Quantum walks as simulators of neutrino oscillations in a vacuum and matter

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Keywords: quantum walks, neutrino oscillations, quantum simulation

Abstract

We analyze the simulation of Dirac neutrino oscillations using quantum walks, both in a vacuum and in matter. We show that this simulation, in the continuum limit, reproduces a set of coupled Dirac equations that describe neutrino flavor oscillations, and we make use of this to establish a connection with neutrino phenomenology, thus allowing one to fix the parameters of the simulation for a given neutrino experiment. We also analyze how matter effects for neutrino propagation can be simulated in the quantum walk. In this way, important features, such as the MSW effect, can be incorporated. Thus, the simulation of neutrino oscillations with the help of quantum walks might be useful to illustrate these effects in extreme conditions, such as the solar interior or supernovae.

1. Introduction

Quantum simulation is important for the ability to explore the behavior of a quantum system under conditions that are experimentally difficult to access. A clear example is the exploration of the Dirac equation, which allows for the visualization of effects like the Zitterbewegung or the Klein paradox [1–3], which can in fact be easily simulated on a classical computer, but are hard to verify in the laboratory. Related to this application of quantum simulations, we will consider in this paper another problem that concerns the simulation of neutrino oscillations using the quantum walk (QW). Neutrino oscillations were proposed by B Pontecorvo in 1957 [4], under the form of neutrino–antineutrino oscillations, in analogy to Kaon oscillations, and afterwards as ‘flavor transitions’ by Maki, Nakagawa and Sakata in 1962 [5]. These kind of oscillations appear because of the three types of flavor states for neutrinos ($\nu_e$, $\nu_\mu$, and $\nu_\tau$) that have a definite interaction in the Standard Model of particle interactions (SM) and do not coincide with the mass eigenstates of the Hamiltonian described by the same model. Instead, there is a unitary transformation that relates both sets of states. As a consequence, a neutrino which is produced, e.g. as an electron neutrino $\nu_e$, can be detected with a given probability as any of the three flavors at a later time (see, for example [6, 7]). Neutrino oscillations have given rise to very rich phenomena, ranging from the solution to the solar neutrino problem, supernovae [8], reactor neutrinos [9], the early Universe [10], or atmospheric neutrinos [11].

QWs are quantum cellular automata in the one particle sector that can be viewed as formal generalizations of classical random walks. They were first considered by Feynman [12] as a possible discretization of the free Dirac dynamics in flat space-time, and later introduced in physics literature in a systematic way by Meyer [13], following the seminal work of Aharonov [14]. A continuous-time version first appeared in [15]. QWs have been realized experimentally with a wide range of physical objects and setups [16–22], and are studied in a large variety of contexts, ranging from fundamental quantum physics [22, 23] to quantum algorithmics [24, 25], solid-state physics [26–29] and biophysics [30, 31]. Following Feynman’s idea, several authors have studied the connection between quantum automata and quantum field theory [32, 33]. In particular, it is well known that the continuous limit of various QWs formally coincides with the Dirac equation [34–36]. It has been shown recently that several QWs can model the dynamics of free Dirac fermions coupled to electromagnetic [37, 38] and relativistic gravitational fields [3, 39–41].
Here, we will make use of the capabilities of the QW as discretizations of quantum field theories, to establish a connection between QWs and the phenomenology of neutrino oscillations in different scenarios. Given the known bounds to the neutrino masses, we will concentrate on relativistic neutrinos, an approximation that holds in the vast majority of experimental situations. Neutrino oscillations have been demonstrated by experiments using a birefringent crystal [42]. In [43] the authors discuss the idea of simulating the coupled Dirac equations describing the neutrino propagation with trapped ions. A different proposal [44] consists in using waveguide arrays. The QW, however, offers the possibility to perform the simulation by using a suitable modification of the multi-atomic setups already available, or proposed, for the QW dynamics. Experimental procedures allowing the implementation of DTQWs with wave functions having more than two components have been proposed in [45, 46]. In these procedures, the DTQWs are implemented with single photons or classical light, for example in optical cavities or with atoms in optical lattices.

