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Numerical comparison of 1D quantum lattice Boltzmann models

Miguel Alfonso Valdivieso Colmenares and José Daniel Muñoz Castaño

Simulation of Physical Systems Group, CEiBA-Complejidad, Universidad Nacional de Colombia, Departamento de Fisica, Crr 30 # 45-03, Ed. 404, Of. 348, Bogotá DC, Colombia
E-mail: mavaldiviesoc@bt.unal.edu.co and jdmunozc@unal.edu.co

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Abstract. Lattice Boltzmann (LB) methods have proven to be powerful tools for simulating classical physical systems such as waves, diffusion and fluid dynamics. For quantum mechanics in one dimension there are two main schemes: one proposed by Meyer, where the Schrödinger equation is interpreted as a diffusion equation with imaginary diffusion constant; the other, proposed by Succi, is based on the Dirac equation, which in the mesoscopic limit reproduces the non-relativistic quantum behaviour in a similar way to lattice Boltzmann models for fluids. In the present work we compare these models by testing the quantum time evolution of a free Gaussian wavepacket. It is found to be in close correspondence with the results of the two models. Time oscillations are found both for the mean and variance of the wavepacket. Also we found their dependences from factors not present in the predicted values. These elements could provide clues for developing a good adaptation of lattice Boltzmann method for the quantum world.

Keywords: lattice Boltzmann methods, quantum transport

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1. Introduction

The development of lattice Boltzmann models [1]–[4] has created a wide range of research and applications in fields like fluid dynamics, waves, diffusion phenomena [5, 7] and even magnetic reconnection in plasmas [6]. Because of the similarities between some formulations of quantum mechanics and fluid dynamics or diffusion, several schemes regarding the adaptation of lattice Boltzmann models to the quantum realm have been proposed [8]–[10], [12, 13, 11, 16]; however, each algorithm has its own results. It could be interesting to put the basic models under the same conditions.

In this paper we develop a concise comparison of two LB models suited for quantum mechanics: one given by Meyer [8]–[10], which resembles the Schrödinger equation as a diffusion equation with imaginary diffusion constant, and another given by Succi [12]–[14], which exploits some similarities between the Dirac equation and the Boltzmann transport equation for fluid dynamics. Section 2 describes both models. The two approaches are used to find the time evolution of a free Gaussian wavepacket, with the results given in section 3.

2. Quantum lattice Boltzmann models

Let us start by describing both models.

2.1. Meyer's model

Meyer's model [8, 9] is based on a classical cellular automaton for diffusion [5]. In the 1D version of this automaton, each cell has two velocities connecting with the next neighbouring cells and each velocity can be empty or filled with a single particle. At each time step, the contents of every cell are flipped at random with probability $(1 - p)$ (the collision step) and thereafter all particles move one cell ahead (the advection step).

The scheme proposed by Meyer's model takes into account a Hilbert space H given by the one-dimensional integer lattice L, where $|x\rangle$ is the discrete basis for this space, $x \in L$ represents the position of each cell and only two velocities are allowed [8, 9]. Meyer's model

replaces the occupation numbers of each velocity with complex numbers standing for the probability amplitudes $\phi^{(\mathrm{l})}$ and $\phi^{(\mathrm{r})}$, which move left or right at each cell with coordinate x, at time t, i.e. $\phi_t^{(\mathrm{l})}(x)$. At each lattice point with the two probability amplitudes, a two-component vector $\psi(t,x) := (\phi_t^{(\mathrm{r})}(x), \phi_t^{(\mathrm{l})}(x))^{\mathrm{T}}$ can be constructed in order to write the state vector of the system:

$$\Psi(t) = \sum_x \psi(t,x)|x\rangle. \tag{1}$$

The condition of unitary evolution for a quantum system

$$\Psi_{t+1} = U\Psi_t,$$

U being a unitary operator on H, is unitarily equivalent [8, 9] to the evolution rule for the probability amplitudes $\phi_t^{(\mathrm{r,l})}(x)$ in the form

