Propagating Quantum Walks: the origin of interference structures.

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Abstract
We analyze the solution of the coined quantum walk on a line. First, we derive the full solution, for arbitrary unitary transformations, by using a new approach based on the four "walk fields" which we show determine the dynamics. The particular way of deriving the solution allows a rigorous derivation of a long wavelength approximation. This long wavelength approximation is useful as it provides an approximate analytical expression that captures the basics of the quantum walk and allows us to gain insight into the physics of the process.

1 Introduction
Consider a two–state particle, e.g. a two–level atom, moving along a one–dimensional lattice. The displacement is conditional; that is, the particle jumps one site at each time to the right or to the left depending on its internal state. The movement of such a particle is rather trivial: If the particle is in its "up" or "down" internal state it moves to the right or to the left, respectively, and it undergoes a superposition of right and left displacements if it is in a superposition of its "up" and "down" states. But the movement becomes nontrivial if

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after each displacement a suitable unitary transformation, e.g. the Hadamard transformation, leads to a superposition of the internal states of the particle. Now the probability distribution that the particle would be found at a given position is quite rich: It is null at odd (even) positions at odd (even) times, shows two strong peaks near the right and left edges, develops strong oscillations near these peaks and has a smooth plateau in the central region. This process is known as the (coined) quantum walk.

In a sense, the quantum walk, which we refer to as QW, is the quantum generalization of the classical random walk, and as such was first introduced ten years ago by Aharonov et al. [1]. It was later rediscovered by Meyer [2] in the context of quantum cellular automata, and more recently by Watrous [3] in the context of quantum algorithms. The QW introduced in these papers is called the discrete QW (be it coined [1,2] or not [3]), and must be distinguished from the so-called continuous QW, introduced by Farhi and Gutmann in 1998 [4], which realizes to some extent a quantum version of continuous time classical Markov chains. The connection between these two types of QWs is still unclear [5].

The QW, both in its discrete and continuous versions, is a process that has recently attracted the attention of many workers in the quantum computing community; see, for example, the recent review by Julia Kempe [5]. Of interest is the possibility that QWs will give rise to new quantum algorithms that show clear speedups over classical algorithms. The first results in this direction have been obtained by Shenvi et al. [6], who have shown that a QW can perform the same tasks as Grover’s search algorithm [7], and by Childs et al. [8], who have introduced an algorithm for crossing a special type of graph exponentially faster than can be done classically.

In the present communication we give an alternate description of the discrete QW that we feel gives physical insight into the nature of that process. This paper is an extension of our previous work [9], in which we showed that the QW on the line is not a characteristically quantum process in the specific sense that it can be understood simply as a wave phenomenon, thus opening the possibility of entirely classical implementations [10]. Indeed, wave implementations [11,12] of the QW have already been discussed. In other words, the characteristic quantum feature of entanglement does not seem to play any central role in the QW, at least in the unidimensional case. The situation could be different for higher dimensional QWs; see the discussion in Knight et al. [10] for some insight into the role of entanglement in higher dimensional QWs.

The rest of the article is organized as follows. In Section 2 we give the evolution equations for the standard discrete coined QW, and reformulate them in a way that directly exhibits an important property: The two coin states evolve independently of each other, the coupling between them entering only through the first iteration of the walk. In Section 3 we derive the formal solution of the QW in a manner different to those already carried out [13,14]. This alternative derivation allows a rigorous derivation of the long wavelength approximation that corresponds to the continuous limit of the QW we pointed out earlier [9]. In Section 4 we give the solution of this long wavelength limit and discuss some
of its properties. Finally in Section 5 we give our conclusions.

2 Equations of evolution

Let $H_P$ be the Hilbert space of the particle positions and $\{|m\rangle, m \in \mathbb{Z}\}$ a basis of $H_P$; and let $H_C$ be the Hilbert space describing the two states of the qubit associated with the internal states of the particle (usually referred to as the coin), and $\{|R\rangle, |L\rangle\}$ a basis of $H_C$. The state of the total system belongs to the space $\mathcal{H} = H_C \otimes H_P$. The dynamics of the system is governed by two operations, the conditional displacement

$$\hat{D} |m, R\rangle = |m + 1, R\rangle,$$

$$\hat{D} |m, L\rangle = |m - 1, L\rangle,$$

and the transformation acting on the internal states of the coin

$$\hat{H} |m, R\rangle = \sqrt{\rho} |m, R\rangle + \sqrt{1 - \rho} |m, L\rangle,$$

$$\hat{H} |m, L\rangle = \sqrt{1 - \rho} |m, R\rangle - \sqrt{\rho} |m, L\rangle,$$

