# UNIVERSIDAD NACIONAL DE COLOMBIA


Physics

# Study, implementation and validation of the Lattice Boltzmann method for quantum systems.

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# Contents

# Introduction

The main objective of this work is to study the theoretical and practical background of the Lattice Boltzmann method for simulating quantum systems (QLB, from now on). This computational method is of great interest because it can be used as a framework for studying complex and relevant problems, such us those arising in quantum computation and quantum optics. As a matter of fact, the QLB method is inspired by this very area of research and can also be applied to elucidate fundamental questions in Quantum Theory, such as the pilot-wave interpretation of quantum mechanics [3][7]. The QLB method appears to be a good algorithm for future quantum computers. The most natural application of quantum computers would be for solving and modeling problems in quantum mechanics, as proposed by Feynman [5]. The lattice kinetic approach is well suited for real-life implementations of quantum networks and quantum computers.

Common computational methods for solving problems in quantum mechanics use finite-difference and finite-element schemes for solving numerically the Schrödinger equation. Other common approaches use Runge-Kutta methods and variational methods by direct minimization of the energy functional. The QLB method is a *modern* method that was first formulated in 1993 by S. Succi and then reformulated independently by D. Meyer in 1996, resulting in two equivalent schemes for the same model. It is considered a simulation method, and not simply one for solving numerically the equations, as it emerges from first physical principles and laws to numerically model the quantum system. Since it was first proposed and reformulated, only a few important contributions mainly by S. Palpacelli in 2009 have been published, where she extended the method to multiple dimensions and applied to non-trivial and closer to real-life situations for interactions with scalar potentials[8].

In Chapter 1, we show a summary of the main theoretical background required for studying quantum systems in the context of the QLB method. Here, we discuss the non-relativistic Schrödinger equation, as well as the Dirac equation for relativistic quantum mechanics, which are the most fundamental equations used in the QLB model. Schrödinger equation is presented putting emphasis on the similarity it has with a diffusive process, meanwhile Dirac equation is presented in the Majorana form to easily note its similarities with the Boltzmann equation for fluid dynamics.

Chapter 2 is devoted completely to the QLB method, enumerating and explaining the two standard schemes for approaching it, explicitely, the Meyer's

and Succi's schemes. We review how Meyer's scheme approaches the problem via a diffusive cellular automata, whilst Succi's exploits the formal similarity between the hydrodynamic Boltzmann equation and the Dirac equation. We give some hints on how to intuitively obtain the relevant equations and give some hints on how to implement them in a computer by explicitely writing them in matrix notation.

In Chapter 3, we show the results of applying the method using both schemes to common cases, free particle propagation and dynamics in a square well potential, which are well-known to the literature and are used to validate the method. We use the case of free particle propagation to compare how accurate and exact both schemes are, noting that taking both schemes as they were originally proposed, Meyer's is the most accurate.

Finally, in Chapter 4, we show the most significant results from this work and some perspectives for future work, specially in terms of the potential application of this method to study interesting problems in the areas of quantum information and quantum optics.

# 1 Basics and theory

## 1.1 Modelling the behaviour of quantum systems: a summary

### 1.1.1 Non-relativistic Schrödinger equation

Imagine we are trying to study the dynamics of a particle that moves freely along a line (one dimension movement). Suppose we know its wave function at some instant $t$; that is, we know the probability amplitude of finding the particle at any point at time $t$. Let us divide the domain where the particle is moving into small intervals, of length $l$ each, as shown in Figure 1 [1].

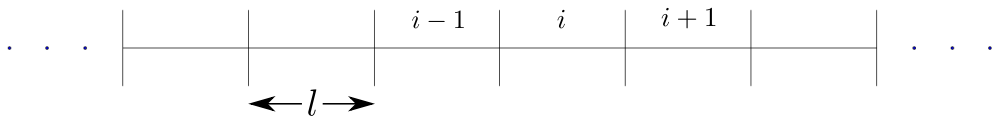


Figure 1: One dimensional domain divided in intervals of length $l$.

Let $\psi_i(t)$ to be the probability amplitude to find the particle in the interval $i$ at time $t$; then, $|\psi_i(t)|^2$ is the probability of finding the particle in the interval i at time $t$. The particle cannot escape this setup, it must be "somewhere" along the line. Thus,

$$\sum_i |\psi_i(t)|^2 = 1 \quad .$$

Therefore, the complex amplitudes $\psi_i(t)$ can be seen as components of the total state vector (ket vector) $|\Psi\rangle$. Now, since the particle is free to move along the line, the probability amplitude at some interval $i$ may travel to the neighboring intervals, $i-1$ and $i+1$. If we define the probability amplitude to pass from one interval to the neighboring ones as $-iA\Delta t/\hbar$, we can write the probability amplitude (wave function) at a later time $t + \Delta t$ as

$$\psi_i(t+\Delta t) = \psi_i(t) + \frac{iE_0\Delta t}{\hbar}\psi_i(t) - \frac{iA\Delta t}{\hbar}\psi_{i+1}(t) - \frac{iA\Delta t}{\hbar}\psi_{i-1}(t) \quad . \quad (1.1)$$

[1] This is the same reasoning followed by Baym and Feynman in references [1] and [10], respectively.

