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Zachycení v kvantových procházkách

Trapping in Quantum Walks

Summary

The basic concepts of quantum walks, which represent a generalization of classical random walks to iterative evolution of a quantum particle on a discrete lattice or a graph, are first illustrated on the example of a two-state quantum walk on a line with the Hadamard coin. Various properties of the quantum walk, e.g. ballistic spreading of the walker's wave function, the shape of the position probability distribution and its limit density, are identified with the help of the Fourier transformation. Next, we discuss that allowing the quantum walker to remain at its present position might lead to the so-called trapping effect, where part of the wave function is exponentially confined in the vicinity of the starting point. It is shown that trapping emerges when the evolution operator of the quantum walk has both continuous and point spectrum. For the particular case of the three-state quantum walk on a line with the Grover coin we evaluate the explicit form of the trapping probability at a finite position in the limit of infinite number of steps. It is shown how does the trapping effect limits the transport into an absorbing center. Finally, extensions of the trapping effect to different types of coin operators and graph topologies are discussed.

Souhrn

Základní koncepty kvantových procházek, které představují zobecnění náhodných procházek na iterativní vývoj kvantové částice na diskrétní mřížce nebo grafu, jsou nejprve představeny na příkladu procházky na přímce o dvou stavech s Hadamardovou mincí. Různé vlastnosti procházky, jako například balistické šíření vlnové funkce, tvar pravděpodobnostního rozdělení a jeho limitní přiblížení, jsou nalezeny pomocí Fourierovy transformace. Dále ukážeme, že pokud kvantové částici umožníme zůstat na místě, pak může dojít k tzv. efektu zachycení, kdy je část vlnové funkce exponenciálně lokalizovaná v blízkosti výchozího bodu procházky. K zachycení dochází pokud má evoluční operátor kvantové procházky kromě spojitého i bodové spektrum. Pro konkrétní příklad kvantové procházky na přímce o třech stavech s Groverovou mincí určíme pravděpodobnost zachycení na konečné pozici v limitě nekonečného počtu kroků. Ukážeme, jakým způsobem efekt zachycení omezuje přenos do absorbujícího centra. Na závěr je diskutován efekt zachycení v kvantových procházkách pro obecnější typy grafů a operátory mince.

Klíčová slova: náhodná procházka, kvantová procházka, Fourierova transformace, limitní rozdělení, zachycení, pravděpodobnost zachycení, přenos excitace

Keywords: random walk, quantum walk, Fourier transformation, limit density, trapping, trapping probability, excitation transport

Contents

1 Introduction

Discrete-time quantum walks have emerged as analogues of classical random walks [1, 2]. They describe iterative evolution of a quantum particle on a graph or a lattice. Soon after the introduction of quantum walks their potential for quantum information processing was identified [3], in particular, in problems related to graphs. The most promising applications are the quantum walk based algorithms for searching an unsorted database [4] which can be formulated as finding a marked vertex of a graph. The quantum walk search offers a quadratic speed-up over its classical counterpart. In addition, quantum walks have been applied to the problem of graph isomorphism testing [5] or detecting anomalies in graphs [6]. Outside of quantum information processing quantum walks were applied to various tasks in the field of quantum simulations. They represent natural candidates for modeling of coherent transport on graphs and networks [7]. Quantum walks are instrumental in discretization of Weyl [8] and Dirac [9] equations. Great attention has been recently focused on the abilities of quantum walks to simulate various topological phases of matter [10] and the properties of the resulting topologically protected bound states [11].

In this thesis we focus on the homogeneous discrete-time quantum walks on infinite lattices, in particular, on a line. Generally speaking, quantum walk mimics a wave propagation. The interference of probability amplitudes results in a ballistic spreading with linear growth of the standard deviation of the walker's position [12]. Hence, it spreads quadratically faster than the classical random walk, which shows a diffusive behaviour. However, in certain cases the ballistic spreading of the quantum walk is complemented with the so-called trapping effect [13], where part of the wave-function is exponentially confined in the vicinity of the origin of the walk. This effect, which has no classical analogue, significantly limits transport by a quantum walk.