$0 \leq \rho \leq 1$, which is the most general unitary transformation that one needs to consider [15] (notice that $\hat{H}$ is the Hadamard transformation when $\rho = 1/2$). The QW is implemented by the repeated action of the operator $\hat{H}\hat{D}$, i.e. if $|\psi\rangle_0$ denotes the state of the system after $n$ iterations then

$$|\psi\rangle_n = (\hat{H}\hat{D})^n |\psi\rangle_0,$$

which can be written as

$$|\psi\rangle_n = \sum_{m=-n}^{+n} [R_{m,n} |m, R\rangle + L_{m,n} |m, L\rangle],$$

with the equations of evolution of the probability amplitudes given by

$$R_{m,n} = \sqrt{\rho} R_{m-1,n-1} + \sqrt{1 - \rho} L_{m+1,n-1},$$

$$L_{m,n} = \sqrt{1 - \rho} R_{m-1,n-1} - \sqrt{\rho} L_{m+1,n-1}.$$

Finally, the probability of finding the particle at position $m$ at iteration (time) $n$, is given by

$$P_m(n) = P^R_m(n) + P^L_m(n),$$

$$P^R_m(n) = |R_{m,n}|^2, \quad P^L_m(n) = |L_{m,n}|^2.$$

Eqs. (7) and (8) are the discrete QW equations as can be found e.g. in the work of Carteret [14] for the specific case of the fair coin $\rho = 1/2$. Different equations of evolution, but still leading to the same final probability, can be found by defining the walk as the repeated action of the operator $\hat{D}\hat{H}$, instead
of $\hat{H} \hat{D}$, as is done by Nayak and Vishwanath [13]. In the Appendix we identify
the transformations that connect these different conventions for the probability
amplitudes.

There is a crucial feature in Eqs. (7) and (8) that is at the heart of our
treatment of the QW. Substituting Eq. (8) into Eq. (7) and rearranging the terms
one easily gets

$$R_{m,n} = \sqrt{\rho} R_{m-1,n-1} + R_{m,n-2} - \sqrt{\rho} \left( \sqrt{\rho} R_{m,n-2} + \sqrt{1-\rho} L_{m+2,n-2} \right). \quad (10)$$

Noticing that the last term in the right–hand side is nothing but $R_{m+1,n-1}$, and
making the change $n \rightarrow n+1$, we can write

$$R_{m,n+1} = R_{m,n-1} + \sqrt{\rho} R_{m-1,n} - \sqrt{\rho} R_{m+1,n}. \quad (11)$$

A similar equation for $L_{m,n}$ can be derived. That is, Eqs. (7) and (8) are equiv-
alent to

$$a_{m,n+1} - a_{m,n-1} = \sqrt{\rho} [a_{m-1,n} - a_{m+1,n}], \quad a = R, L \quad (12)$$

which is a remarkable equation, as it shows that the evolutions of the two coin
states are independent. That is, $R_{m,n}$ does not depend on $L_{m,n}$ at previous
times, and vice versa. The only coupling between $R_{m,n}$ and $L_{m,n}$ appears at
the first interaction. Notice that in Eq. (12) one needs to specify two initial
conditions (both $a_{m,0}$ and $a_{m,1}$) and one needs Eqs. (7) and (8) for calculating
$a_{m,1}$ from $a_{m,0}$. But apart from this initial coupling, the evolution is completely
independent for the two coin states. In other words: The QW is composed of
two independent QWs, one for each coin state, coupled only at initialization.

Eq. (12) is interesting for another reason already discussed in [9] in the special
case of the Hadamard transformation ($\rho = 1/2$). Simple inspection leads to
the idea that Eq. (12) can be understood as the discretization of a differential
equation involving all the odd derivatives with respect to space and time of a
continuous field $a(x,t)$

$$\sum_{k=0}^{\infty} \frac{\Delta t^{2k+1}}{(2k+1)!} \frac{\partial^{2k+1}}{\partial t^{2k+1}} a(x,t) = -\frac{1}{\sqrt{2}} \sum_{k=0}^{\infty} \frac{\Delta x^{2k+1}}{(2k+1)!} \frac{\partial^{2k+1}}{\partial x^{2k+1}} a(x,t). \quad (13)$$

This is too naive an approximation, as the above equation does not respect
the symetries of the solutions of Eq. (12); Eq. (13) describes the propagation of
waves in the positive position $x$ direction, whilst the probability distribution of
the quantum walk clearly shows propagation in both the positive and negative
directions. But it is clear that Eq. (12) suggests the existence of some kind of
continuous description of the discrete coined QW. Earlier [9] we obtained such
a continuous description by introducing, without justification, new amplitudes
$A_{m,n}^{\pm}$, through the definition

$$a_{m,n} = A_{m,n}^{+} + (-1)^{n} A_{m,n}^{-}, \quad (14)$$
and then we derived continuous differential equations for the continuous fields $A^\pm(x,t)$. These equations are similar to Eq. (13) but with a velocity that differs in its sign for the fields $A^+(x,t)$ and $A^-(x,t)$. From these equations we obtained an approximate evolution equation by neglecting higher order derivatives

$$\frac{\partial}{\partial t} A^\pm(\xi,\tau) = \mp \frac{1}{\sqrt{2}} \left[ \frac{\partial}{\partial \xi} + \frac{1}{12} \frac{\partial^3}{\partial \xi^3} \right] A^\pm(\xi,\tau), \quad (15)$$

with $\xi = x/\Delta x$ and $\tau = t/\Delta t$. Eq. (13) can be solved explicitly in terms of Airy functions, and shows that to this degree of approximation the quantum walk fields $A^\pm_{m,n}$ satisfy the same equation as the evolution of an optical pulse in a medium with third order dispersion.