$$\begin{pmatrix} \phi_{t+1}^{(\mathrm{r})}(x+1) \\ \phi_{t+1}^{(\mathrm{l})}(x-1) \end{pmatrix} = \begin{pmatrix} \cos\theta & \mathrm{i}\sin\theta \\ \mathrm{i}\sin\theta & \cos\theta \end{pmatrix} \begin{pmatrix} \phi_t^{(\mathrm{r})}(x) \\ \phi_t^{(\mathrm{l})}(x) \end{pmatrix}, \tag{2}$$

where θ is related to the particle mass by $m = \tan(\theta)$.

This model reproduces in the continuum limit the time dependent Schrödinger equation for a free particle with probability amplitude at each lattice point $\phi(x,t) = \phi^{(\mathrm{l})}(x,t) + \phi^{(\mathrm{r})}(x,t)$ and probability density $\rho(x,t) = |\phi(x,t)|^2$. This scheme has been extended to many dimensions [10] and classical solitons [11].

In order to implement a free particle going to the right, we assign values for the probability amplitudes based on the initial wavefunction $\Phi(x)$ as

$$\begin{pmatrix} \phi^{(\mathrm{r})}(x) \\ \phi^{(\mathrm{l})}(x) \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \Phi(x). \tag{3}$$

2.2. Succi's model

Following a completely different path, Succi proposed a lattice Boltzmann model that uses a BGK evolution equation [12]–[17]. From the Dirac equation in the Majorana form, he obtains a discretization scheme for the spatial and time derivatives of the Dirac quadrispinor

$$\psi = \begin{pmatrix} u_1 \\ u_2 \\ d_1 \\ d_2 \end{pmatrix}. \tag{4}$$

Let us work in atomic ($c = \hbar = 1$) and lattice units ($\Delta z = \Delta t = 1$). The streaming of this model is given by [12, 13, 16]

$$\begin{aligned} \hat{u}_1 &= au_1 + bd_2, \qquad & \hat{u}_2 &= au_2 + bd_1, \\ \hat{d}_1 &= ad_1 - bu_2, \qquad & \hat{d}_2 &= ad_2 - bu_1, \end{aligned} \tag{5}$$

where $\hat{u}_{1,2} = u_{1,2}(z+1, t+1)$ and $\hat{d}_{1,2} = d_{1,2}(z-1, t+1)$ stand for the evolved probability amplitudes, $u_{1,2} = u_{1,2}(z,t)$ and $d_{1,2} = d_{1,2}(z,t)$ stand for the original amplitudes, m is

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the particle's mass, and the constants a and b are given by

$$a = \frac{(1-\Omega/4)}{(1+\Omega/4-\mathrm{i}g),} \qquad b = \frac{m}{(1+\Omega/4-\mathrm{i}g)}, \tag{6}$$

with $\Omega = m^2 - g^2$.

In order to obtain the behaviour of a non-relativistic quantum particle, a linear combination of the quadrispinor functions is performed. Defining the functions

$$\varphi_1^+ = \frac{1}{\sqrt{2}}(u_1 + d_2)\exp(\mathrm{i}mt), \tag{7}$$

$$\varphi_2^+ = \frac{1}{\sqrt{2}}(u_2 + d_1)\exp(\mathrm{i}mt), \tag{8}$$

and the probability density $\rho = |\varphi_1^+|^2 + |\varphi_2^+|^2$, it can be shown that the Schrödinger equation is reproduced in the continuum limit [13, 16]. This model has been implemented in two and three dimensions [16] and in the solution of ground state Bose–Einstein condensates [17].