The rest of the thesis is organized as follows: In Section 2 we introduce the concept of a quantum walk on the example of a two-state walk on a line and illustrate its basic properties. Next, in Section 3 we consider the three-state walk, where the walker is allowed to remain at its present position. This is the simplest non-trivial model which can result in the trapping effect. The implications of trapping for quantum transport are discussed in Section 4. We conclude and discuss the trapping effect in a broader scope in Section 5.

2 Two-state quantum walk

Before turning to the quantum walk let us first briefly review the classical random walk on a line. Here we consider a memory-less stochastic process where the walker moves on an integer lattice in discrete time steps. In an unbiased simple random walk the walker has two possibilities: from its present position x it can move in a single step to the neighbouring lattice points

$x \pm 1$ with equal probability $\frac{1}{2}$. Let us denote by $p(x,t)$ the probability that the walker is at position x at time t. The time evolution of the probability distribution is governed by the following difference equation

$$p(x,t) = \frac{1}{2}p(x-1,t-1) + \frac{1}{2}p(x+1,t-1), \qquad x \in \mathbb{Z}. \tag{1}$$

Suppose that the particle starts the walk from the origin of the lattice $x = 0$, i.e. the initial condition for the time evolution equation is $p(x,0) = \delta_{x,0}$. The solution of (1) is then easily found to be

$$p(x,t) = \frac{1}{2^t}\binom{t}{\frac{t+x}{2}}. \tag{2}$$

From the expression (2) it is straightforward to calculate various attributes of the random walk. The mean value vanishes since the random walk we consider is unbiased. The standard deviation grows with the square root of the number of steps which corresponds to the fact that the classical random walk is a diffusion process. For large number of steps t one can approximate the exact probability distribution (2) with the Gaussian distribution

$$p(x,t) \approx \frac{1}{\sqrt{2\pi t}}e^{-\frac{x^2}{2t^2}},$$

with vanishing mean and a standard deviation $\Delta x = \sqrt{t}$.

Let us now turn to the quantum counterpart of the simple random walk on a line. The classical walker is now replaced with a quantum particle that propagates on an integer lattice under iterative unitary evolution. Let us denote by $|x\rangle, x \in \mathbb{Z}$, the state of the quantum walker being located at site x. These vectors form an orthonormal basis of the position space $\mathcal{H}_P$, i.e.

$$\mathcal{H}_P = \mathrm{Span}\left\{|x\rangle | x \in \mathbb{Z}\right\} = l^2(\mathbb{C}), \quad \langle x|y\rangle = \delta_{xy}, \quad \sum_x |x\rangle\langle x| = \hat{I}_P.$$

The propagation of the quantum particle resembles that of the classical random walker, however, instead of choosing the particular direction randomly the quantum walker evolves into a superposition. As shown by Meyer [2], one can achieve non-trivial evolution for a homogeneous quantum walk only if the walker is not a scalar. Hence, we consider a quantum walker with an internal degree of freedom, usually referred to as coin, which is used to control the propagation on the lattice. In our particular case the coin has two orthogonal states corresponding to the steps to the left and right denoted by $|L\rangle$ and $|R\rangle$. These two vectors form a basis of the two-dimensional coin space $\mathcal{H}_C$. The complete Hilbert space of our two-state quantum walk on a line is given by the tensor product of the position space $\mathcal{H}_P$ and the coin space $\mathcal{H}_C$, i.e.

$$\mathcal{H} = \mathcal{H}_P \otimes \mathcal{H}_C = l^2(\mathbb{C}) \otimes \mathbb{C}^2.$$

The unitary evolution operator $\hat{U}$ which performs a single step of the quantum walk is given by

$$\hat{U} = \hat{S} \cdot \left(\hat{I}_P \otimes \hat{C}\right).$$

Here $\hat{S}$ is the conditional shift operator, which moves the walker one step to the left or to the right according to its coin state

$$\hat{S} = \sum_{x=-\infty}^{\infty} \left(|x-1\rangle\langle x| \otimes |L\rangle\langle L| + |x+1\rangle\langle x| \otimes |R\rangle\langle R| \right).$$