The weak points of this approach [9] are that the fields $A^\pm$ are introduced without justification, that only the special case of the Hadamard transformation is considered, and that the continuum limit is not clearly derived. The goal of this paper is to present a rigorous derivation of Eq. (13) for arbitrary values of $\rho$. For that purpose, we first turn to a new derivation of the full solution of the quantum walk on the line.

3 The exact solution: an approach based on four fields

As at a given time identified by the index $n$ the amplitudes $a_{m,n}$ depend on the discrete variable $m$. So it is usual [13] [14] to define a continuous function of $\kappa$, periodic over a range of $2\pi$, such that the $a_{m,n}$ are the Fourier components of that function $f_n(\kappa)$,

$$f_n(\kappa) \equiv \sum_{m=-\infty}^{\infty} a_{m,n} e^{im\kappa}. \quad (16)$$

It is then possible to formulate the problem in terms of the continuous function $f_n(\kappa)$ of $\kappa$ rather than the discrete function $a_{m,n}$ of $m$. A similar strategy can be implemented with respect to the dependence on the time step $n$. We essentially follow this approach below, but our perspective is slightly different. Because we want to be able to understand Eq. (12) as the discretization of certain linear partial differential equations, we introduce Fourier expansions such as (16) in a more physical way.

3.1 Fourier amplitudes

From the amplitudes $a_{m,n}$ defined at discrete points in space, labeled by $m$, and time, labeled by $n$, we can formally introduce a field $a(x,t)$ at arbitrary points in space and time defined by

$$a(x,t) = \sum_{m,n=-\infty}^{\infty} a_{m,n} \delta(x-\Delta X) \delta(t-nT), \quad (17)$$
which produces appropriately weighted delta functions at the positions in space and time where \(a_{m,n}\) is defined. Here \(X\) is the distance between the sites in the one-dimensional lattice, and \(T\) is the time between steps in the walk. We can formally introduce the Fourier transform of this function

\[
a(x,t) = \frac{1}{(2\pi)^2} \int_{-\infty}^{+\infty} d\tilde{k} d\tilde{\omega} a(\tilde{k}, \tilde{\omega}) e^{i\tilde{k}x} e^{-i\tilde{\omega}t},
\]

(18)

where from Eq. (17) we find that

\[
a(\tilde{k}, \tilde{\omega}) \equiv \int_{-\infty}^{+\infty} a(x,t) e^{-i\tilde{k}x} e^{i\tilde{\omega}t} = \sum_{m,n=\infty}^{+\infty} a_{m,n} e^{-ikmX} e^{i\omega nT}.
\]

(19)

Next, note that we can write each \(\tilde{k}\) and \(\tilde{\omega}\) uniquely as

\[
\tilde{k} = k + \frac{2\pi p}{X}, \quad \tilde{\omega} = \omega + \frac{2\pi q}{T},
\]

(20)

with \(p\) and \(q\) integers, and \(k\) and \(\omega\) lying within the ranges

\[
-\frac{\pi}{X} < k \leq \frac{\pi}{X}, \quad -\frac{\pi}{T} < \omega \leq \frac{\pi}{T}.
\]

(21)

Then using the identity

\[
\sum_{p=\infty}^{+\infty} \delta(y - 2\pi p) = \frac{1}{2\pi} \sum_{p=\infty}^{+\infty} e^{ipy},
\]

(22)

which follows immediately from identifying the Fourier sum representing the periodic function of \(y\) on the left-hand side, we easily find from Eq. (19) that \(a(\tilde{k}, \tilde{\omega}) = a(k, \omega)\). Then, making use of Eqs. (17)–(19) and (22), we can write

\[
a(x,t) = \bar{a}(x,t) \sum_{m,n=\infty}^{+\infty} \delta(x-mX) \delta(t-nT)
\]

(23)

where

\[
\bar{a}(x,t) = \frac{1}{(2\pi)^2} XT \int_{-\pi/X}^{+\pi/X} dk \int_{-\pi/T}^{+\pi/T} d\omega a(k, \omega) e^{ikx} e^{-i\omega t}
\]

(24)

\[
a(k, \omega) = \sum_{m,n=\infty}^{+\infty} a_{m,n} e^{-ikmX} e^{i\omega nT},
\]

(25)

cf. Eq. (10).

3.2 Dispersion relation

Returning now to the discrete QW Eqs. (12), we multiply each side by \(e^{-i\omega nT}\) and \(e^{ikmX}\) and sum over \(m\) and \(n\). This yields the equation

\[
\sin \omega T = \sqrt{p} \sin kX,
\]

(26)
which identifies the dispersion relations \( \omega = \omega(k) \). Because of the range of \( k \) and \( \omega \) appearing in Eq. (24), we need only consider such solutions over the ranges (21). There are then two such solutions. One solution, which we label \( \omega_0(k) \), is that for which \( \omega \to 0 \) as \( k \to 0 \). The second, which we label \( \omega_1(k) \), is given by

\[
\omega_1(k) = -\omega_0(k) \pm \frac{\pi}{T},
\]

for \( k \) respectively > 0 and < 0. These relations are represented in Fig.1.