A previous work has already motivated such a study [47]. Here, we extend this work in two crucial directions. First, we analyze the continuous version (in space and time) of the proposed model. In this way, we can obtain the resulting equations that describe the well known Hamiltonian dynamics of (relativistic) neutrinos. This result, not only is a verification of the model describing neutrino oscillations, but also allows one to establish a clear correspondence between the parameters of the simulation and the neutrino data for a given experiment. Secondly, we show how matter effects can be incorporated into the simulation. As it is well known, matter effects are crucial for the explanation of the solar neutrino problem, specially for the higher energy $^8\text{B}$ neutrinos [7], and for long baseline experiments [48, 49]. A quantum simulator can then be used as an extra tool to visualize these effects from the point of view of a discretized field theory.

This paper is organized as follows. In section 2 we give a short introduction to the phenomenon of neutrino oscillations, and illustrate it for the case of two flavors. In section 3 we define the dynamics of the QW model, and we show that, in the continuous space-time limit, we recover the dynamics of a set of coupled Dirac equations that can be put in correspondence with the Hamiltonian formulation of neutrino oscillations, thus allowing one to identify the value of the parameters needed to simulate a given neutrino experiment. We make use of this correspondence, in section 4, to give an example of the simulation of three flavors in a vacuum. In section 5, we show how matter effects in the neutrino propagation can be incorporated in the QW model. Our main conclusions are summarized in section 6. Along this paper we use natural units, defined by $\hbar = c = 1$.

2. Neutrino oscillations

Neutrinos are produced as ‘flavor states’ via charged or neutral currents in nuclear reactors, stars, cosmic rays and many other scenarios, in the way described by the SM. These flavor states $\Psi_i (\alpha = e, \mu, \tau)$ are related, at a given space-point $(t, x)$, to the mass eigenstates by an unitary transformation $R$, such that

$$\Psi_i(t, x) = \sum_i R_{ni} \Psi_i(t, x),$$

(1)

where $\Psi_i(t, x)$ is the neutrino field with mass $m_\nu$. The field can, in principle, take either a Dirac or a Majorana form although we will consider, for definiteness, a Dirac field: the precise nature of the neutrino field is still undetermined and, although important for the fundamental knowledge of neutrinos, is irrelevant in the case of relativistic neutrinos considered here. Equation (1) actually refers to the left chiral components of the neutrinos, since only these components interact within the SM. We will restrict ourselves to propagation along one spatial dimension, then $x$ refers to the coordinate along that dimension.

We will concentrate on neutrino eigenstates, with momentum $\vec{k}$ and energy $E_\nu = \sqrt{\vec{k}^2 + m_\nu^2}$ of the Hamiltonian $H$ of the theory:

$$H \left| \nu_\alpha \right\rangle = E_\nu \left| \nu_\alpha \right\rangle.$$

Suppose that, at time $t = 0$, a flavor neutrino $|\nu_\alpha\rangle$ is produced, then at time $t$ the neutrino state evolves according to

$$\left| \nu_\alpha \right\rangle_t = e^{-iHt} \sum_{i=1}^3 R_{ni} \left| \nu_i \right\rangle = \sum_i \left| \nu_i \right\rangle e^{-iE_i t} R_{ni}^\text{M}.\$$

(3)

Therefore, at time $t$, the initial neutrino can be detected as any flavor $\nu_\beta$. The probability of the $\nu_\alpha \rightarrow \nu_\beta$ transition after a time $t$ is then given by the following expression

$$P (\nu_\alpha \rightarrow \nu_\beta; t) = \left| \sum_{i=1}^3 R_{ni} e^{-iE_i t} R_{ni}^\text{M} \right|^2.$$  

(4)
To illustrate the latter formula, let us analyze the case with only two neutrino states (some interesting cases, such as solar and atmospheric neutrinos, can be effectively described in this way). The matrix $R$ can be taken as

$$ R = \begin{pmatrix} \cos \phi_{12} & \sin \phi_{12} \\ -\sin \phi_{12} & \cos \phi_{12} \end{pmatrix}, $$