By $\hat{C}$ we have denoted the quantum coin operator which rotates the coin state before the shift. This operator ensures that the evolution of the quantum walk is non-trivial. In principle, $\hat{C}$ can be any $U(2)$ matrix. For simplicity we restrict ourselves to a particular choice of the coin given by the Hadamard transformation $\hat{H}$ which is defined by its action on the basis states

$$\hat{H}|L\rangle = \frac{1}{\sqrt{2}}\left(|L\rangle + |R\rangle\right), \qquad \hat{H}|R\rangle = \frac{1}{\sqrt{2}}\left(|L\rangle - |R\rangle\right).$$

We refer to the two-state quantum walk with the choice of the coin operator $\hat{C} = \hat{H}$ as the Hadamard walk. The state of the quantum walker after t steps of the Hadamard walk is determined by successive applications of the unitary evolution operator $\hat{U}$ to the initial state

$$|\psi(t)\rangle = \hat{U}^t|\psi(0)\rangle. \tag{3}$$

To compare with the classical random walk we also suppose that the quantum walker starts from the origin of the lattice. In addition, we have to specify the initial orientation of the quantum coin which can be described by some vector $|\psi_C\rangle = \psi_L|L\rangle + \psi_R|R\rangle \in \mathcal{H}_C$. The state vector after t steps can be written as a superposition

$$|\psi(t)\rangle = \sum_{x=-\infty}^{\infty} \left(\psi_L(x,t)|x\rangle|L\rangle + \psi_R(x,t)|x\rangle|R\rangle \right),$$

where $\psi_{L,R}(x,t)$ are the probability amplitudes of finding the particle at position x with the coin state $|L\rangle$, $|R\rangle$ after t steps of the walk. We note that there is no randomness in the time evolution of the Hadamard walk. Indeed, equation (3) describes unitary evolution of a closed quantum mechanical system. Nevertheless, position of the quantum walker is a random variable which is not determined prior to measurement. According to the standard rules of quantum mechanics the probability to find the quantum walker at position x after t steps of the walk is given by

$$p(x,t) = |\langle x|\langle L|\psi(t)\rangle|^2 + |\langle x|\langle R|\psi(t)\rangle|^2 = |\psi_L(x,t)|^2 + |\psi_R(x,t)|^2.$$

For comparison we show in Figure 1 the probability distributions of the classical random walk and the Hadamard walk after $t = 100$ steps. Classical random walk results in a Gaussian distribution with zero mean value and standard deviation proportional to the square-root of the number of steps. On the other hand, the probability distribution of the Hadamard walk is characterized by two dominant peaks on the edges. Due to the choice of the initial coin state $|\psi_C\rangle = |L\rangle$ the peak on the left is more pronounced.

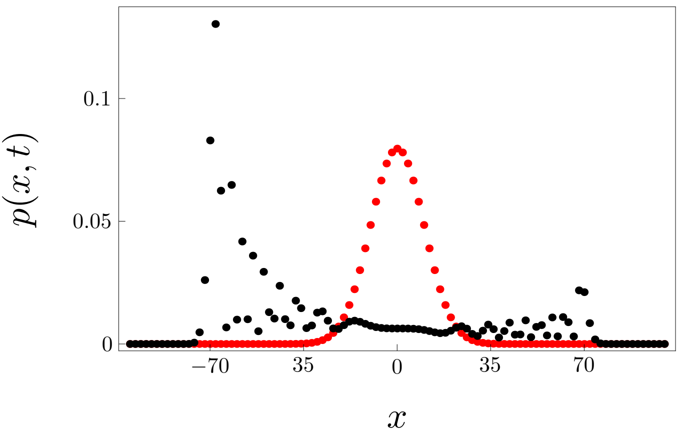

Figure 1: The probability distribution $p(x,t)$ of the classical random walk (red dots) and the Hadamard walk (black dots) after 100 steps. The width of the distribution is proportional to $\sqrt{t}$ in the classical case and t in the quantum case.