3.3 Separation into two fields

Solutions of Eqs. (12) must respect the dispersion relations, and thus for Eq. (25) to represent an actual solution we must have

\[
a(k, \omega) = \frac{(2\pi)^2}{XT} \left[ a^+(k) \delta(\omega - \omega_0(k)) + a^-(k) \delta(\omega - \omega_1(k)) \right],
\]

for some amplitudes \( a^+(k) \) and \( a^-(k) \). Thus from Eq. (24) we find

\[
\bar{a}(x, t) = \int_{-\pi/X}^{+\pi/X} dk \ a^+(k) e^{ikx} e^{-i\omega_0(k)t} + \int_{-\pi/X}^{+\pi/X} dk \ a^-(k) e^{ikx} e^{-i\omega_1(k)t}.
\]

Using this expression for \( \bar{a}(x, t) \) in Eq. (23) for \( a(x, t) \), employing Eq. (27) to write \( \omega_1(k) \) in terms of \( \omega_0(k) \), and recalling that \( \exp(\pm i\pi n) = (-1)^n \) we can write

\[
a(x, t) = a^+(x, t) \sum_{m, n = -\infty}^{+\infty} \delta(x - mX)\delta(t - nT) + a^-(x, t) \sum_{m, n = -\infty}^{+\infty} (-1)^n \delta(x - mX)\delta(t - nT),
\]

where

\[
a^\pm(x, t) = \int_{-\pi/X}^{+\pi/X} dk \ a^\pm(k) e^{ikx} e^{\mp i\omega_0(k)t}.
\]

Obviously, we can also write Eq. (24) in the form

\[
\bar{a}(x, t) = a^+(x, t) + (-1)^n a^-(x, t),
\]

which will be used in the next section.

Clearly the fields \( a^+(x, t) \) and \( a^-(x, t) \) represent disturbances propagating (at least for small \( k \)) to the right and the left respectively, both with a dispersion relation \( \omega_0(k) \). The effect of the second dispersion relation \( \omega_1(k) \) is to introduce a kind of “temporally antiferromagnetic” behavior, indicated by the \( (-1)^n \), associated with the leftward going wave. The solution seems the simplest when formulated in terms of these two fields \( a^+(x, t) \) and \( a^-(x, t) \). Since we have dynamical equations, Eqs. (12), for both the \( R_{m,n} \) and the \( L_{m,n} \), we will have four fields in all as \( a \) ranges over \( R \) and \( L \): \( R^+(x, t), R^-(x, t), L^+(x, t), \) and \( L^-(x, t) \).
3.4 Initial conditions

Eqs. (12) requires two sets of initial conditions: the value of \( R_{m,n} \) and \( L_{m,n} \) at both \( n = 0 \) and \( n = 1 \). We can now see how these are built into the fields \( a^\pm(x,t) \). We begin by noting that from Eqs. (17) and (30) we can immediately identify

\[
\begin{align*}
    a_{m,0} &= a^+ (mX,0) + a^- (mX,0), \\
    a_{m,1} &= a^+ (mX,T) - a^- (mX,T).
\end{align*}
\]

(33) \hspace{2cm} (34)

So to construct the \( a^\pm(k) \) appropriate for our initial conditions we must invert Eqs. (31) to find the \( a^\pm(k) \) in terms of \( a^\pm(x,t) \). This is easily done by focusing on points \( x = mX \); writing Eqs. (31) at such points and performing the sums indicated below, we find

\[
a^\pm(k) = \frac{1}{2\pi} X e^{\pm i\omega_0(k)T} \sum_{m=-\infty}^{\infty} a^\pm (mX,t) e^{-i k m X}.
\]

(35)

As the left hand side is independent of time, so must be the right hand side. Writing down these equations for \( t = 0 \) and \( t = T \) we can then use Eqs. (33) and (34) to solve for the \( a^\pm(k) \) in terms of the \( a_{m,0} \) and the \( a_{m,1} \). The result is

\[
a^\pm(k) = \frac{1}{4\pi} X \sum_{m=-\infty}^{\infty} \frac{e^{\pm i\omega_0(k)T} a_{m,0} \pm a_{m,1}}{\cos [T \omega_0(k)]} e^{-i k m X},
\]

(36)

where in the second expression we have used the dispersion relation (26).

3.5 Full solution

The solution of the walk problem subject to arbitrary initial conditions can then be written in the form of Eq. (30) or, identifying the discrete points of interest in space and time, in the form

\[
a_{m,n} = a^+ (mX, nT) + (-1)^n a^- (mX, nT),
\]

(37)

where \( a^\pm(x,t) \) are given by Eqs. (31) with the Fourier components given by Eq. (36). Inserting those Fourier components we find that we can write the full solution for \( a^\pm(x,t) \) in terms of a single Green function \( g(x;t) \),

\[
a^\pm(x,t) = \sum_{m=-\infty}^{\infty} g(\pm(x-mX); t-T) a_{m,0} \pm \sum_{m=-\infty}^{\infty} g(\pm(x-mX); t) a_{m,1},
\]

(38)

where

\[
g(x;t) = \frac{X}{4\pi} \int_{-\pi/X}^{\pi/X} dk \frac{e^{ikx} e^{-i\omega_0(k)t}}{\sqrt{1 - \rho \sin^2 kX}}.
\]

