Appendix

A.1 Notation and conventions list

Efforts have been made to stick to consistent notation in this paper and to introduce the relevant conventions when they are first used. This appendix section serves as a further reference to how different symbols and notations are used in this paper.

Notation	Name	Defined by
ψ	Schrödinger wave function	$\langle x \vert \psi \rangle$
u	Pauli 2-spinor	$u := \begin{pmatrix} u_1 \\ u_2 \end{pmatrix}$
$\mathbf{E}$	Electric vector field	See Maxwell equations
$\mathbf{B}$	Magnetic vector field	See Maxwell equations
$\mathbf{A}$	Magnetic vector potential	via $\nabla \times \mathbf{A} := \mathbf{B}$
ϕ	Electric scalar potential	via $\mathbf{E} = -\nabla\phi - \frac{\partial \mathbf{A}}{\partial t}$
$\hat{H}$	Hamiltonian operator	determined by physical system
∇u	-	$\nabla u := \begin{pmatrix} \partial_x u_1 & \partial_y u_1 & \partial_z u_1 \\ \partial_x u_2 & \partial_y u_2 & \partial_z u_2 \end{pmatrix}$
$\nabla^2 u$	-	$\nabla^2 u := \begin{pmatrix} \nabla^2 u_1 \\ \nabla^2 u_2 \end{pmatrix}$
$(\mathbf{A} \cdot \nabla) u$	-	$(\mathbf{A} \cdot \nabla) u := \begin{pmatrix} \partial_x u_1 & \partial_y u_1 & \partial_z u_1 \\ \partial_x u_2 & \partial_y u_2 & \partial_z u_2 \end{pmatrix} \begin{pmatrix} A_1 \\ A_2 \\ A_3 \end{pmatrix}$
$\nabla \cdot (\mathbf{A} u)$	-	$\nabla \cdot (\mathbf{A} u) = \mathrm{div}(\mathbf{A}) u + \mathbf{A} \cdot \nabla u$
ρ	probability density	$\vert\psi\vert^2$ or $\vert u\vert^2$
$\nabla \cdot \mathbf{j}$	divergence of current	via $\frac{\partial \rho}{\partial t} + \nabla \cdot \mathbf{j} = 0$
$\bar{\mathbf{A}}$	Scaled $\mathbf{A}$	$\bar{\mathbf{A}} = \frac{\mathbf{A}}{A_0}$
$\bar{\phi}$	Scaled ϕ	$\bar{\phi} = \frac{\phi}{\phi_0}$
L_0	Reference length	e.g. numerical space step
T_0	Reference time period	e.g. numerical time step
m, M_0	Reference mass	particle or system mass
q, q_0	Reference charge	particle or system charge
σ	Vector of Pauli matrices	$\sigma = \begin{pmatrix} \sigma_1 \\ \sigma_2 \\ \sigma_3 \end{pmatrix} = \begin{pmatrix} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \\ \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \\ \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \end{pmatrix}$
ϵ	scaling parameter	see section 3.1.3
$\hbar$	scaled Planck constant	physical constant $\hbar = \frac{h}{2\pi}$
c	speed of light	c velocity of special relativity

Table 1: Notation used throughout this master's thesis.

B Deutsche Zusammenfassung (German Abstract)

Diese Arbeit diskutiert numerische Ansätze zur Pauli Gleichung, welche ein semi-relativistisches quantenphysikalisches Modell für geladene Fermionen wie z.B. Elektronen in einem elektromagnetischen Feld darstellt. Zunächst werden dafür die allgemeine Schrödinger Gleichung sowie der mathematische Formalismus der Quantenphysik und Spin sowie klassische Elektrodynamik basierend auf Lorentz-Kraft und Maxwell Gleichungen kurz eingeführt, gefolgt von einer kurzen Diskussion zweier fundamental relativistischer Quantenfeldgleichungen: der Klein-Gordon und Dirac Gleichung. Darauf aufbauend werden zwei verschiedene Motivationen für die Pauli Gleichung als sinnvolles Modell präsentiert: Ein Bottom-up Ansatz basierend auf experimentellen Resultaten und ein Top-down Ansatz als semi-relativistischer Limes der Dirac Gleichung.
Nachdem die Pauli Gleichung auf diese Art motiviert und eingeführt wurde werden numerische Ansätze zum Pauli System wie auch der magnetischen Schrödinger Gleichung diskutiert. Dabei wird eine mögliche Skalierung dieser Gleichungen hergeleitet. Den Kern der Arbeit bildet die Erweiterung eines bekannten numerischen Ansatzes zur magnetischen Schrödinger Gleichung [1] auf das Pauli Gleichungssystem, inklusive einer numerischen Implementation dieser Methode in der Programmiersprache Julia.

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