The standard tool to solve the time-evolution equation (3) of homogeneous quantum walks is the Fourier transformation [12]. In our case the Fourier transformation $\hat{F}$ is an isometry between $l^2(\mathbb{C}) \otimes \mathbb{C}^2$ and $L^2((0,2\pi), dk) \otimes \mathbb{C}^2$ defined by

$$\tilde{\psi}(k) = (\hat{F}\psi)(k) = \sum_{x=-\infty}^{\infty} e^{ixk}\psi(x).$$

The time evolution equation (3) is in the Fourier picture reduced to

$$\tilde{\psi}(k,t) = \tilde{U}(k)^t \psi_C, \tag{4}$$

where $\tilde{U}(k)$ is the Fourier transformation of the evolution operator $\hat{U}$

$$\tilde{U}(k) = D(k)\cdot H = \begin{pmatrix} e^{-ik} & 0 \\ 0 & e^{ik} \end{pmatrix} \cdot \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix},$$

and $\psi_C = (\psi_L, \psi_R)^T$ is the Fourier transformation of the initial state. The time evolution equation (4) is readily solved by diagonalizing the matrix $\tilde{U}(k)$. Let us denote the eigenvalues of $\tilde{U}(k)$ by $e^{i\omega_j(k)}$ and the corresponding eigenvectors by $v_j(k)$. We find that the explicit form of $\omega_j(k)$ is given by

$$\omega_1(k) = -\arcsin\left(\frac{\sin k}{\sqrt{2}}\right), \quad \omega_2(k) = \arcsin\left(\frac{\sin k}{\sqrt{2}}\right) + \pi.$$

We note that the fact that both $\omega_j(k)$ depend on the momentum k shows that the spectrum of the evolution operator of the Hadamard walk is purely continuous. The solution of (4) can then be written in the form

$$\tilde{\psi}(k,t) = e^{i\omega_1(k)t} v_1(k) f_1(k) + e^{i\omega_2(k)t} v_2(k) f_2(k), \tag{5}$$

where $f_j(k)$ denotes the overlap of the eigenvector $v_j(k)$ with ψ_C. Finally, with the help of the inverse Fourier transformation we obtain the solution of the time-evolution equation in the position representation in the form

$$\psi(x,t) = \mathcal{I}_1(x,t) + \mathcal{I}_2(x,t), \quad \mathcal{I}_j(x,t) = \int_0^{2\pi} \frac{dk}{2\pi} e^{-ixk} e^{i\omega_j(k)t} v_j(k) f_j(k). \tag{6}$$

This form of solution allows one to employ the method of stationary phase [14] to investigate the asymptotic behaviour of the wave function $\psi(x,t)$ and the corresponding probability distribution $p(x,t)$. We find that $p(x,t)$ decays exponentially for $|x| > t/\sqrt{2}$, while for $|x| < t/\sqrt{2}$ it behaves like $p(x,t) \sim t^{-1}$. Near the points $x = \pm t/\sqrt{2}$ the probability distribution decays the slowest according to $p(x,t) \sim t^{-\frac{2}{3}}$, which explains the two peaks in Figure 1 and the ballistic spreading of the Hadamard walk.

Moreover, using the solution in the Fourier picture (5) we can prove the weak-limit theorem [15], which says that the pseudo-velocity $\frac{x}{t}$ of a quantum walker converges weakly in the asymptotic limit of $t \to +\infty$ to a random variable v. This is shown by the convergence of moments of the pseudo-velocity, which can be written explicitly in the form

$$\lim_{t\to\infty}\left\langle\left(\frac{x}{t}\right)^n\right\rangle = \int\limits_{-\frac{1}{\sqrt{2}}}^{\frac{1}{\sqrt{2}}} dv\ v^n w(v),$$

where the limit density of v is given by

$$w(v) = \mathcal{M}(v) f_K\left(v;\frac{1}{\sqrt{2}}\right),\quad f_K(v;a) = \frac{\sqrt{1-a^2}}{\pi(1-v^2)\sqrt{a^2-v^2}}.$$

Here $f_K(v;a)$ is the Konno's density function [16] and $\mathcal{M}(v)$ denotes the weight function which is a first order polynomial in v with coefficients depending on the initial coin state. The weak-limit theorem shows that the Hadamard walk is indeed a ballistic process with $\Delta x \sim t$.