(39)
and we have used the fact that \( g(x; -t) = g(-x; t) \). Using the original walk equations (7) and (8) we can then find the \( a_{m,1} \) in terms of the \( a_{m,0} \), for \( a = R, L \). Then our final solution is given by Eq.(37) with

\[
L^\pm(x, t) = \sum_m g(\pm(x - mX); t - T) L_{m,0} \mp \sqrt{\rho} \sum_m g(\pm(x - mX); t) L_{m+1,0} \\
\pm \sqrt{1 - \rho} \sum_m g(\pm(x - mX); t) R_{m-1,0},
\]

(40)

and

\[
R^\pm(x, t) = \sum_m g(\pm(x - mX); t - T) R_{m,0} \mp \sqrt{\rho} \sum_m g(\pm(x - mX); t) R_{m-1,0} \\
\pm \sqrt{1 - \rho} \sum_m g(\pm(x - mX); t) L_{m+1,0}.
\]

(41)

Earlier, Nayak and Vishwanath [13] formally solved the discrete QW and analyzed the asymptotic behaviour of the solution. In the Appendix we show that our formal solution and theirs are the same. More recently, Carteret et al. [14] have reviewed previous results concerning the asymptotics of the QW and presented new asymptotics. Of course, all those asymptotic results fully apply to our solution; we do not pursue this further here.

4 An approximate approach: the long wavelength limit

The solution in the form we have constructed leads naturally to a passage to the continuum limit, which we identify by focusing on the continuous functions of space and time \( \bar{a}(x, t) \), and constructing simplified equations for their evolution in the long wavelength limit.

4.1 Derivation of the equation of evolution in the long wavelength limit

Our starting points are Eqs.(31) and (32), which we write again here for clarity:

\[
\bar{a}(x, t) = a^+(x, t) + (-1)^n a^-(x, t),
\]

(42)

\[
a^\pm(x, t) = \int_{-\pi/X}^{+\pi/X} dk \, a^\pm(k) e^{ikx} e^{\mp i\omega_0(k)t},
\]

(43)

with \( a^\pm(k) \) given by Eqs.(36). We consider the long wavelength limit by neglecting high frequency (and small wavelength) effects. For that purpose we introduce low–frequency fields

\[
\hat{A}^\pm(x, t) = \int_{-\pi/L}^{+\pi/L} dk \, \mathcal{G}(kX) a^\pm(k) e^{ikx} e^{\mp i\omega_0(k)t}.
\]

(44)
which in the long wavelength limit take the place of the fields \( a^\pm(x,t) \). Here \( G(kX) \) is a function that vanishes at high spatial frequencies \( k \); that is, it plays the role of a low-pass filter. The cut-off that it provides is assumed to be such that we can make a series expansion in \( \omega_0(k) \). Taking the dispersion relation Eq.(26) and expanding as a power series one gets

\[
\omega T - \frac{1}{6} \omega^3 T^3 + \ldots = \sqrt{\rho} X k - \frac{1}{6} \sqrt{\rho} X^3 k^3 + \ldots
\]  

(45)

Using the lowest order, \( \omega T = \sqrt{\rho} X k \), we approximate \( (\omega T)^3 \approx (\sqrt{\rho} X k)^3 \) and write \( \omega \approx \hat{\omega}(k) \) with

\[
\hat{\omega}(k) = \sqrt{\rho} X k - \frac{1}{6} \sqrt{\rho}(1 - \rho) X^3 T k^3.
\]  

(46)

Now, we take this approximate dispersion relation in Eq.(44) and write

\[
\hat{A}^\pm(x,t) \approx \int_{-\infty}^{\infty} dk a^\pm(k) G(kX) e^{ikx} e^{\pm i\hat{\omega}(k)t},
\]  

(47)

where \( \omega_0(k) \) has been approximated by \( \hat{\omega}(k) \) and the integration limits have been extended to infinity. Finally from Eqs.(47) it is easy to derive the equations of evolution of \( \hat{A}^\pm(x,t) \). The equations can be written in the form

\[
\frac{\partial}{\partial \tau} \hat{A}^\pm(\xi,\tau) = \mp \sqrt{\rho} \left[ \frac{\partial}{\partial \xi} + \frac{1 - \rho}{6} \frac{\partial^3}{\partial \xi^3} \right] \hat{A}^\pm(\xi,\tau)
\]  

(48)

where we have introduced the new functions \( \hat{A}^\pm(\xi,\tau) = \hat{A}^\pm(X\xi,T\tau) \), and the normalized time and space variables \( \tau = t/T \) and \( \xi = x/X \). Notice that the form of this equation is independent of the particular form chosen for the cut-off function \( G(kX) \).

This is the differential equation derived earlier (Eq.(15) of [9]) for the special case \( \rho = 1/2 \). It can be identified with the equation the envelope function of a light pulse would satisfy in a description of propagation through a material medium with no group velocity dispersion at the lowest order – such lowest order dispersion would appear through a term involving a second derivative with respect to \( \xi \) – but with higher order dispersion described by the third derivative term. The equation is well known in fiber optics, where it is used to describe pulse propagation near the zero-dispersion wavelength [16]. Notice that the effective “dispersion coefficient” in Eq. (48) is proportional to \( (1 - \rho) \) and thus, interestingly, can be varied by modifying the unitary transformation applied in the QW after each displacement.

