Fractional scaling of quantum walks on percolation lattices

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Abstract. Quantum walks can be used to model processes such as transport in spin chains and bio-molecules. The enhanced spreading and mixing properties of quantum walks compared with their classical counterparts have been well-studied on regular structures and also shown to be sensitive to defects and imperfections. Using numerical simulation, we study the spreading properties of quantum walks on percolation lattices for both bond and site percolation. The randomly missing edges or sites provide a controlled amount of disorder in the regular Cartesian lattice. In one dimension (the line) we introduce a simple model of quantum tunneling to allow the walk to proceed past the missing edges or sites. This allows the quantum walk to spread faster than a classical random walk for short times, but at longer times the disorder localises the quantum walk. In two dimensions, we observe fractional scaling of the spreading with the number of steps of the walk. For percolation above the 85\% level, we obtain faster spreading than classical random walks on the full lattice.

1. Introduction

Quantum versions of random walks have been used as simple models of quantum transport phenomena, applicable to systems as diverse as spin chains \cite{1} and bio-molecules \cite{2}. Here we investigate the properties of quantum walks on percolation lattices, disordered structures appropriate for modelling biological and experimentally realistic systems.

Quantum walks have continuous-time \cite{3} and discrete-time (coined) versions \cite{4,5}, in this work, we use only the coined quantum walk. We consider the effects of missing edges or sites for both the line and the 2D Cartesian lattice. In one dimension, a missing edge or site halts the progress of both quantum and classical random walks. Variants that allow progress to be made have been studied previously, e.g., dynamic broken links that change location at each time step \cite{6}. In this work we introduce a simple model of quantum tunnelling \cite{7} that also allows the quantum walker to make progress beyond the gaps. On 2D percolation lattices, there is in general more than one possible path between two sites, allowing the quantum walk to proceed around the missing edges without any tunnelling.

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1
2. Quantum walks

Quantum walks are quantum versions of classical random walks and are defined analogously. For a coined quantum walk, the quantum walker carries a quantum coin of dimension \( d \), the maximum number of edges at any site. For the walk on the line, the coin has dimension \( d = 2 \) and the most common choice of coin operator to “toss” the coin is the Hadamard operator,

\[
C_2^{(\text{Had})} = \frac{1}{\sqrt{2}} \begin{pmatrix}
1 & 1 \\
1 & -1
\end{pmatrix}. \tag{1}
\]

We write the basis states of the quantum walker as \(|c, x\rangle\), where \( c \) is the state of the coin (one of the \( d \) directions, for the line \( c = \pm 1 \)) and \( x \) is the position on the line. After “tossing” the coin with the coin operator, the particle moves to adjacent positions according to the coin state; this is expressed mathematically as a conditional shift operator,

\[
S|\pm 1, x\rangle = |\pm 1, x \pm 1\rangle. \tag{2}
\]

One step of the quantum walk is produced by the unitary operator \( U = S(C \otimes 1_x) \). A quantum walk of \( t \) steps starting from an initial state \(|\psi_0\rangle\) is thus

\[
|\psi(x, t)\rangle = U^t|\psi_0\rangle. \tag{3}
\]

Each vertex in a two-dimensional lattice has four edges connected to it, so the quantum walker needs a four-dimensional coin. We label the four directions \(|L\rangle, |R\rangle\) corresponding to \(|-1\rangle\) and \(|+1\rangle\) on the \( x \) axis and \(|D\rangle, |U\rangle\) for \(|-1\rangle\) and \(|+1\rangle\) on the \( y \) axis. The operator for “tossing” the coin can be any \( 4 \times 4 \) unitary. The most common choice is based on Grover’s diffusion operator,

\[
C_4 = \frac{1}{2} \begin{pmatrix}
-1 & 1 & 1 & 1 \\
1 & -1 & 1 & 1 \\
1 & 1 & -1 & 1 \\
1 & 1 & 1 & -1
\end{pmatrix}. \tag{4}
\]

To complement this choice of coin operator, the shift operator \( S_4 \) must also invert the coin states,

\[
S_4|L, x, y\rangle = |R, x - 1, y\rangle \\
S_4|R, x, y\rangle = |L, x + 1, y\rangle \\
S_4|D, x, y\rangle = |U, x, y - 1\rangle \\
S_4|U, x, y\rangle = |D, x, y + 1\rangle. \tag{5}
\]

This ensures that the coin operator is then applied to a coin state that labels the edge from which the walker arrived, which is the one that receives the minus sign from the Grover coin operator. This preserves the symmetry of the walk.

The quantum walk on both the line and on the full Cartesian lattice spread at a rate proportional to \( t \), a quadratic speed up over the classical \( \sqrt{t} \). This can be quantified by calculating the root mean square distance of the walker from the starting point. On the line this is just \( x_{rms}(t) = \sqrt{\sum_{c, x} (x - x_0)^2 |\psi(x, t)|^2} \) for a walk starting at \( x_0 \). On the 2D lattice,

\[
r_{rms}(t) = \sqrt{\sum_{c, x} [(x - x_0)^2 + (y - y_0)^2] |\psi(x, t)|^2}. \tag{6}
\]
3. Percolation lattices
Both bond (edge) and site percolation have similar definitions: with independent randomly chosen probability \( p \), the bond or site is present in the lattice. In two and higher dimensions, percolation lattices exhibit a phase transition from a set of small disconnected regions to a more highly connected structure (“one giant cluster”). On 2D Cartesian lattices, the critical probability \( p_c = 0.5 \) (bond) and \( p_c = 0.5927... \) (site[8, 9]).