The second term in the right hand side of the equation is the amplitude for the particle to stay in the interval $i$ (related to the "zero" energy level), the third term is the amplitude to leak out from the $i+1$-th interval into the $i$-th one and the fourth one is the amplitude for the particle to leak from the $i-1$-th interval into the $i$-th one.

For a sufficiently small $\Delta t$ we can arrange and rewrite the previous expression such that

$$i\hbar\frac{\partial\psi_i}{\partial t} = E_0\psi_i - A\psi_{i+1} - A\psi_{i-1} \quad . \tag{1.2}$$

The solutions of this first order linear differential equation can be written as

$$\psi_i(t) = a_i e^{-iEt/\hbar} \quad . \tag{1.3}$$

Replacing (1.3) into (1.2), we get

$$Ea_i = E_0 a_i - Aa_{i+1} - Aa_{i-1} \quad . \tag{1.4}$$

By using spatial coordinates instead of interval indices (such that $i = x_i$ and $i \pm 1 = x_i \pm l$), we can rewrite (1.4) as

$$Ea(x_i) = E_0 a(x_i) - Aa(x_i + l) - Aa(x_i - l) \quad , \tag{1.5}$$

which looks very similar to a differential equation. By assuming solutions of the form $a(x_i) = e^{ikx_i}$, Eq. (1.5) becomes

$$\begin{aligned} E &= E_0 - Ae^{ikl} - Ae^{-ikl} & (1.6)\\ &= E_0 - 2A\cos(kl) \quad . & (1.7) \end{aligned}$$

This means that for any choice of $k$ there is a solution with energy $E$ given by equation (1.7) and that the solutions for (1.2) can be written as

$$\psi_i = e^{ikx_i}e^{-iEt/\hbar} \quad . \tag{1.8}$$

By taking the limit $l \to 0$ but keeping the wave number $k$ constant, Eq. (1.7) transforms into $E = E_0 - 2A$, and Eq. (1.2) becomes

$$i\hbar\frac{\partial\psi(x_i)}{\partial t} = (E_0 - 2A)\psi(x_i) + A\left[2\psi(x_i) - \psi(x_i + l) - \psi(x_i - l)\right] \quad . \tag{1.9}$$

Moreover, we can choose our reference zero energy such that $E_0 - 2A = 0$, so that the first term in the right-hand side vanishes.

The second term in Eq. (1.9) should be somewhat related to a second derivative of $\psi(x)$. Actually, by taking a Taylor expansion of that term as $l \to 0$ (and keeping $k$ and $E$ constants), the term can be written as

$$2\psi(x) - \psi(x+l) - \psi(x-l) \approx -l^2 \frac{\partial^2 \psi(x)}{\partial x^2} \quad . \tag{1.10}$$

So, Eq. (1.9) becomes

$$i\hbar \frac{\psi(x)}{\partial t} = -Al^2 \frac{\partial^2 \psi(x)}{\partial x^2} \quad , \tag{1.11}$$

where the coefficient $Al^2$ can be interpreted as an effective mass $m$, such that $Al^2 = h^2/2m$; that is,

$$i\hbar \frac{\partial \psi(x)}{\partial t} = -\frac{\hbar^2}{2m} \frac{\partial^2 \psi(x)}{\partial x^2} \quad . \tag{1.12}$$

This is the Schrödinger equation, the quantum mechanical equation that give us the rate of change of the amplitude $\psi(x)$ of finding the particle at position $x$. This equation was first discovered by Erwin Schrödinger (1926), and can be imagined as a diffusion equation with an imaginary diffusion coefficient $\kappa = i\hbar/2m$. This important analogy suggests the possibility to model the Schrödinger equation via a lattice gas cellular automata for diffusion[7].

### 1.1.2 The Dirac equation

Historically, as soon as the Schrödinger equation was discovered, attempts to create a relativistic quantum theory were made. This is how the first relativistic version of the Schrödinger equation was born, commonly known as the Klein-Gordon equation, which succesfully described the relativistic motion of spinless particles; nevertheless, there were no description for the behaviour of spin-1/2 elementary particles. It was in 1928 when Paul Dirac first proposed a formulation that was consistent with both quantum mechanics (including spin) and special relativity. Inspired by a Hamiltonian equation of the form

$$i\hbar \frac{\partial \psi}{\partial t} = H\psi \quad , \tag{1.13}$$

Dirac naturally realized that the hamiltonian $H$ must also be linear in the spatial derivatives; assuming an the equation with the form

$$i\hbar \frac{\partial \psi}{\partial t} = \frac{\hbar c}{i} \left( \alpha_1 \frac{\partial \psi}{\partial x^1} + \alpha_2 \frac{\partial \psi}{\partial x^2} + \alpha_3 \frac{\partial \psi}{\partial x^3} \right) + \beta mc^2 \psi \equiv H\psi \quad , \tag{1.14}$$

where the coefficients $\alpha_i$ and $\beta$ are matrices fulfilling the following relations (written in $2 \times 2$ blocks):

$$\alpha_i = \begin{pmatrix} 0 & \sigma_i \\ \sigma_i & 0 \end{pmatrix}, \quad \beta = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \tag{1.15}$$

where the $\sigma_i$ are the familiar Pauli matrices [2]. The symmetry between the time and spatial coordinates makes them transform in the same way when applying linear transformations (such as the Lorentz transformations), that is, the equation (1.14) satisfies Lorentz invariance and covariance, two requirements for a correct relativistic model in quantum mechanics.