**4.2 Solution of the differential equation**

Let us proceed now to analyze the solution of Eq.(48). By Fourier transforming Eq.(48) one easily gets

\[
\hat{A}^\pm(\xi,\tau) = \int_{-\infty}^{\infty} dq \hat{\bar{A}}^\pm(q,0) e^{iq\xi} e^{\mp i\sqrt{\rho}(1 + \frac{1 - \rho}{6} q^2)\tau}.
\]  

(49)
with
\[ \tilde{A}^\pm(q, 0) = \frac{1}{2\pi} \int^{+\infty}_{-\infty} d\xi \, A^\pm(\xi, 0) e^{-iq\xi}. \] (50)

The initial conditions \( A^\pm(\xi, 0) \) can be calculated from Eqs. (36) and (47). First we rewrite Eqs. (36) in the long–wavelength limit
\[ a^\pm(k) = \frac{1}{4\pi} X \sum_{m=-\infty}^{\infty} (a_{m,0} \pm a_{m,1}) e^{-imkX} \] (51)
where we have approximated \( \exp[T\omega_0(k)] \approx 1 \). Substituting this into Eq.(47), and using the normalized spatial frequency \( q = Xk \) we get
\[ A^\pm(\xi, 0) = \frac{1}{4\pi} \sum_{m=-\infty}^{\infty} (a_{m,0} \pm a_{m,1}) \int^{+\infty}_{-\infty} dq \, G(q) e^{iq(\xi-m)}. \] (52)

Now we need to choose a particular cut–off function. To obtain an explicit solution of Eq. (48) we adopt a Gaussian,
\[ G(q) = e^{-w^2q^2}, \] (53)
where \( w \) is a free parameter. We further consider the usual case that the QW starts with the particle at position \( m = 0 \), and we get
\[ A^\pm(\xi, 0) = a_{0,0}G(0) \pm a_{-1,1}G(-1) \pm a_{1,1}G(1), \] (54)
\[ G(m) = N \exp\left[ -\frac{(\xi-m)^2}{4w^2} \right], \]
with \( N \) a normalization factor that can be fixed by imposing
\[ \sum_{j=+, -, } \left[ \int^{+\infty}_{-\infty} d\xi \, |R_j(\xi, 0)|^2 + \int^{+\infty}_{-\infty} d\xi \, |L_j(\xi, 0)|^2 \right] = 1, \] (55)
for the total probability remains equal to unity at all times. In the following we omit this constant, as it is nothing but a scaling factor.

In substituting the initial condition (54) into Eq. (50) and this into Eq.(49), we are left with integrals of the form
\[ Z(\xi, \tau) = \int^{+\infty}_{-\infty} dk \exp\left( iAk + i\frac{1}{3}Bk^3 - Ck^2 \right), \] (56)
\[ A = \xi - \sqrt{\rho}\tau, \] (57)
\[ B = \frac{1}{2}\sqrt{\rho}(1-\rho)\tau, \] (58)
\[ C = w^2, \] (59)
whose solution can be expressed in terms of the Airy function \( A_i(x) \) [17][18]
\[ Z(\xi, \tau) = \frac{2\pi}{B^{3/3}} \exp\left( \frac{3ABC + 2C^3}{3B^2} \right) A_i\left( \frac{AB + C^2}{B^{4/3}} \right). \] (60)
Then the final result reads, up to a normalization factor,
\[
\bar{a}(\xi, \tau) = A^+(\xi, \tau) + (-1)^n A^-(\xi, \tau) \tag{61}
\]
\[
A^\pm(\xi, \tau) = a_0 Z(\pm \xi, \tau) \pm a_{-1,1} Z(\pm (\xi + 1), \tau) \pm a_{1,1} Z(\pm (\xi - 1), \tau),
\]

or, explicitly,
\[
\bar{R}(\xi, \tau) = R^+(\xi, \tau) + (-1)^n R^-(\xi, \tau) \tag{62}
\]
\[
\bar{L}(\xi, \tau) = L^+(\xi, \tau) + (-1)^n L^-(\xi, \tau) \tag{63}
\]
with
\[
R^\pm(\xi, \tau) = R_{0,0}[Z(\pm \xi, \tau) \pm \sqrt{\rho} Z(\pm (\xi + 1), \tau)] \tag{64}
\]
\[
\pm \sqrt{1 - \rho} L_{0,0} Z(\pm (\xi + 1), \tau),
\]
\[
L^\pm(\xi, \tau) = L_{0,0}[Z(\pm \xi, \tau) \mp \sqrt{\rho} Z(\pm (\xi + 1), \tau)] \tag{65}
\]
\[
\pm \sqrt{1 - \rho} R_{0,0} Z(\pm (\xi - 1), \tau),
\]

where use was made of the discrete QW Eqs.\(^7\) and \(^8\).

Notice that while the form of Eq. 48 is independent of the particular form of \(G(kX)\), this solution depends explicitly on \(w\) because the application of the initial condition does depend on the details of that cut-off function.