A typical percolation lattice will have sites with four, three, two, one and no edges. A suitable coin operator is needed for each, we used the Grover coin appropriate for the number of edges, padded with (minus) the identity for the missing edges (details in [7]). In one dimension (the line) any missing edge will stop the progress of the walker, effectively \( p_c = 1 \).

4. Numerical method
Numerical simulation of a quantum walk is a straightforward evaluation of equation (3) for chosen parameters. In high level computational environments such as Matlab, it takes only a few lines of code. However, we wrote our own routines in C and C++ to ensure they were efficient enough to run up to 140 time steps for the walk on a two-dimensional lattice (the memory required scales linearly in the number of lattice sites). It was also necessary to repeat the simulations over a sufficient number of random percolation lattices to ensure reasonable statistics were obtained. The largest of our simulations took over a week on a 3GHz processor to complete this averaging for 5,000 random lattices. This was in fact largely due to the time required to generate the random numbers for specifying the percolation lattice (one per walk). We used routines from Park and Miller [10] freely available online for generating the random numbers, although the quality of the random numbers is not particularly important for this type of simulation.

5. Tunnelling on a broken line
Tunnelling is a generic property of quantum systems whereby a quantum particle has a small probability of passing through a barrier that prevents the passage of a classical particle. We model this using a biased Hadamard operator,

\[
C^{(\eta)}_2 = \begin{pmatrix}
\sqrt{\eta} & \sqrt{1-\eta} \\
\sqrt{1-\eta} & -\sqrt{\eta}
\end{pmatrix},
\]

where \( \eta \) gives the probability of passing to the next site while \( 1 - \eta \) is the probability of being reflected back. For a line with a random subset of edges missing, the quantum walk proceeds by using the standard Hadamard where both edges are present at a site, while the biased Hadamard is used at sites with one or both edges missing.

After 100 steps, the effect of the missing edges with tunnelling is not significantly different from the walk on the full line. However, by 1000 steps the spreading has significantly slowed, and after 10,000 steps the spreading rate has dipped below the classical \( \sqrt{t} \) scaling. This is shown in figure 1. The random missing edges and consequent random use of different coin operators causes the walk to localise. Note that \( p = 0 \) (no edges) returns to quantum spreading, because there is no randomness to disrupt the quantum coherences if the tunnelling coin is used everywhere. Regular patterns of varying coin bias have been studied by Linden and Sharam [11], who find quantum spreading in most cases, but with widely varying spreading rates. Generalisation of this model by Shikano and Katsura [12] suggests that localization vs spreading depends on whether the variation in the coin is commensurate with the lattice spacing. Since our randomly missing edges do not have any periodicity, we expect to find localisation in all cases, with the range explored by the quantum walk governed by both the tunnelling probability \( \eta \) and the percolation probability \( p \). Comparison of figures 1 and 2 show these effects clearly. Reducing \( \eta \)
by a factor of two (figure 2) reduces the range by roughly a factor of three, from around 70 to 23 for $p = 0.2$ or $0.8$.

6. **Spreading on 2D percolation lattices**

On a 2D lattice there is no need for tunnelling, so we studied the basic quantum walk only. Below $p_c$, the quantum walk will not be able to spread as there are only small connected structures. Approaching $p_c$ from above, the spreading slows down completely, as the number of long-distance connected paths reduces to zero. For $p = 1$, the lattice is fully connected, and the standard quantum walk spreading applies (linear in $t$). In between, we find the quantum walks show fractional scaling of the spreading, i.e., proportional to $t^{\alpha}$ for $(0.5 < \alpha < 1)$. The numerically determined scaling exponents $\alpha$ are shown in figure 3.

Our (numerical) results are skewed by finite size effects: the increase in $\alpha$ from zero begins slightly before $p = p_c$. The rise tails off at $\alpha = 0.5$, then rises again steeply to $\alpha = 1$ for the full lattice ($p = 1$). At this stage, we do not have enough data to predict the large $t$ behaviour, but one possibility is that the steep rise to the quantum value of $\alpha = 1$ at $p = 1$ will becomes a “step” function at $p = 1$ as $t \to \infty$. The randomness in the percolation lattice would thus act as
decoherence in the large $t$ limit, reducing the behaviour to that of a classical random walk. The classical behaviour is shown for numerical simulation using the same parameters. This data has much larger finite size effects. This is due to the classical spread of $\sqrt{t}$, which is only around 12 lattice units for 140 time steps. A classical random walk with equivalent spread (around 30 lattice units would require 900 steps.

7. Summary
We have found localisation on a line for quantum walks tunnelling through missing edges. However, the short time behaviour is still faster than classical spreading. In two dimensions we have found faster than classical scaling with fractional exponents. Although we conjecture this will disappear in the long time limit, again this would only be approached for quite large values of $t$, and from the point of view of models for disordered systems on smaller scales (tens to hundreds of sites), the faster-than-classical fractional scaling is very much the dominant feature.

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