**1.1.2.1 Majorana form of the Dirac Equation:** It will be useful in the next sections to write the Dirac equation in such a way that all the coefficients and streaming matrices in (1.14) are real. This is called the **Majorana form** of the Dirac equation and, it is achieved by applying to (1.14) the following unitary transformation

$$S = \frac{1}{\sqrt{2}}(\alpha_2 + \beta) = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 0 & 0 & -i \\ 0 & 1 & i & 0 \\ 0 & -i & -1 & 0 \\ i & 0 & 0 & -1 \end{pmatrix} \quad , \tag{1.16}$$

which results in the following transformed matrices

$$\alpha_1^S \equiv \begin{pmatrix} 0 & 0 & 0 & -1 \\ 0 & 0 & -1 & 0 \\ 0 & -1 & 0 & 0 \\ -1 & 0 & 0 & 0 \end{pmatrix} = -\alpha_1, \quad \alpha_2^S \equiv \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix} = \beta$$

$$\alpha_3^S \equiv \begin{pmatrix} 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 1 \\ -1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix} = -\alpha_3, \qquad \beta^S \equiv \begin{pmatrix} 0 & 0 & 0 & -i \\ 0 & 0 & i & 0 \\ 0 & -i & 0 & 0 \\ i & 0 & 0 & 0 \end{pmatrix} = \alpha_2 \quad .$$

So, (1.14) can be written as

$$\frac{\partial \psi}{\partial t} + c\left(-\alpha_1 \frac{\partial \psi}{\partial x^1} + \beta \frac{\partial \psi}{\partial x^2} - \alpha_3 \frac{\partial \psi}{\partial x^3}\right) = -i\omega_c \alpha_2 \psi \quad , \tag{1.17}$$

where the *quadrispinor* $\psi$ has also been transformed by applying $S$, and $\omega_c = \frac{mc^2}{\hbar}$ is the well known Compton frequency.

**1.1.2.2 Adding a potential to the Dirac equation:** Adding an interaction with a potential in equation (1.14) is done by making the usual replacement of operators:

$$\begin{aligned} i\hbar\partial_t &\rightarrow i\hbar\partial_t + qV \\ -i\hbar\nabla &\rightarrow -i\hbar\nabla + \frac{q}{c}\mathbf{A} \quad , \end{aligned} \tag{1.18}$$

which results in the following expression for the Dirac equation with electromagnetic potential interaction:

$$\partial_t\psi + c\alpha\cdot\nabla\psi = -i\omega_c\beta\psi + i\frac{q}{\hbar}V\psi - i\frac{q}{\hbar}(\mathbf{A}\cdot\alpha)\psi \equiv iM\psi \quad , \tag{1.19}$$

where

$$M = -\omega_c + \frac{q}{\hbar}V - \frac{q}{\hbar}(\mathbf{A}\cdot\alpha) \quad . \tag{1.20}$$

# 2 The Quantum Lattice Boltzmann method

The Quantum Lattice Boltzmann (QLB) method has two common schemes which were developed independently and proven to be equivalent.

## 2.1 Meyer's Scheme (1996)

The Meyer's scheme for the QLB method is based on a diffusion cellular automata, that is, looking at the evolution of the wavefunction for the system as a quantum lattice gas. The wavefunction evolves according to some local rule of the form

$$\phi_{t+1} = f\left(\phi_t(x+e) | e \in E(t,x)\right) \quad , \tag{2.1}$$

where $E(x,t)$ is a set of lattice vectors that define the neighborhood of the automaton [7].

As usual in the Schrödinger picture of quantum mechanics, a unitary and local evolution of the state vector is required, *i.e.*,

$$\phi_{t+1} = U\phi_t \quad , \tag{2.2}$$

where $U$ is a unitary operator ($U^*U = UU^* = I$). Therefore, we can write (2.1) as

$$\phi_{t+1} = \sum_{e \in E(t,x)} w(t, x+e)\phi_t(x+e) \quad , \tag{2.3}$$

where the coefficients $w$ are constrained by the unitary condition given by (2.2). In one dimension, this translates to a band diagonal system (due to the local and homogeneous evolution), as follows:

$$\begin{pmatrix} \vdots \\ \phi_{t+1}(x-e) \\ \phi_{t+1}(x) \\ \phi_{t+1}(x+e) \\ \vdots \end{pmatrix} = \begin{pmatrix} \ddots & & & & & & \\ & w_- & w_0 & w_+ & & & \\ & & w_- & w_0 & w_+ & & \\ & & & w_- & w_0 & w_+ & \\ & & & & & & \ddots \end{pmatrix} \begin{pmatrix} \vdots \\ \phi_t(x-e) \\ \phi_t(x) \\ \phi_t(x+e) \\ \vdots \end{pmatrix} \quad , \tag{2.4}$$

where $w_\pm \equiv w(t, x \pm e)$. A problem arises when trying to find a matrix $U$ to satisfy (2.4), known as the NO-GO LEMMA, formulated by Grössing and Zeilinger in the following way[6][7]:

NO-GO LEMMA. *In one dimension there exists no nontrivial, homogeneous, local, scalar Quantum Cellular Automata (QCA).*

