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# Survival probability in a one-dimensional quantum walk on a trapped lattice

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**Abstract.** The dynamics of the survival probability of quantum walkers on a one-dimensional lattice with random distribution of absorbing immobile traps is investigated. The survival probability of quantum walkers is compared with that of classical walkers. It is shown that the time dependence of the survival probability of quantum walkers has a piecewise stretched exponential character depending on the density of traps in numerical and analytical observations. The crossover between the quantum analogues of the Rosenstock and Donsker–Varadhan behavior is identified.

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## 1. Introduction

The classical random walk (CRW) is a prototype model of the stochastic processes that occur in many physical systems [1]. Extension of the random walk concept from the stochastic classical realm to the unitarily evolving quantum world is motivated by the promise of quantum walks (QWs) [2, 3] as quantum algorithms [4] outperforming their classical counterparts, and as a simple model for quantum computation.

In parallel with the remarkable developments in the experimental ability to control single atoms and photons, early proposals and demonstrations of QWs are followed by more robust and controllable implementations [5]–[7]. The superiority of a QW algorithm [4] was experimentally demonstrated very recently [8]. In a very recent experiment [9], the effect of absorbing boundaries on the QW was examined. The QW on a line segment with absorbing boundaries [2, 10] is a special case of a more general situation of QW in the presence of absorbing traps.

A QW on a trapped lattice exhibits a transition to CRW [11]; therefore, traps can be characterized as a quantum decoherence mechanism [12, 13], similar to broken links [14] or environmental noise [15]. Controlling the trap density in the lattice allows for a tunable decoherence mechanism, which is beneficial to fundamental investigations of quantum decoherence and to efficient implementation and speeding up of quantum algorithms [16, 17].

In addition to their role as a source of quantum decoherence, traps can play another role in the dynamics of QW. It is known that their presence causes different dynamical regimes on the evolution of CRW. Our aim is to explore whether such distinct dynamical regimes can emerge in QW without changing its quantum nature. Earlier occurrences of such a crossover between different dynamical regimes other than quantum-to-classical transition should be taken into account for potential applications of trapped QW.

Trapped CRW was extensively explored earlier [18]–[20]. A practical quantity of interest is the survival probability of diffusing particles, which is the mean probability that a walker can still be found on the lattice after some time $t$. It can be analytically calculated for a one-dimensional (1D) CRW [21]. In the early times of CRW on a 1D lattice with low trap

concentration, survival probability decays exponentially with the square root of time, $t^{1/2}$, which is known as the Rosenstock (RS) [22] behavior. At asymptotically large times, this behavior makes a crossover [23] to a qualitatively different scaling form, which is called the Donkser and Varadhan (DV) regime [24]–[27], in which the survival probability exponentially decays with $t^{1/3}$. Similar scaling forms also appear in the closely related problem of the Lifshitz tail or Griffiths singularity of the density of states at the band edge for a quantum electron in a random potential [28]–[30].

It is neither intuitively nor quantitatively obvious to extend the classical results to characterize the survival probability of quantum walkers on a trapped land, because of the curious role played by quantum coherence and path interference in a QW, which is associated with the characteristic strong de-localization of quantum walkers. This paper specifically addresses the question of quantum diffusion dynamics on a trapped chain; in particular it investigates the quantum analogues of the RS and DV dynamical regimes of the classical diffusion problem.

It is difficult to observe the RS-to-DV crossover in CRW. Time dependence of classical survival probability makes the crossover happen only after a long time, although it can happen relatively earlier for larger trap concentrations or for larger diffusive constants [31]. Motivated by the role of the diffusive constant in shortening the crossover time in CRW, we predict that highly de-localized quantum walkers can enter the DV regime earlier than classical walkers. Furthermore, the qualitatively different DV scaling form in CRW is attributed to the existence of large voids, or absorber-free regions, which are exponentially rare among the possible configurations [26]. Their contribution can dominate the time dependence of the survival probability only at large times, after the more common smaller voids have lost their walkers. In QW, we expect that, due to the larger spread of the walkers, such voids should be larger, and hence rarer. An average over such clusters, with their corresponding large decay times, would lead to slower decay of quantum walkers compared with their classical counterparts. Indeed, for a continuous-time 1D quantum transport problem, it is found that the survival probability exponentially decays with $t^{1/4}$ [32]. This asymptotically slower decay of quantum coherent particles compared with the diffusive classical particles is explained by the existence of slowly decaying asymptotically large trap-free segments [32]. In QW-based search algorithms with multi-agents, such a slowing down of quantum coherent dynamics would cause the additional limitation of the quantum speeding up even for small target (or trap) concentrations. It should be taken into account in addition to the usual quantum-to-classical decoherence problem.