Finally, the probability distribution is given by
\[
P(\xi, \tau) = P^R(\xi, \tau) + P^L(\xi, \tau), \tag{66}
\]
\[
P^A(\xi, \tau) = |A^+(\xi, \tau) + (-1)^n A^-(\xi, \tau)|^2, \quad A = R, L.
\]

Let us now compare the above long wavelength approximation with the solution of the original discrete QW Eqs.\(^7\) and \(^8\). In the left column of Fig.2 we present the total probability distribution \(P_m(n)\), as well as the partial probabilities \(P^R_m(n)\) and \(P^L_m(n)\), as obtained from Eqs.\(^7\) and \(^8\) for \(n = 200\), \(R_{0,0} = 1/\sqrt{2}\) and \(L_{0,0} = i/\sqrt{2}\) (a value of the initial conditions for which the mean displacement is null) and \(\rho = 1/2\) (which corresponds to the Hadamard walk). In the right column of Fig.2 we present the solution of the long wavelength approximation \(P(\xi, \tau)\) (and \(P^R(\xi, \tau)\) and \(P^L(\xi, \tau)\)) for \(\tau = 200\) and the same value of \(\rho\) and of the initial conditions and for \(w = 0.4\). Finally, in the central column of the figure we present the long wavelength approximation evaluated only at integer values of the position \(\xi\). These last plots are given in order to make a better comparison with the exact solution, as the latter is nonvanishing only at even (odd) positions at even (odd) times. Although we only show plots for a particular initial condition and value of \(\rho\), similar correspondence between the exact solution and the long wavelength limit results for other sets of initial conditions and values of \(\rho\) as well.

In Fig. 2 we chose the value \(w = 0.4\) because for that particular value the agreement of the long wavelength approximation with the exact solution is close to the best that can be achieved. In Fig. 3 we plot the long wavelength approximation for three different values of \(w\). Note that for the largest \(w = 0.55\).
the long wavelength approximation yields values that are too low, compared to the exact solution, for small $\xi$, while for the smallest $w = 0.25$ the long wavelength approximation extends to $|\xi|$ beyond the range of the exact solution.

We see from Fig. 2 that the main trends of the exact QW solution are well captured by the long wavelength approximation, although obvious quantitative differences appear. The main discrepancy between the exact solution and the long wavelength approximation is the presence of the oscillations that appear in the latter. By taking into account higher order terms in the expansion of a more accurate approximation to the exact solution could be obtained, but the corresponding differential equation would not have a simple analytic solution. In any case, our main thesis is not that Eqs. (42) and (43) are a good quantitative approximation to the exact solution. Rather, our central result is that comparisons such as those in Fig. 2 demonstrate that the propagation and dispersion effects described by Eq. (48) capture the qualitative nature of the QW.

5 Conclusions

In this paper we have rigorously derived both the exact solution of the coined QW for arbitrary unitary transformations, and a long wavelength approximation that constitutes an approximate continuous limit of the QW.

The long wavelength approximation identified here corresponds to the dynamical equation of an envelope function characterizing a light pulse propagating in a medium with higher order dispersion, for example in an optical fiber close to the zero-dispersion wavelength [16]. This, together with the fact that entirely classical implementations of the unidimensional QW are possible [9, 10], lead us to the conclusion that entanglement does not play a central role in the unidimensional QW, and that the walk can be regarded as a pure wave phenomenon. This conclusion cannot, however, be generalized to higher dimensional QWs [19]. There several coins are needed, and it would in such a scenario that the entanglement characteristic of an essential quantum nature might appear, as already discussed [10]. It would then be very interesting to generalize the work we have carried out here by deriving long wavelength descriptions of multidimensional QWs. This could help elucidate any role played by entanglement in such processes.

Another point of interest is the effect of decoherence on QWs. Kendon and Tregenna [20] have shown that decoherence modifies the probability distribution of the QW in somewhat unsuspected ways. In particular, it can lead to quite smooth, and at the same time wide, probability distributions. It would be interesting to investigate the role of decoherence in continuous descriptions of the QW, such as that we have presented here. In this sense, the recent work by Romanelli et al. [21], in which Markovian and intereference terms of the quantum evolution are separated, provides a new interesting tool for this type of analysis.
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7 Appendix

In this appendix we show the relation between the walk definition we use here and that used by Nayak and Vishwanath [13], and confirm that our solution reproduces theirs. We begin with our walk in the case of a Hadamard transformation,

\[ R_{m,n} = \frac{1}{\sqrt{2}} (R_{m-1,n} - L_{m+1,n}) , \quad (67) \]
\[ L_{m,n} = \frac{1}{\sqrt{2}} (R_{m-1,n} + L_{m+1,n}) . \quad (68) \]

and define new variables

\[ \hat{R}_{m,n} \equiv L_{-m+1,n} , \quad \hat{L}_{m,n} \equiv R_{-m+1,n} , \quad (69) \]

so

\[ L_{m,n} = \hat{R}_{-m+1,n} , \quad R_{m,n} = \hat{L}_{-m+1,n} . \quad (70) \]