To solve this problem, Meyer relaxes the homogeneity condition but keeps intact the local and unitary evolution of the system. He makes the $U$ operator 2-step invariant; that is, instead of having $TUT^{-1} = U$ we now require $T^2UT^{-2} = U$ (where $T$ is the spatial translation operator); therefore, the operator $U$ can be written as

$$U = \begin{pmatrix} \ddots & & & & & & & \\ & a & b & c & & & & \\ & & d & e & f & & & \\ & & & a & b & c & & \\ & & & & d & e & f & \\ & & & & & & & \ddots \end{pmatrix} \quad . \tag{2.5}$$

By applying the unitarity condition, we are left with the following system of equations for the elements of $U$:

$$\begin{aligned} aa^* + bb^* + cc^* &= 1 & dd^* + ee^* + ff^* &= 1 \\ bd^* + ce^* &= 0 & ea^* + fb^* &= 0 \\ ca^* &= 0 & fd^* &= 0 \quad . \end{aligned} \tag{2.6}$$

The nontrivial solutions are such that $c = d = 0$ (or $a = f = 0$, conversely). That makes $U$ a block diagonal matrix,

$$U = \begin{pmatrix} \ddots & & & & \\ & S & & & \\ & & S & & \\ & & & S & \\ & & & & \ddots \end{pmatrix} \quad , \tag{2.7}$$

where $S$ is a $2 \times 2$ block acting only on a pair of adjacent cells, defined as

$$S := \begin{pmatrix} e & f \\ a & b \end{pmatrix} \quad . \tag{2.8}$$

Now, let us see how this relates to the structure of the wavefunction itself. In the one dimensional case, the state vector can be thought of as made of two components, one moving to the right and one, to the left; that is

$$|\Psi\rangle = |x\rangle \otimes |i\rangle \,, \quad i = r, l \quad , \tag{2.9}$$

where the indices $r$ and $l$ designate the right and left components, respectively. This means that the $S$ operator in (2.8) can be interpreted as a

collision operator between pairs of cells and its components can be thought as transition amplitudes for the wavefunction to go to the left or to the right direction. Since the system does not have a preferred direction of movement, we force $e = b \equiv p$ and $a = f \equiv q$, such that $S$ is now written as

$$S = \begin{pmatrix} p & q \\ q & p \end{pmatrix} \tag{2.10}$$

where the coefficient $p$ is the transition amplitude for the wavefunction to mantain its direction and $q$ is the amplitude to go in the opposite direction,

$$\begin{aligned} \psi_r(x, t + \Delta t) &= p\psi_r(x, t) + q\psi_l(x, t) \\ \psi_l(x, t + \Delta t) &= q\psi_r(x, t) + p\psi_l(x, t) \end{aligned} \quad . \tag{2.11}$$

If we just let the system evolve by applying $U$ in (2.7) at each time step, we would just end up with having noninteracting sets of pairs of adjacent cells. Instead of that, Meyer's scheme evolves by $U$ and by $TUT^{-1}$ at alternating time steps: the collision operator $U$ acts on a pair of cells at instants $t$ and then, at the following time step $t + \Delta t/2$, as a "*staggered* rule for a *checkerboard* model" (Fig. 2): Cells can be paired in two ways, starting with an even cell or with an odd one. In even time steps, we pair cells starting with an even cell, and viceversa; and the unitary matrix $U$ acts on paired cells only. So, two time steps add an evolution time $\Delta t$ .

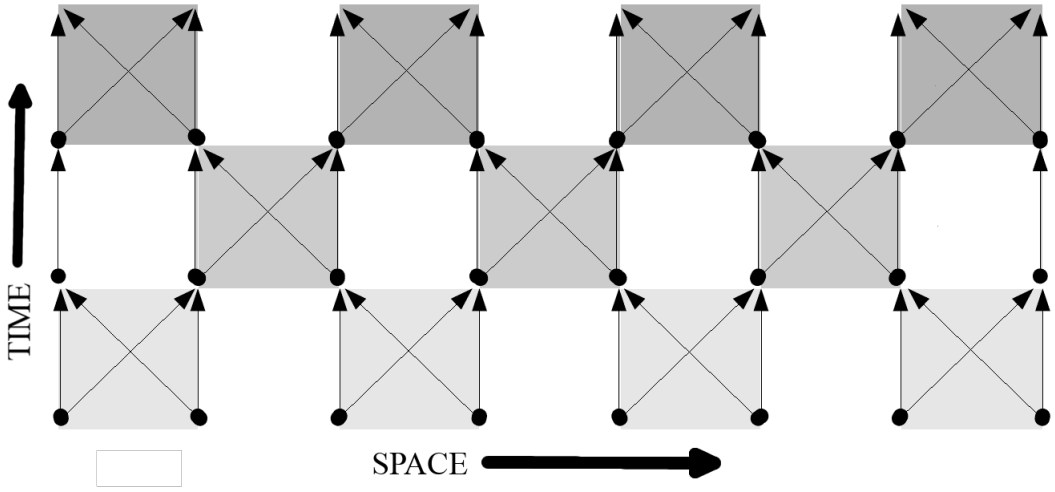


Figure 2: "2-step" *staggered* rule for the *checkerboard* model in a CA.