3 Three-state quantum walk

Let us now turn to the three-state walk on a line where we allow the walker to remain at its present position. From the point of view of a classical random walk this is not very interesting, as one can easily see that one step of such a three-state classical random walk is equivalent to two steps of the usual random walk discussed in the previous section. However, for a quantum walk this equivalence does not hold any more. Indeed, in a three-state quantum walk we have a larger coin space compared to the two-state quantum walk. The additional degrees of freedom might lead to effects which are not present in the two-state quantum walks. One of them is trapping which we illustrate on the example of a three-state Grover walk on a line.

For a three-state quantum walk we have to extend the coin space with an additional basis state $|S\rangle$ corresponding to the walker staying at its present position, i.e.

$$\mathcal{H}_C = \mathrm{Span}\left\{|L\rangle, |S\rangle, |R\rangle\right\} = \mathbb{C}^3.$$

The step operator has to be modified accordingly

$$\hat{S} = \sum_{x=-\infty}^{\infty}\Big(|x-1\rangle\langle x|\otimes|L\rangle\langle L| + |x\rangle\langle x|\otimes|S\rangle\langle S| + |x+1\rangle\langle x|\otimes|R\rangle\langle R|\Big).$$

Finally, the coin operator now acts on the three-dimensional coin space. We choose it as the Grover operator $\hat{G}$ which is defined by

$$\hat{G} = 2|w\rangle\langle w| - \hat{I}_C, \tag{7}$$

where $|w\rangle$ denotes the uniform superposition of all basis states

$$|w\rangle = \frac{1}{\sqrt{3}}\left(|L\rangle + |S\rangle + |R\rangle\right).$$

The unitary evolution operator of the three-state Grover walk then reads

$$\hat{U} = \hat{S}\cdot(\hat{I}_P \otimes \hat{G}).$$

The time evolution equation has the same form as for the Hadamard walk (3). We again choose the initial state to be localized at the origin with some initial coin state $|\psi_C\rangle$. After t steps of the Grover walk the walker is in a state of superposition

$$|\psi(t)\rangle = \sum_{x=-\infty}^{\infty}\Big(\psi_L(x,t)|x\rangle|L\rangle + \psi_S(x,t)|x\rangle|S\rangle + \psi_R(x,t)|x\rangle|R\rangle\Big),$$

where $\psi_j(x,t)$ are the probability amplitudes of finding the walker at position x with the coin state j ($j = L, S, R$). Let us denote by $\psi(x,t)$ the vector of probability amplitudes corresponding to the position x after t steps

$$\psi(x,t) = \left(\psi_L(x,t), \psi_S(x,t), \psi_R(x,t)\right)^T.$$

The probability distribution of the walker's position generated by the three-state Grover walk is then given by $p(x,t) = ||\psi(x,t)||^2$. For illustration, we show in Figure 2 a generic probability distribution obtained for the three-state Grover walk with the initial state $|\psi_C\rangle = |S\rangle$ after $t = 100$ steps.

The probability distribution presented in Figure 2 has three characteristic peaks. Two peaks are located at the edges of the probability distribution and their properties are similar to those of the Hadamard walk presented in Figure 1. The height of these peaks decreases with the number of steps, while their distance from the origin increases linearly. This part of the probability distribution, which spreads ballisticaly across the lattice, can be analyzed along the same lines as for the Hadamard walk. One can prove the weak limit theorem [17, 18, 19] in the form

$$\lim_{t\to\infty}\left\langle\left(\frac{x}{t}\right)^n\right\rangle = \int_{-\frac{1}{\sqrt{3}}}^{\frac{1}{\sqrt{3}}} v^n w(v)dv. \tag{8}$$