$\phi_{12}$ being the mixing angle. By approximating $E_{\nu} \approx |k| \pm \frac{m_e^2}{2|k|}$, equation (4) gives, for $\beta = \alpha$:

$$ P(\nu_e \rightarrow \nu_{\varnothing}; t) = \sin^2 2\phi_{12} \sin^2 \varphi(t), $$

where

$$ \varphi(t) \equiv \frac{\Delta m_{12}^2 t}{2|k|}, $$

with the notation $\Delta m_{12}^2 = m_1^2 - m_2^2$. Notice that, in the latter equation, one can replace $|k|$ by $E$ within the same order of approximation as above, where $E = E_1 \approx E_2$. Also, it is customary to use the distance $L = t$ traveled by the neutrinos from the production to the detection point. Then, the argument of the oscillatory function in (6) becomes

$$ \varphi(L) \approx 5.08 \frac{\Delta m_{12}^2 L}{2E}, $$

when $\Delta m_{12}^2$ is expressed in $eV^2$, $L$ in Km and $E$ in GeV units.

### 3. The model

Consider a QW defined over discrete time and discrete one dimensional space, labeled respectively by $j \in \mathbb{N}$ and $p \in \mathbb{Z}$. This QW is driven by an homogeneous coin acting on the $2n$-dimensional tensor-product Hilbert space $\mathcal{H} = \mathcal{H}_{\text{spin}} \otimes \mathcal{H}_n$, where $\mathcal{H}_{\text{spin}}$ is 2-dimensional and $\mathcal{H}_n$ describes the $n$-flavor Hilbert space of the walker. The evolution equations read

$$ \begin{bmatrix} \psi_{j+1,p}^1 \\ \vdots \\ \psi_{j+1,p}^n \end{bmatrix} = \left( \bigoplus_{h=1,n} \mathcal{S} Q_h^2 \right) \begin{bmatrix} \psi_{j,p}^1 \\ \vdots \\ \psi_{j,p}^n \end{bmatrix}, $$

where $Q_h^2 \in SU(2), h = 1 \ldots n$, and

$$ Q_h^2 = \begin{pmatrix} \cos(\theta_h) & i \sin(\theta_h) \\ i \sin(\theta_h) & \cos(\theta_h) \end{pmatrix}, $$

is the quantum coin acting on each flavor state of the walker depending on dimensionless real parameters $(\epsilon, \theta_h)$. The operator $\mathcal{S}$ is the usual spin-dependent translation acting on each flavor component, $\psi_{j,p}^h = (\psi_{j,p}^1, \psi_{j,p}^2, \psi_{j,p}^3) \in \mathcal{H}_{\text{spin}}$ and defined as follows:

$$ S \psi_{j,p}^h = (\psi_{j,p+1}^h, \psi_{j,p}^h, \psi_{j,p-1}^h)^T. $$

We note $\Psi = (\bigoplus_{h=1,n} \psi_{j,p}^h) \in \mathcal{H}_n$.

Equation (9) describe the evolution of $n$ independent two-level systems, and it has been shown that each of them recover, in the continuous limit, the Dirac equation [3, 37, 39], where the parameter $\theta_h$ corresponds to the mass of the fermion. Let us now consider an additional unitary operator $R$ and its inverse $R^{-1} = R^T$ acting on $\mathcal{H}_n \otimes \mathcal{H}_2$. The specific role of this operator is to mix the flavor degrees of freedom, as in equation (1). The evolution equation becomes:

$$ \Psi_{j+1,p}^h = R (\bigoplus_{h=1,n} \mathcal{S} Q_h^2) R^T \Psi_{j,p}^h, $$

where we call $\tilde{\Psi}_{j,p} = R \Psi_{j,p}$ the flavor eigenstates. In the next section we will prove that this simple model recovers, in the continuous limit, the oscillatory dynamical behavior of Dirac neutrinos in vacuum.

#### 3.1. Generalized Dirac equation for neutrinos

In order to compute the continuous limit of equations (9), we first consider that $\tilde{\Psi}_{j,p}$ are the ‘values’ $\psi(t_j, x_p)$ taken by a two-component wave-function $\tilde{\Psi}$ at space-time point $(t_j = j\epsilon, x_p = p\epsilon)$. We assume that $\tilde{\Psi}$ is at least twice differentiable with respect to both space and time variables for all sufficiently small values of $\epsilon$. Assuming the existence of the continuous limit imposes the following constraint on the coin:
The above equation (13) is directly verified because $Q^i = I_2$ as $\epsilon \to 0$ and $RR^\dagger = I_{2n}$ by definition.