This means that to actually evolve the system we now have two collision steps, one for the actual collision between vecinities and one for the *staggered*

rule, and in-between these two collision steps we have advection processes. In this way we are left with the following evolution operators for this scheme. For $t \to t + \Delta t/2$:

$$C_1 = \begin{pmatrix} p & q & 0 & 0 & 0 & 0 & 0 & 0 \\ q & p & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & p & q & 0 & 0 & 0 & 0 \\ 0 & 0 & q & p & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & p & q & 0 & 0 \\ 0 & 0 & 0 & 0 & q & p & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & p & q \\ 0 & 0 & 0 & 0 & 0 & 0 & q & p \end{pmatrix} \quad A = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix} \quad , \tag{2.12}$$

for $t + \Delta t/2 \to t + \Delta t$:

$$C_2 = \begin{pmatrix} 0 & p & q & 0 & 0 & 0 & 0 & 0 \\ 0 & q & p & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & p & q & 0 & 0 & 0 \\ 0 & 0 & 0 & q & p & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & p & q & 0 \\ 0 & 0 & 0 & 0 & 0 & q & p & 0 \\ q & 0 & 0 & 0 & 0 & 0 & 0 & p \\ p & 0 & 0 & 0 & 0 & 0 & 0 & q \end{pmatrix} \quad A = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix} \quad , \tag{2.13}$$

such that, in conclusion

$$|\Psi\rangle_{t+\Delta t} = AC_2AC_1 |\Psi\rangle_t \tag{2.14}$$

## 2.2 Succi's Scheme (1993)

The Succi's scheme was the first one to be proposed for a QLB method. This scheme exploits the formal similarity when comparing the Dirac equation (see section 1.1.2) to the hydrodynamic Lattice Boltzmann equation.

The hydrodynamic Lattice Boltzmann equation is a discrete relation of the form

$$f_i(\vec{r} + \vec{c}_i\Delta t, t + \Delta t) - f_i(\vec{r}, t) = \Omega_{ij}(f_j - f_j^{eq}), \quad i = 1, \ldots, b \quad , \tag{2.15}$$

where $f_i$ is the probability distribution of finding a particle at position $\vec{r}$ and time $t$ with velocity $\vec{v} = \vec{c}_i$, $\Omega_{ij}$ is the scattering matrix mediating collisions among distributions and $b$ is the number of discrete speeds connecting each

site to its nearest neighbors. The left-hand side is the exact discrete-velocity representation of the Boltzmann streaming operator $\partial_t f + \vec{v} \cdot \nabla f$ and the right-hand one represents the particle collisions (collision operator). At second order in space, Eq. (2.15) can be written as[9][11]

$$\partial_t f + \vec{c} \cdot \nabla f = \Omega(f, f^{eq}), \quad i = 1, \ldots, b \quad . \tag{2.16}$$

By direct comparison of Eqs. (1.17) and (2.16) one can see the formal parallel between Lattice Boltzmann (LBE) and Dirac equations, summarized as follows:

$$\begin{aligned} \text{Boltzmann} &\rightarrow \text{Dirac} \\ f_i &\rightarrow \psi_i \\ \vec{c} &\rightarrow c\,(-\alpha^x, \beta, -\alpha^z) \equiv \mathbf{L} \\ \Omega &\rightarrow -i\frac{mc^2}{\hbar}\alpha^y \equiv M \quad , \end{aligned}$$

where the number of speeds $b$ is now fixed to 4 (since $\psi$ is a quadrispinor). The streaming operator $\mathbf{L}$ can't be diagonalized simultaneously in 2D or beyond (this rises subtleties and difficulties when using the QLB method in more than one dimension) and the collision operator $M$ is now antisymmetric, in contrast to the symmetric $\Omega$ matrix in the LBE.

Now, if we take the one-dimensional Dirac equation in Majorana form (Eq. 1.17), written in matrix notation, we are left with a system of two independent subsystems:

$$\begin{aligned} \partial_t \begin{pmatrix} u_1 \\ u_2 \end{pmatrix} + \partial_z \begin{pmatrix} u_1 \\ u_2 \end{pmatrix} &= \omega_c \begin{pmatrix} d_2 \\ d_1 \end{pmatrix} \\ \partial_t \begin{pmatrix} d_1 \\ d_2 \end{pmatrix} - \partial_z \begin{pmatrix} d_1 \\ d_2 \end{pmatrix} &= -\omega_c \begin{pmatrix} u_2 \\ u_1 \end{pmatrix} \quad , \end{aligned} \tag{2.17}$$

where the Dirac quadrispinor is written as $\psi = (u_1, u_2, d_1, d_2)^T$ and different letters label different spin states.

The Succi's QLB model is obtained by a convenient discretization of equation (2.17). As a first approach, a time-explicit Euler method could be applied to obtain the following discrete evolution equations:

$$\begin{aligned} u_{1,2}(z + \Delta z, t + \Delta t) - u_{1,2}(z, t) &= \Delta t \omega_c d_{2,1}(z, t) \\ d_{1,2}(z - \Delta z, t + \Delta t) - d_{1,2}(z, t) &= -\Delta t \omega_c u_{2,1}(z, t) \quad , \end{aligned}$$

where $\Delta z = c\Delta t$ (light-cone rule). Nevertheless, this discretization is known to be unconditionally unstable for any choice of $\Delta t$ and also results in a non-unitary evolution [12].