The explicit form of the limit density is again given in terms of the Konno's function

$$w(v) = \mathcal{M}(v) f_K\left(v; \frac{1}{\sqrt{3}}\right), \tag{9}$$

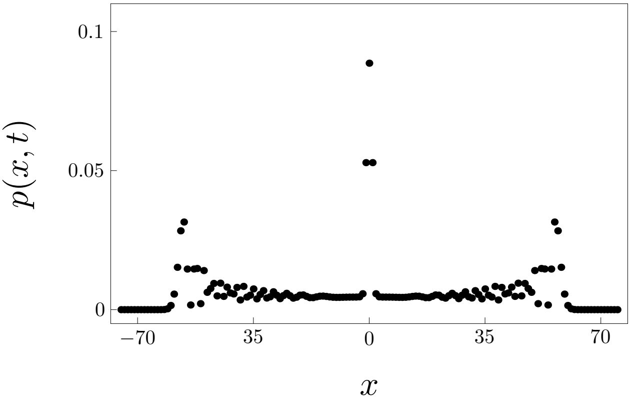

Figure 2: Probability distribution of the three-state Grover walk for the initial coin state $|\psi_C\rangle = |S\rangle$ after $t = 100$ steps.

where now the weight $\mathcal{M}(v)$ is a second-order polynomial in v. However, the relation (8) holds only for $n \geq 1$, since the limit density is not normalized to unity. Indeed, $w(v)$ does not capture the additional sharp peak at the origin which is stationary and does not contribute to the growth of the moments. We find that the height of the peak does not decrease with the increasing number of steps. In fact, one can show [13] that the probability $p(x,t)$ of the three-state Grover walk at any finite position x has a non-vanishing limit

$$\lim_{t\to\infty} p(x,t) \equiv p_\infty(x) \neq 0,$$

except for a particular initial coin state. This feature, which is not present in a two-state quantum walk, is defined as trapping. The trapping effect stems from the fact that the evolution operator of the three-state Grover walk has, apart from the continuous spectrum, also a non-empty point spectrum. Indeed, one can easily check that the vectors

$$|s_x\rangle = |x\rangle\left(|L\rangle + \frac{1}{2}|S\rangle\right) + |x+1\rangle\left(|R\rangle + \frac{1}{2}|S\rangle\right), \quad x \in \mathbb{Z}. \tag{10}$$

are eigenvectors of $\hat{U}$ corresponding to an infinitely degenerate eigenvalue 1. This result is also easily obtained with the Fourier transformation, which is defined similarly as in the previous section. The evolution operator in the Fourier picture is given by the matrix

$$\tilde{U}(k) = D(k)\cdot G = \left(\begin{array}{ccc} e^{-ik} & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & e^{ik} \end{array}\right)\cdot\frac{1}{3}\left(\begin{array}{ccc} -1 & 2 & 2 \\ 2 & -1 & 2 \\ 2 & 2 & -1 \end{array}\right).$$

We easily find that the eigenvalues of $\tilde{U}(k)$ are given by

$$\lambda_{1,2}(k) = e^{i\omega_{1,2}(k)}, \quad \omega_{1,2}(k) = \pm \arccos\left(-\frac{1}{3}(2+\cos k)\right), \quad \lambda_3 = 1.$$

We note that the k dependent eigenvalues $\lambda_{1,2}(k)$ correspond to the continuous spectrum of the evolution operator $\hat{U}$, while the k independent $\lambda_3 = 1$ determines its point spectrum. As we have illustrated in the previous section, the continuous spectrum determines the spreading part of the probability distribution. On the other hand, the point spectrum determines the trapped part of the probability distribution. Indeed, we can write the wave function of the Grover walk in a form similar to that for the two-state walk

$$\psi(x,t) = \mathcal{I}_1(x,t) + \mathcal{I}_2(x,t) + \mathcal{I}_3(x), \quad \mathcal{I}_3(x) = \int_0^{2\pi} \frac{dk}{2\pi} e^{-ixk} v_3(k) f_3(k),$$