When we Taylor-expand (12) at first order in $\epsilon$, the zero-order terms cancel each other, since (13) is satisfied, and the first-order terms provide the following system of partial differential equations (PDEs):

$$\left[\partial_t - (\bigoplus_{h=1,n} \sigma_z) \partial_s - iM] \Psi(t, x) = 0,\right.$$  \hspace{1cm} (14)

where $M_{rs}$ is the mass tensor, with indices $r, s = \{1, \ldots, n\}$:

$$M_{rs} = \sum_{c=1, \ldots, n} R_{rc} \tilde{Q}_c R_{rc}^{-1} \tilde{Q}_c = \bar{\theta}_r \sigma_c.$$  \hspace{1cm} (15)

Equation (14) are standard Dirac equations for $n$ relativistic flavor neutrinos in $(1 + 1)$ continuous space-time. Notice that, because $\Psi(t, x)$ is a solution of the Dirac equation, it is also a solution of the Klein–Gordon (KG) equation. As usual, we can expand the neutrino field in plane waves of the form $\Psi(t, x) = \tilde{\Psi}(t) e^{i k x}$, so that equation (14) transcribes in $(\partial_x^2 + k^2 + M^\dagger M) \tilde{\Psi}(t) = 0$, where $M^\dagger M = \text{diag}[\bar{\theta}_1^2, \ldots, \bar{\theta}_n^2]$. To describe relativistic neutrinos, however, the condition $k \gg \bar{\theta}_r$ has to be fulfilled. In this limit, one can linearize the previous KG equation as follows:

$$i\partial_t \tilde{\Psi}_k(t) - \Omega_k \tilde{\Psi}_k(t) = 0, \quad \Omega_k = \left(k + R^\dagger \frac{|M|^2}{2k} - R\right).$$  \hspace{1cm} (16)

where we have considered only the positive-energy probability amplitudes (neutrinos), and defined $|M| = \sqrt{M^\dagger M}$. For negative-energy states (antineutrinos) a global minus sign appears in equation (16).

Following a similar procedure as in section II one can obtain, starting from equation (16), the transition probability, which can be written as

$$P(\nu_i \to \nu_j; t) = \left| \sum_k \tilde{\psi}_k^\alpha (0) \tilde{\psi}_k^\beta (t) \right|^2.$$  \hspace{1cm} (17)

For example, in the case of two neutrino flavors, one would arrive to equation (6), but with the phase $\varphi(t)$ given by

$$\varphi(t) = \frac{\bar{\theta}_1^2 - \bar{\theta}_2^2}{2k} t.$$  \hspace{1cm} (18)

4. Simulation of neutrino oscillations in vacuum

The above equations were derived for any number of neutrino generations. Writing them explicitly in terms of mixing angles is extremely cumbersome in general. Let us consider the three neutrino generations $\{\nu_e, \nu_\mu, \nu_\tau\}$ in vacuum, respectively the electron, the muon and the tau neutrino. The transformation $R$ recovers the Pontecorvo–Maki–Nakagawa–Sakata (PMNS) mixing matrix and depends on three real parameters$^3$:

$$R = e^{i0_1 \lambda_1} e^{i0_2 \lambda_2} e^{i0_3 \lambda_3},$$  \hspace{1cm} (19)

where the $\lambda$ are the Gell–Mann matrices that correspond to the spin-one matrices of $SO(3)$. Each angle $\phi_{ij}$ corresponds to the mixing between two neutrino species. Let us remark that when $R$ is the identity, the solutions of equation (16) are propagating plane waves $\propto e^{-i(Et - kx)}$, where $k^2 = E^2 - \bar{\theta}_e^2$, $h \in \{e, \mu, \tau\}$.