Instead, a Crank-Nicolson method is chosen (based on its stability when applied to diffusion) to discretize the right hand side of equation (2.17) and the left hand side is discretized by a plain foward-in-time finite difference scheme. The result reads

$$\begin{aligned} u_{1,2}(z+\Delta z, t+\Delta t) - u_{1,2}(z,t) &= \frac{1}{2}\omega_c \Delta t \left[ d_{2,1}(z-\Delta z, t+\Delta t) + d_{2,1}(z,t) \right] \\ d_{1,2}(z-\Delta z, t+\Delta t) - d_{1,2}(z,t) &= -\frac{1}{2}\omega_c \Delta t \left[ u_{2,1}(z+\Delta z, t+\Delta t) + u_{2,1}(z,t) \right] \end{aligned} \quad , \tag{2.18}$$

which is a numerically stable and implicit scheme. By solving for the relevant terms $u_{1,2}(z+\Delta z, t+\Delta t)$ and $d_{1,2}(z-\Delta z, t+\Delta t)$ we finally get the explicit QLB equations for the Succi's scheme

$$\begin{aligned} u(z+\Delta z, t+\Delta t) &= a(z,t)u(z,t) + b(z,t)d(z,t) \\ d(z-\Delta z, t+\Delta t) &= a(z,t)d(z,t) - b(z,t)u(z,t) \end{aligned} \quad , \tag{2.19}$$

where the coefficients $a(z,t)$ and $b(z,t)$ are given by

$$\begin{aligned} a(z,t) &= \frac{1 - \frac{1}{4}\omega_c^2 \Delta t^2}{1 + \frac{1}{4}\omega_c^2 \Delta t^2}, \\ b(z,t) &= \frac{\omega_c \Delta t}{1 + \frac{1}{4}\omega_c^2 \Delta t^2} \quad . \end{aligned} \tag{2.20}$$

This is the central point of the Succi's scheme for the QLB method respect to its implementation on a computer. It is interesting to note that the components $u$ and $d$ of the Dirac quadrispinor in this scheme are analogues of the components $\psi_r$ and $\psi_l$ of Meyer's scheme (see section 2.1). This is a direct but superficial confirmation of the equivalence between both schemes[2].

### 2.2.1 Adding a scalar potential to the Succi's scheme for QLB method

Interactions with an external scalar field are included in this model by extending the collision operator in the right-hand side of (2.17). For example,

[2]The formal equivalence between both schemes was proven by Meyer himself (see reference [7]).

for a electrostatic potential, the scheme is transformed as follows:

$$\begin{aligned} \partial_t \begin{pmatrix} u_1 \\ u_2 \end{pmatrix} + \partial_z \begin{pmatrix} u_1 \\ u_2 \end{pmatrix} &= \omega_c \begin{pmatrix} d_2 \\ d_1 \end{pmatrix} + ig \begin{pmatrix} u_1 \\ u_2 \end{pmatrix} \\ \partial_t \begin{pmatrix} d_1 \\ d_2 \end{pmatrix} - \partial_z \begin{pmatrix} d_1 \\ d_2 \end{pmatrix} &= -\omega_c \begin{pmatrix} u_2 \\ u_1 \end{pmatrix} + ig \begin{pmatrix} d_1 \\ d_2 \end{pmatrix} \end{aligned} \tag{2.21}$$

with $g = qV/\hbar$ the coupling to the electrostatic potential $V$ and $q$ the particle's electric charge. Furthermore, by applying the same discretization method as before we are left with the same evolution equations given by (2.19), but now the coefficients $a$ and $b$ are

$$\begin{aligned} a(z,t) &= \frac{1 - \frac{1}{4}\Delta t^2(\omega_c^2 - g(z,t)^2)}{1 - ig(z,t)\Delta t + \frac{1}{4}\Delta t^2(\omega_c^2 - g(z,t)^2)}, \\ b(z,t) &= \frac{\omega_c \Delta t}{1 - ig(z,t)\Delta t + \frac{1}{4}\Delta t^2(\omega_c^2 - g(z,t)^2)} \quad . \end{aligned} \tag{2.22}$$

# 3 Applications for the QLB model

Both schemes of the QLB model were implemented and validated by applying them to two common pedagogical cases: Free particle propagation and the propagation inside a square well. For both cases periodic boundary conditions were used.

## 3.1 Free particle

In this first case both schemes were applied to a minimum uncertainty free wave packet as initial condition, working with atomic units ($\hbar = c = 1$ and $q = -1$), written as

$$\psi_0(z) = (2\pi\Delta_0)^{-1/2} \exp\left(-\frac{(z-z_0)^2}{4\Delta_0^2}\right) \exp\left(-imv_z z\right) \tag{3.1}$$

This is a one dimensional wave packet centered at $z_0$ with initial spread $\Delta_0$ and propagating along $z$ at speed $v_z$. This means that our Dirac quadrispinor, $\psi = (u_1, u_2, d_1, d_2)$, is given by setting

$$\begin{aligned} u_1 = u_2 &= \frac{1}{2}\psi_0, \\ d_1 = d_2 &= -i\frac{1}{2}\psi_0. \end{aligned}$$