A particle going to the right of the initial wavefunction $\Phi(x)$ is mapped onto the quadrispinor functions as

$$\begin{pmatrix} u_1(x) \\ u_2(x) \\ d_1(x) \\ d_2(x) \end{pmatrix} = \begin{pmatrix} 1/2 \\ 1/2 \\ -\mathrm{i}/2 \\ -\mathrm{i}/2 \end{pmatrix} \Phi(x). \tag{9}$$

3. Simulations

In order to test the behaviour of both models, we simulate the time evolution of a Gaussian wavefunction for a single free particle,

$$\Phi(x) = \frac{\mathrm{e}^{\mathrm{i}kx}}{2\sigma\sqrt{2\pi}} \exp\left[-\frac{1}{2}\left(\frac{x-\mu}{\sigma}\right)^2\right], \tag{10}$$

with k the wavenumber, μ the initial position of the Gaussian centroid and σ the variance. This wavepacket has analytical solutions for the mean displacement d and the variance σ [13], in terms of the centroid's position of the wavepacket X, the velocity β (in terms of c) and the initial parameters of centroid μ and variance σ_0,

$$X(t) = \mu + \beta t; \qquad d = X - \mu, \tag{11}$$

$$\sigma(t) = \left(\sigma_0^2 + \frac{t^2}{4m^2\sigma_0^2}\right). \tag{12}$$

The question is, therefore, how both algorithms reproduce the time evolution for the Gaussian wavepacket (10). For this purpose we used a simulation space of length $L = 2048$ cells with periodic boundary conditions and we set $m = 0.5$, $\mu = L/2$, $\sigma = 50$ lattice units and a speed of $\beta = 0.2$.

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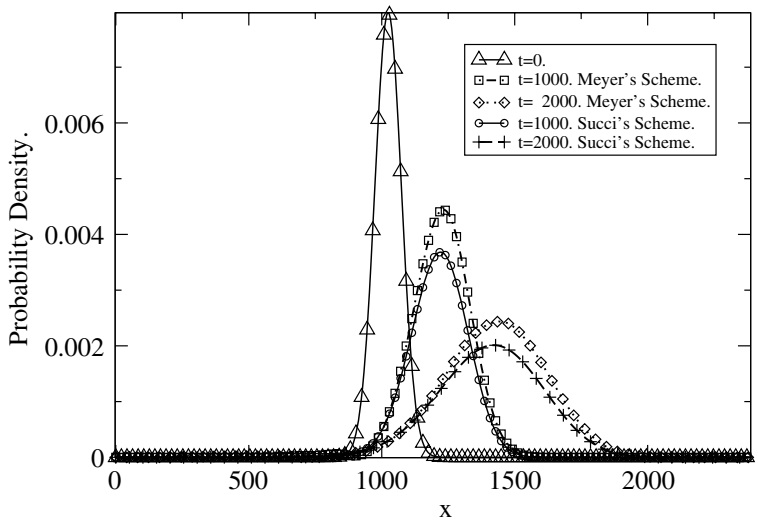

Figure 1. Probability density from the two models. Note the nice agreement between them in centroid and variance at different times; however, there is a difference in height of the probability density between the two models.

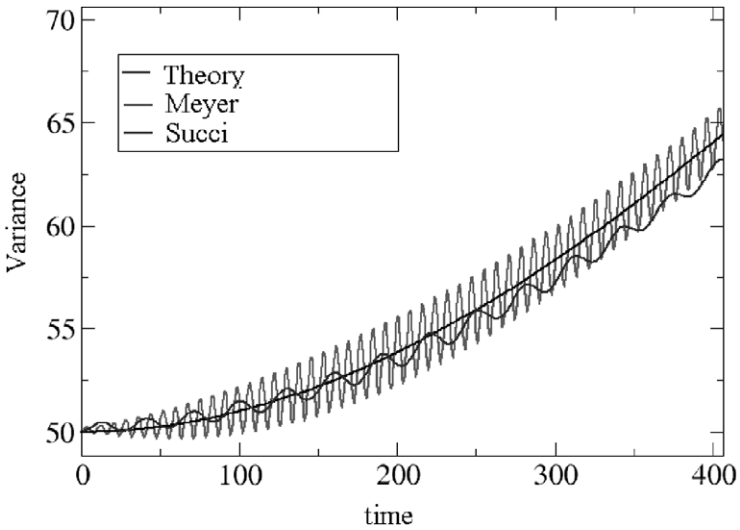

Figure 2. Variance of the Gaussian wavepacket. An unexpected oscillatory behaviour can be observed for both models.