where the integrals $\mathcal{I}_{1,2}(x,t)$ are defined similarly to (6). As follows from the Riemann-Lebesque lemma the two time-dependent integrals $\mathcal{I}_{1,2}(x,t)$ vanish for fixed x as t approaches infinity. However, the last integral is time-independent. Hence, we find that the probability amplitude at position x in the asymptotic limit $t \to +\infty$ is given by

$$\lim_{t\to+\infty} \psi(x,t) = \mathcal{I}_3(x),$$

which can be non-zero. This results in the non-vanishing probability of finding the particle at a finite position x in the limit of infinite number of steps

$$\lim_{t\to+\infty} p(x,t) = p_\infty(x) = ||\mathcal{I}_3(x)||^2 \neq 0,$$

which we refer to as trapping probability. For the three-state Grover walk the trapping probability can be evaluated explicitly [17, 18, 19]. With the substitution $z = e^{ik}$ the integral $\mathcal{I}_3(x)$ is transformed into a contour integral over a unit circle in a complex plane, which can be evaluated using the method of residues. In [19] we have shown that the trapping probability reads

$$p_\infty(x) = \begin{cases} 12(5-2\sqrt{6})^{2|x|}|g_+ - g_2|^2, & x < 0 \\ (5-2\sqrt{6})\left(3|g_+|^2 + 2|g_2|^2\right), & x = 0 \\ 12(5-2\sqrt{6})^{2x}|g_+ + g_2|^2, & x > 0 \end{cases} . \tag{11}$$

Here g_+ and g_i are amplitudes of the initial coin state

$$|\psi_C\rangle = g_+|\gamma^+\rangle + g_1|\gamma_1^-\rangle + g_2|\gamma_2^-\rangle,$$

in terms of the basis formed by the eigenvectors of the Grover operator

$$\hat{G}|\gamma^+\rangle = |\gamma^+\rangle, \quad \hat{G}|\gamma_i^-\rangle = -|\gamma_i^-\rangle.$$

The advantage of using the eigenvector basis is that the resulting formula for the trapping probability (11) has a considerably simpler form than in the standard basis [17, 18]. One can clearly see that the trapping probability decreases exponentially with the distance from the origin. Moreover, the trapping probability can be highly asymmetric, since the dependence on the initial coin state is different for positive and negative x. As we have discussed in [19] the asymmetry can be made such that the trapping appears only on the positive or negative half-line by a proper choice of the initial coin state. Finally, we note that the trapping probability (11) is independent of the amplitude g_1. Indeed, $|\gamma_1^-\rangle$ is the so-called leaving state for which the trapping effect does not emerge [13].

Finally, we note that the trapping probability (11) together with the limit density (9) can be used to approximate the exact probability distribution of the three-state Grover walk according to

$$p(x,t) \approx \frac{1}{t} w\left(\frac{x}{t}\right) + p_\infty(x). \tag{12}$$

The trapping probability $p_\infty(x)$ dominates near the the origin, while the density $w(v)$ governs the behaviour at larger distances. One can check that

$$\sum_{m=-\infty}^{\infty} p_\infty(m) + \int\limits_{-\frac{1}{\sqrt{3}}}^{\frac{1}{\sqrt{3}}} w(v)\ dv = 1,$$

i.e. within the approximation (12) the probability distribution is properly normalized to unity.

4 Implications of trapping for quantum transport

The trapping effect considerably limits complete spreading of the walker's wave-function. This has crucial implications on the transport properties of the quantum walk. Let us now illustrate it on the example of excitation transport to an absorbing sink modelled by a quantum walk, which we have investigated in detail in [20]. Consider a ring graph with $2N$ vertices with periodic boundary conditions $-N \equiv N$. On the vertex N, i.e. opposite the starting point of the walk, is a sink which absorbs the walker. The action of the sink is described by the projection operator

$$\hat{\pi} = \left(\hat{I}_P - |N\rangle\langle N|\right) \otimes \hat{I}_C.$$

Time evolution of the quantum walk on a ring graph with a sink is not unitary and the state of the excitation after t steps is described by the vector