The analytical solution of the Schrödinger equation for a freely propagating particle is

$$\begin{aligned} \psi(z,t) = (2\pi)^{-1/4} &\left(\Delta_0 + \frac{it}{2m\Delta_0}\right)^{-1/2} \exp\left(-\frac{(z-z_0-v_z t)^2}{4\Delta_0^2 + (2it/m)}\right) \\ &\times \exp\left(imv_z z\right) \exp\left(-\frac{imv_z^2 t}{2}\right) \end{aligned} \tag{3.2}$$

and by using the definitions for mean position $Z(t)$ and mean spread $\Delta_z(t)$

$$\begin{aligned} Z(t) &= \int z|\psi(z,t)|^2 dz, \\ \Delta_z(t) &= \int (z - Z(t))^2 |\psi(z,t)|^2 dz \end{aligned}$$

we obtain that these quantities should evolve according to

$$\begin{aligned} Z(t) &= z_0 + v_z t, \\ \Delta_z^2(t) &= \Delta_0^2 + \frac{t^2}{4m\Delta_0^2} \quad . \end{aligned}$$

The time evolution of the wave packet with momentum is shown in Fig. 3, where the following parameters where used: $m = 0.2$, $\Delta_0 = 50$, $v_z = 0.1$ and $z_0 = 1024$ on a lattice of size $L = 2048$ nodal points. Here you can see how the wave packet moves linearly along the $x$ axis for both schemes implemented in the simulation.

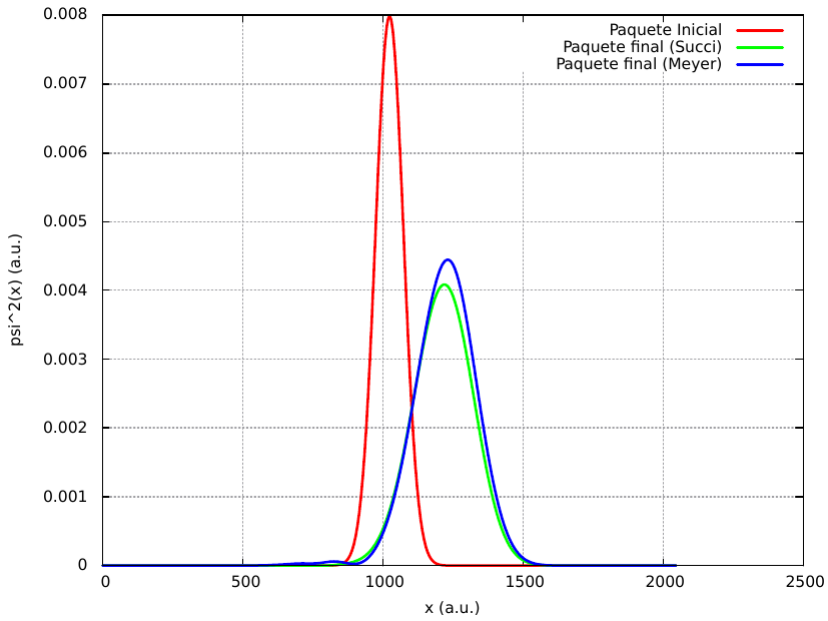


Figure 3: Time evolution of a free gaussian wave packet at $t = 1000$ in lattice units. Results from Meyer's scheme (blue) and Succi's scheme (green) are shown, using the same initial condition for both cases (red).

In Fig. 4 we show the time evolution of the variance of the wave packet, where a good agreement between the analytical behavior and the numerical solution is shown, thus proving that both schemes correctly model the behavior of a free gaussian wave packet according to the non-relativistic Schrödinger dynamics. It must be noted that Succi's scheme has a first-order accuracy in time, whilst the accuracy in Meyer's is of second order, this explains the differences between both schemes and why it becomes larger as time increases. The plot also shows a somewhat unexpected oscillatory behavior, that can be related to the *Zitterbewegung* effect or "trembling motion", which is part of the physics involved in modelling elementary particles with the Dirac equation [4], once again, qualitatively showing an equivalence between both schemes, specially since Meyer's scheme does not part from the discretizacion of the Dirac equation. These results are the same as the ones obtained by Valdivieso and Muñoz in 2009 [13].

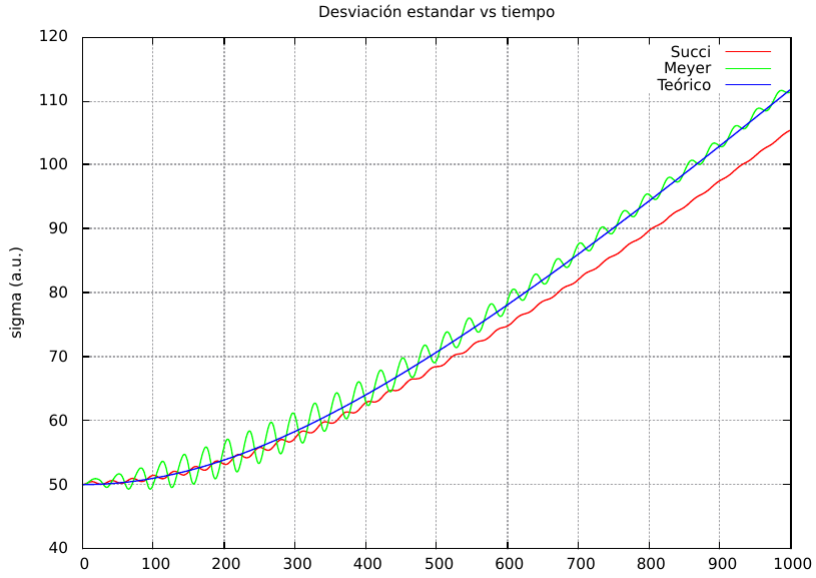


Figure 4: Time evolution of the variance of a free gaussian wave packet for $t = 1000$ in lattice units. Results from Meyer's (green) and Succi's (red) schemes are shown compared to the theoretical expected result (blue).