The first results can be observed in figure 1, which shows the probability density $\rho = \|\psi\|^2$ at two different time steps for both models. One can see a nice agreement between $X(t)$ and $\sigma(t)$ with just a slight difference in the amplitude. Figure 2 shows unexpected oscillations in the variance for both models. These oscillations tend to disappear when time increases. The situation can be influenced by the mass term in (12) and therefore we ran for each model a set of simulations with the same initial variance, but different masses. The results are shown in figure 3.

In figure 3(a) (Meyer's model), one sees that the frequency rises when the mass increases but the amplitude remains almost the same. In contrast, in figure 3(b)

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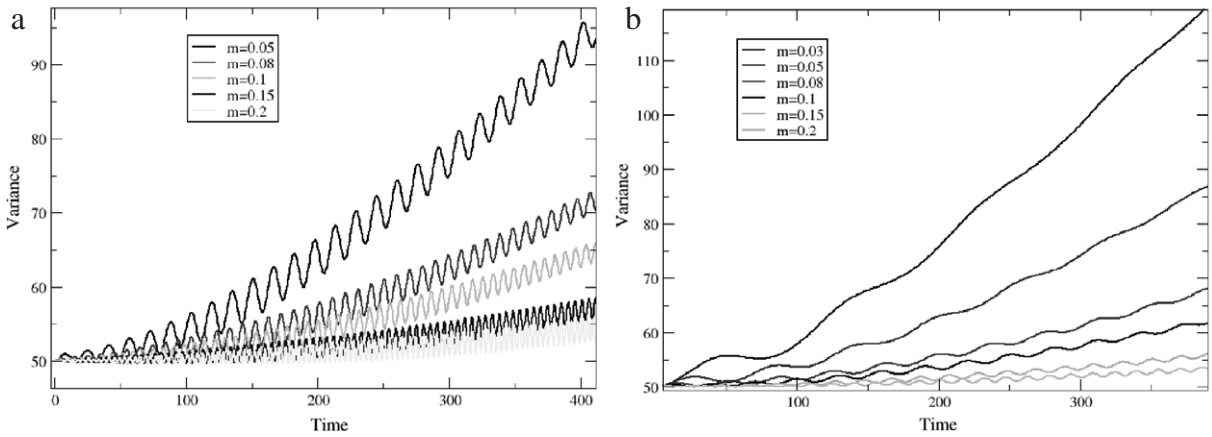

Figure 3. Variance of the Gaussian wavepacket in (a) Meyer's model and (b) Succi's model as a function of mass.

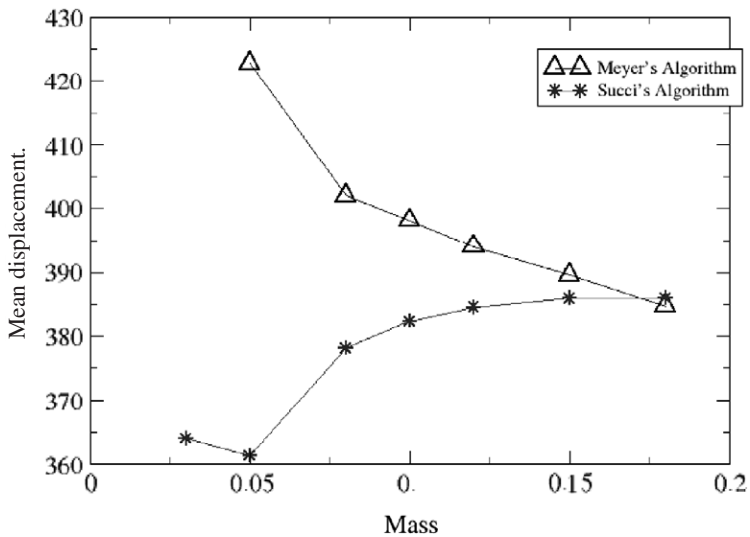

Figure 4. Final data for the mean displacement plotted versus the mass of the Gaussian wavepacket. The analytical result in this case is 400 lattice units.