The comparison between equations (7) and (18) allows us to establish a criterion to simulate a given neutrino oscillation experiment, by requiring that the accumulated phase $\varphi(t)$ takes the same value in both cases, where $t$ represents the number of time steps in the QW simulation. For example, one can choose the values $\bar{\theta}_2$ as given the neutrino square masses $m_2^2$, expressed in eV$^2$, and $k$ given by the energy in GeV. This will, in turn, fix the number of required time steps, for a given distance $L$. A second condition, of course, is that the mixing angles $\phi_{ij}$ correspond to the observed values (see [30] for recent results).

In figure 1 we can observe the oscillatory behavior of three flavor neutrinos starting from a pure electron-neutrino initial state:

$$\psi_{k}^{i, \nu_e}(0) = \frac{1}{\sqrt{n}} \sum_{p=0}^{n-1} e^{-i(k - k_0)x_p} \otimes (1, 0, 0, 0, 0, 0)^T.$$  \hspace{1cm} (20)

One can observe that these plots reproduce the ones corresponding to actual calculations of neutrino oscillations (see for example [51]).

$^3$We do not include CP symmetry violation effects in this model.
5. Neutrino oscillations in matter

Wolfenstein (1978) was first to recognize that the medium induces a modification of the neutrino dispersion relation [52], and then Mikheyev and Smirnov showed that oscillations can be resonant when neutrinos pass through a density gradient, so that the flavor branches of the dispersion relations have an avoided crossing [53]. This Mikheyev–Smirnov–Wolfenstein (MSW) effect is very important in astrophysics because neutrinos are naturally produced in the interior of stars and stream through a density gradient into empty space.

In order to model neutrino oscillations in a medium, let us consider the case with only two flavors, which we freely denote as $\nu_e$ and $\nu_{\mu}$. Notice that, as already mentioned, many realistic experiments can be effectively reduced to a two-neutrino oscillation. In that case we consider one mixing angle and a 2-dimensional matrix $R$:

$$R = \begin{pmatrix} \cos \phi & \sin \phi \\ -\sin \phi & \cos \phi \end{pmatrix} \otimes \mathbb{I}_2$$ (21)

Matter interaction is modeled by introducing a position-dependent phase:

$$\Psi_{j+1,p} = V_p R (\bigoplus_{h=1,2} S Q^h) R^\dagger \Psi_{j,p},$$ (22)

where

$$V_p = \text{diag}(e^{i\theta_{\nu_e}}, 1) \otimes \mathbb{I}_2$$ (23)

By the same procedure presented in section A we can derive the following Dirac equations:

$$i \partial_t \Psi(t, x) - \mathcal{H}_m \Psi(t, x) = 0,$$ (24)

$$\mathcal{H}_m = i (\sigma_2 \otimes T) \partial_x - \mathcal{M} + \mathcal{V}(x)$$ (25)

where the potential $\mathcal{V}$ reads as follows:

$$\mathcal{V}(x) = \gamma^5 \mathbb{I}_4 \rho(x),$$ (26)

with $\mathbb{I}_4$ the 4-dimensional identity matrix, and $\gamma^5 = \frac{1}{2}(1 + \sigma_2)$. The transition probability from an electron neutrino to the muon neutrino is given by:

![Figure 1. Time evolution of the probability $P(\nu_i \to \nu_j, t)$, $\beta \in \{e, \tau, \mu\}$ of a three flavor neutrino oscillation in vacuum, simulated by a QW. (Top) Short (inset) and medium time range (200 time steps). (Bottom) Long time range (1000 time steps). The mass differences are $\Delta m^2_{21} = 0.003$ rad, $\Delta m^2_{32} = 0.32$ rad, $\Delta m^2_{43} = 0.31$ rad, and the mixing angles $\theta_{12} = 0.34$ rad, $\theta_{13} = 0.54$, $\theta_{23} = 0.45$ rad, whereas $k_0 = 100$. The initial condition is defined in equation (20).](image)
where $U = U(x)$ is position-dependent and reads:

$$U(x) = \begin{pmatrix} \cos \Phi(x) & \sin \Phi(x) \\ -\sin \Phi(x) & \cos \Phi(x) \end{pmatrix},$$

and the mixing angle $\Phi(x)$ is related to the mixing angle in vacuum $\phi$ via the well known relation:

$$\sin^2 2\Phi(x) = \frac{\sin^2 2\phi}{A(x)},$$

with $A(x) = \left[ \cos(2\phi) - \frac{2E(x)}{2m} \right]^2 + \sin^2 2\phi$ the resonance factor. Notice that, if matter density is not constant, it is necessary to take into account the effect of $\partial_x U(x)$ in the evolution equation in mass eigenstates. In fact:

$$U \mathcal{H}_m U^{-1} = iU (\sigma_\gamma \otimes I) \partial_x U^{-1} + \text{diag. terms}$$