In terms of these new variables the walk Eqs. (67) and (68) are specified by

\[ \hat{L}_{m,n} = \frac{1}{\sqrt{2}} \left( \hat{L}_{m+1,n} + \hat{R}_{m+1,n} \right) , \quad (71) \]
\[ \hat{R}_{m,n} = \frac{1}{\sqrt{2}} \left( \hat{L}_{m-1,n} + \hat{R}_{m-1,n} \right) . \quad (72) \]

These are the walk equations of Nayak and Vishwanath [13]. Then, in terms of our functions \( a^{\pm}(x,t) \), where \( a \) is \( R \) or \( L \), we have from Eqs. (67) and (68),

\[ \hat{R}_{m,n} = L^{\pm}((-m+1)X,nT) + (-1)^n L^-((-m+1)X,nT) , \quad (73) \]
\[ \hat{L}_{m,n} = R^{\pm}((-m-1)X,nT) + (-1)^n R^-((-m-1)X,nT) . \quad (74) \]

In writing out the expressions for \( R^{\pm} \) and \( L^{\pm} \) at the lattice sites indicated we do a change of variables, putting \( k = k' + \pi/X \). We use

\[ \omega_0(k' + \pi/X) = -\omega_0(k') , \quad (75) \]
\[ \exp[i(k' + \pi/X)X] = -\exp[ik'X] , \quad (76) \]
\[ \exp[-i(k' + \pi/X)mX] = (-1)^m \exp[-ik'mX] , \quad (77) \]
and can then adjust the limits of integration of the function back to $-\pi/X$ to $\pi/X$ in the new variable $k'$, since the function is periodic over $2\pi/X$. Changing the name of the new variable back to $k$ we can collect the terms and write

$$\hat{R}_{m,n} = \int_{-\pi/X}^{\pi/X} dk \, e^{ikX} \left[ L^+(k) - (-1)^{n+m} L^-(k + \frac{\pi}{X}) \right] \cdot e^{-ikmX} e^{-i\omega_0(k) n T}, \quad (78)$$

$$\hat{L}_{m,n} = \int_{-\pi/X}^{\pi/X} dk \, e^{-ikX} \left[ R^+(k) - (-1)^{n+m} R^-(k + \frac{\pi}{X}) \right] \cdot e^{-ikmX} e^{-i\omega_0(k) n T}. \quad (79)$$

Now the initial condition adopted in [13] is $\hat{L}_{m,0} = \delta_{m0}$ and $\hat{R}_{m,0} = 0$, which, in our notation Eqs. (70) read $R_{m,0} = \delta_{m-1}$ and $L_{m,0} = 0$. After one time step, see Eqs (67) and (68), we have $R_{m,1} = L_{m,1} = \delta_{m0}/\sqrt{2}$, so we can construct $L^\pm(k)$ and $R^\pm(k)$ from (36), with $\rho = 1/2$. We find

$$L^+(k) = -L^-(k + \frac{\pi}{X}) = \frac{X}{4\pi} \frac{1}{\sqrt{1 + \cos^2 kX}}, \quad (80)$$

$$R^+(k) = -R^-(k + \frac{\pi}{X}) = \frac{X}{4\pi} \frac{\sqrt{2} e^{i\omega_0(k) T} e^{ikX} + 1}{\sqrt{1 + \cos^2 kX}}, \quad (81)$$

and using (26) we recover

$$\hat{R}_{m,n} = \left[ 1 + (-1)^{n+m} \right] \frac{X}{4\pi} \int_{-\pi/X}^{\pi/X} dk \, \frac{e^{ikX}}{\sqrt{1 + \cos^2 kX}} e^{-ikmX} e^{-i\omega_0(k) n T}, \quad (82)$$

$$\hat{L}_{m,n} = \left[ 1 + (-1)^{n+m} \right] \frac{X}{4\pi} \int_{-\pi/X}^{\pi/X} dk \, \left( 1 + \frac{\cos kX}{\sqrt{1 + \cos^2 kX}} \right) e^{-ikmX} e^{-i\omega_0(k) n T}, \quad (83)$$

in agreement with Nayak and Vishwanath [13]

References


Figure Captions

Fig.1. Dispersion relations as given by Eq. 4.

Fig.2. Probability distribution of the QW. The exact solution is presented in the left column ($P_m(n)$, $P_m^R(n)$, $P_m^L(n)$ for $n = 200$ from top to bottom), the long wavelength approximation ($P(ξ,τ)$, $P_m^R(ξ,τ)$, and $P_m^L(ξ,τ)$ for $τ = 200$ from top to bottom) is presented in the right column, and also in the central column but in this case evaluated only at integer even. In the left and central columns the points have been joined to guide the eye. The initial condition is $R_{0,0} = 1/\sqrt{2}$ and $L_{0,0} = i/\sqrt{2}$, and the parameters are $ρ = 1/2$, (Hadamard walk) and $w = 0.4$ for the long wavelength approximation. The probabilities
in the long wavelength approximation have not been normalized, and the units are thus arbitrary.

Fig. 3. $P(\xi, \tau)$ for $\tau = 200$ and the same initial conditions and parameters as in Fig. 3 except for the values of $w$ that are indicated in the figure.
$P(\xi) \text{ (arbitrary units)}$

- $w = 0.25$
- $w = 0.4$
- $w = 0.55$