(Succi's model), both the frequency and the amplitude of the oscillation increase with mass. Similar results arise from other parameter sets.

As regards the mean displacement, it is interesting how near to one another the two algorithms are after 2000 time steps with respect to the analytical configuration given by (11). Note that this value is mass independent. The result of the final displacement, plotted as a function of mass, can be observed in figure 4.

For Meyer's model at low masses, the final displacement lies above the theoretical result and decreases when mass increases, even crossing the theoretical prediction. In contrast, the final displacement in Succi's model increases with mass and reaches a slightly better result for large masses.

The results of the mean displacement can be also investigated when the velocity of the wavepacket changes. Indeed, the result depends on the value of this parameter and

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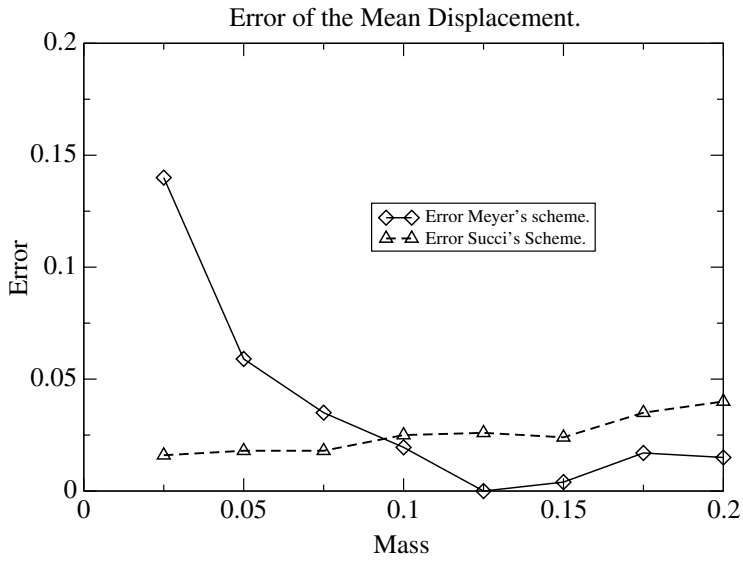

Figure 5. Relative error of the mean displacement as a function of velocity.

therefore a percentage error can be estimated for each one (figure 5). It can be observed that the error level for the Succi model remains almost the same. The errors for the Meyer algorithm, in contrast, start very high and decrease with particle speed to values around half of those for the Succi model.

4. Concluding remarks

Thus far we have compared the predictions of two lattice models for quantum dynamics, namely: a diffusion automaton proposed by Meyer and a lattice Boltzmann model proposed by Succi, when applied to the free propagation of a Gaussian wavepacket. In general, we identify that both models reproduce the basic Gaussian packet propagation with a linear increase in both displacement and variance over time. However, both variance and displacement present unexpected oscillations. These oscillations are less impressive in the Succi model than in the Meyer one. Furthermore, the numerical predictions for the mean displacement and the variance from both models exhibit dependences on the particle mass and speed; however they are in parameters that theoretically do not affect these two quantities.

These results show unexpected elements in both quantum lattice Boltzmann models. Although the theory of these schemes shows an adequate reproduction of the Schrödinger equation, these oscillations and cross-dependences in parameters not involved in the theoretical predictions may hide boundary problems, problems in the discretization of the Hilbert space or even numerical instabilities. These may prove to be fundamental issues for an adequate adaptation of these numerical methods in the quantum realm.

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