$$|\psi(t)\rangle = \left(\hat{\pi}\cdot\hat{U}\right)^t |\psi(0)\rangle,$$

with norm generally less than unity. Let us denote by $\mathcal{P}(t)$ the survival probability , i.e. the probability that the excitation remains on the ring until time t, which is given by

$$\mathcal{P}(t) = \langle\psi(t)|\psi(t)\rangle.$$

The asymptotic transport efficiency η is then defined as

$$\eta = 1 - \lim_{t\to\infty}\mathcal{P}(t).$$

One can show that if the propagation of excitation is modelled by a two-state quantum walk then the survival probability decays exponentially fast

$$\mathcal{P}(t) \sim c\, e^{-\gamma t}, \quad \gamma = 2(1-|\lambda_l|).$$

Here λ_l is the leading eigenvalue of $\hat{\pi}\cdot\hat{U}$, i.e. the largest eigenvalue in absolute value. In such a case, the asymptotic transport efficiency η is unity.

However, for the three-state walk model with the Grover coin we find that $\lambda_l = 1$. Indeed, the stationary states $|s_x\rangle$ of the unitary evolution operator $\hat{U}$ given by (10) are not affected by the presence of the sink at the vertex N for $x\in\{-N+1,\ldots,N-2\}$. Hence, they are eigenvectors of $\hat{\pi}\cdot\hat{U}$ with eigenvalue one and the trapping effect in the three-state quantum walk persists even in the presence of the sink. This result indicates that the survival probability does not vanish and the excitation transport is not efficient. With the knowledge of the stationary states (10) one can evaluate the asymptotic transport efficiency η explicitly for small rings, i.e. small values of N. For larger values of N we can estimate the transport efficiency using the results obtained for the infinite line (11). Within this approximation the limiting value of the survival probability reads

$$\lim_{t\to\infty}\mathcal{P}(t) = \sum_{x=-N+1}^{N-1} p_\infty(x).$$

The asymptotic transport efficiency η is then given by

$$\eta = 1 - \sum_{x=-N+1}^{N-1} p_\infty(x).$$

Since the trapping probability (11) depends on the initial state so does the transport efficiency. It follows that the smallest value of η is obtained when the initial coin state is chosen as the eigenstate $|\gamma^+\rangle$. We note that for the leaving state $|\gamma_1^-\rangle$ the asymptotic transport efficiency reaches unity.

5 Conclusions

We have shown that expanding the coin space of a quantum walk might lead to a novel effect of trapping which is not present in a two-state quantum walk on a line. Trapping is manifested by a stationary peak at the origin which decreases exponentially with the distance. However, part of the wave function still spreads ballistically. The trapping effect emerges when the evolution operator of the quantum walk has both continuous and point spectrum.

We note that the Grover operator (7) is not the only coin for which the trapping effect arises for the three-state quantum walk. In [21] we have found two one-parameter extensions of the Grover matrix for which the point spectrum of the evolution operator is preserved. The properties of the resulting quantum walks were investigated in detail in [19]. We have further extended these results in [22] where we have given full classification of all $U(3)$ matrices which lead to the trapping effect for a three-state quantum walk on a line.

Limitations of quantum transport imposed by the trapping effect, which we have illustrated in the previous section, were analyzed for a broad range of coin operators in [20]. We have also analyzed the effect of dynamical percolation [23] of the ring on the transport efficiency. Improving transport by allowing the edges to break randomly seems to be counterintuitive from a classical point of view. However, percolation can eliminate the trapping effect and thus improve the asymptotic transport efficiency to unity.

Finally, we stress that the trapping effect is not limited to quantum walks where the walker is permitted to stay at its present position. Indeed, it was also identified on higher-dimensional lattices [24] and more complicated graph structures [25], where the walker has to leave the occupied vertex. The additional degrees of freedom offered by larger coin space results in features which do not exist for three-state walks. As an example, the effect of strong trapping was identified in [26]. It was found that for certain $U(4)$ coins the leaving state, i.e. an initial state for which the trapping vanishes, does not exist. Hence, in such walks the trapping effect is always present, irrespective of the initial condition. This is not possible in three-state walks where the leaving state always exists [22].

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