As mentioned above, the eigenvalues $E_{1m}$ and $E_{2m}$ of the Hamiltonian (25) present an avoided crossing (see figure 2) close to the resonance. The effect of the off-diagonal terms proportional to $\partial_x \Phi(x)$ in the evolution is to generate transitions between the energy states close to the resonance. However, if the derivative is much smaller with respect to the diagonal terms such transitions are negligible. To quantify the strength of the off-diagonal terms it is useful to introduce the adiabaticity parameter:

$$\gamma = \frac{\Delta m^2_{\text{sol}}}{4k |\partial_x \Phi(x)|}.$$ 

If $\gamma \gg 1$ for all $x$ the evolution is adiabatic, otherwise the probability of flavor transition reads:

$$P(\nu_e \rightarrow \nu_{\mu}; t_f) = \frac{1}{2} + \left( 1 - P_c \right) \cos 2\Phi(t_f) \cos 2\Phi(t_i)$$

where $t_f$ and $t_i$ are the final and initial times (which can be approximated by the final and initial position $x_f$ and $x_i$, for relativistic neutrinos), $P_c$ is the crossing probability for $x_f \rightarrow \infty$:

$$P_c = \frac{\exp\left(-\frac{\pi}{2} \gamma \right) - \exp\left(\frac{\pi}{\sin \phi^2} \frac{2m \gamma}{2m} \sin \phi^2 \right)}{1 - \exp\left(-\frac{\pi}{2} \gamma \right)},$$

and $\gamma$ is the adiabaticity parameter at the resonance [54].

In figure (3) we have shown that a QW can mimic the time evolution of two neutrino flavors in matter with a linear density and for $\gamma \ll 1$. In the long time behavior the transition probability simulated by the QW converges to the asymptotic probability $P(\nu_e \rightarrow \nu_{\mu}; t_f)$, which confirms the agreement between the QW’s and the neutrino’s dynamics in matter.
6. Conclusions and outlook

In this paper we have analyzed the simulation of Dirac neutrino oscillations both in a vacuum and in the presence of matter effects using quantum walks, which can therefore be regarded as a discretization of the underlying field theory. We showed that, in fact, in the continuous limit one recovers a set of coupled Dirac equations that describe flavor oscillations. This fact allows us to establish a clear connection with the neutrino phenomenology for a particular scenario, such as detection of solar, atmospheric, reactor neutrinos, etc., so as to fix the relevant parameters of the simulation (e.g. the initial state, or the necessary time steps). We have also introduced a way to simulate neutrino propagation in matter, an element which is crucial for some experiments, such as detection of solar neutrinos [7], or long baseline experiments [18, 49]. As discussed in section V, the simulation correctly reproduces the flavor conversion probability for a wide range of values of the adiabaticity parameter. The above results show that quantum walks can be used to simulate these phenomena, thus allowing one for a visualization of the neutrino phenomenology in scenarios like the solar interior or supernovae.

Acknowledgments

This work has been supported by the Spanish Ministerio de Educación e Innovación, MICIN-FEDER project FPA2014-54459-P, SEV-2014-0398 and Generalitat Valenciana grant GVPROMETEOII2014-087. We acknowledge valuable discussions with E Roldán and A Verga.

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Figure 3. Time evolution of the probability $P(\nu_e \rightarrow \nu_x)$ in matter with linear density $\rho(x) = x$ simulated by a QW in 125 time steps. The mass difference and the initial energy is the same of figure 2. The dashed line (black) represents the asymptotic crossing probability at the resonance given by formula (32), for different adiabaticity parameters $\gamma$. The initial and final time steps are $t_i = 0$, $t_f = 125$. The initial condition is as defined in equation (20).
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