## 3.2 Particle propagation in a square potential well

In this second case we consider the dynamics of the same wave packet inside a repulsive square potential well of the form

$$V(x) = \begin{cases} V_0 & x \leq L/3 \\ 0 & L/3 < x < 2L/3 \\ V_0 & x \geq 2L/3 \end{cases} , \tag{3.3}$$

where the expected behavior is to observe a quantum tunneling effect, in which the particle collides with the walls of the well and still can go through these walls even if its energy $E$ is lower than the potential energy wall $V_0$. This effect can be seen in Fig. 5, where the particle is travelling along the positive $x$ axis and "boncing" from the walls and going through at the same time, even when $V_0 >> E$ (quantum tunneling).

These results, when compared to the expected behaviour, show the viability of the QLB schemes in one dimension and validate the method for modelling quantum systems.

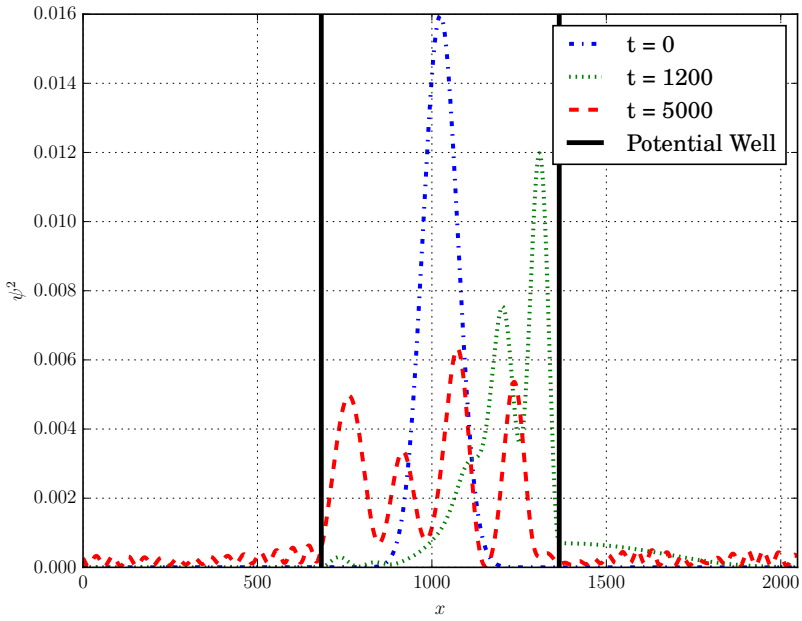


Figure 5: Gaussian wave function density $\psi^2$ moving inside a square potential well at different times in lattice units. Parameters are set as follows: $L = 2048$, $v_z = 0.2$, $m = 0.1$, $V_0 = 0.2$, $\Delta_0 = 50$.

# 4 Conclusions

In this work we have studied and validated the Quantum Lattice Boltzmann (QLB) model in its both variations, the Meyer and Succi schemes for modelling quantum systems in the non-relativistic Schrödinger regime.

As discussed in Chapters 1 and 2, quantum mechanics, in both Schrödinger's and Dirac's pictures, can be formulated as a lattice gas automata or in a fluid dynamics language, respectively. Specifically, Schrödinger equation can be thought of as a diffusive process with an imaginary diffusion coefficient $\kappa = i\hbar/2m$; this is the fundamental idea behind Meyer's scheme, which numerically models quantum systems via a diffusive cellular automata or a lattice gas. On the other hand, Dirac equation can be written in such a way that, when formally related to the Boltzmann equation for fluid dynamics, one realizes that the same process which conduces from the Boltzmann equation to the Navier-Stokes for fluids, can be applied to the Dirac equation to conduct to the Schrödinger equation, this is what is exploited in Succi's scheme for QLB.

Both schemes were implemented from scratch and applied to common pedagogical cases, *i.e.,* free particle propagation and the quantum dynamics inside a square potential well; obtaining results that are in agreement with the analytical expected behavior, therefore validating the usability of the method and its schemes to simulate quantum systems. Moreover, this method formulates a framework for studying "real-time" dynamics of quantum systems at a fundamental level, a subject that is not well studied in most of the common courses regarding Quantum Mechanics.

Once the method is validated, opportunities for future work in the subject are presented for it to be expanded and applied in different and non-trivial cases. One clear possibility is extending the method to include interaction with vector potentials using Eq. (1.19) as starting point, which in turn, can be used to study the dynamics between spin particles and magnetic fields and, even further, this could result in a good method to simulate and measure entanglement in systems relevant to quantum optics and information.

In conclusion, this work shows a theoretical study of the QLB method and discusses it in a practical sense keeping in mind its implementation in a computer program. It also summarizes its variations in a single document, making this work a good tutorial and starting point to study the Lattice Boltzmann model for quantum systems.

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