We perform detailed numerical simulations for settings relevant to current experimental efforts. As such, our discussion is limited to the 1D coined discrete-time QW. Comparative studies of the signatures of coherent and incoherent transport in the case of continuous-time QW were recently reported [32]–[34]. We give particular attention to the practical case of small, finite-size lattices and a small number of time steps. Similar to the classical prototype system of disordered media, randomly distributed static traps are assumed. The trapping process is supposed to be a quenched, instantaneous and perfect absorption of walkers. In a typical scenario of interest there would be few traps, and dynamics would be limited to short times; however, the cases of long-time behavior as well as densely trapped lattices are also analyzed to comprehend differences in both the RS and DV regimes, in addition to the dynamics of quantum-to-classical transition.

We explain our numerical results by the Flory-type heuristic arguments [35] used in polymer chemistry. Spatial arrangements of macromolecules, or conformations of polymers,

are closely related to the diffusion and the random walk problem. In the early 1930s, structural chemistry descriptions of long-chain molecules were based on unconstrained random walks, where the skeletal bonds of the molecule are represented by the uncorrelated steps of random walkers. This analogy yields scaling relations for the root mean square (rms) distance of the chain (squared radius of gyration) depending on the bond length and the number of the bonds. In 1949, P J Florry provided a seminal work that takes into account the volume exclusion effect (no segments of a molecule can overlap in space), in the formation of polymers. This allows for a description of polymer growth in terms of the self-avoiding or repulsive random walks. In self-avoiding walks, the walker would stop or become trapped if there are no more unvisited neighboring sites. Our trapped lattice model is in that sense closely related to such random walk models of polymer growth and size distribution. The movement of a single walker to a nearest neighbor site can be imagined as initiating the formation of an unsaturated bifunctional monomer, while trapping would give polymers of different sizes.

This paper is organized as follows. First we present a short review of the theory and major results of the 1D QW in section 2. The model of CRW and QW with traps is introduced and the survival probability is defined in section 3. In section 4, the numerical simulations on the survival probability are presented and the analytical results are given using the correspondence to the QW with position measurement on the line in the thermodynamic limit. Section 5 is devoted to the conclusions and the outlook.

## 2. Quantum walk

### 2.1. Single-particle walk

We consider a coined discrete-time QW on a finite linear lattice segment with periodic boundary conditions. Denoting the total number of sites on the lattice by $K$, the geometry is equivalent to a ring, or a so-called $K$-cycle [16, 36]. In strict mathematical terms, it is the Cayley graph of the cyclic group of size $K$. The coin (chirality) space of a single walker is described by $\mathcal{H}_{\mathrm{C}}$ with two basis vectors $\{|\uparrow\rangle, |\downarrow\rangle\}$. Also, the position space of a single walker on this chain is described by $\mathcal{H}_{\mathrm{P}}$ with the basis $\{|kt\rangle \ : \ k \in \mathbb{Z}/K\mathbb{Z}\}$. The Hilbert space of the total system is given by $\mathcal{H} = \mathcal{H}_{\mathrm{C}} \otimes \mathcal{H}_{\mathrm{P}}$. We identify the chirality basis vectors as

$$|\uparrow\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad |\downarrow\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}. \tag{1}$$

Each step of the particle[7] consists of a unitary coin operation $\hat{C}$ for the chirality transformation, and a position-shift operation $\hat{S}$. At time $t$, QW is defined by transformation $\hat{U}^t$ with $\hat{U}$ being the unitary operator of a walk step, which is given by

$$\hat{U} := \hat{S}(\hat{C} \otimes \hat{I}), \tag{2}$$

with $\hat{I}$ being the identity operator. Throughout this paper, we assume that the coin operator $\hat{C}$ is the Hadamard operator

$$\hat{H} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} \tag{3}$$

[7] Throughout this paper, we call it the step or the time. It should be noted that these have the same meaning.

for simplifying the discussion. The shift position operator $\hat{S}$ is described by

$$\hat{S} = |\uparrow\rangle\langle\uparrow| \otimes \sum_{k=1}^{K} |k+1\rangle\langle k| + |\downarrow\rangle\langle\downarrow| \otimes \sum_{k=1}^{K} |k-1\rangle\langle k|, \tag{4}$$

with $k \in \mathbb{Z}/K\mathbb{Z}$; $K+1 \equiv 1$ and $0 \equiv K$. The wave function of the quantum walker at time $t$ can be written as $|\psi(t)\rangle = \sum_{c,k} \psi_c(k,t)c, k\rangle|$ with $c = \uparrow, \downarrow$. This can be rewritten as

$$|\psi(k,t)\rangle = \sum_{c\in\{\uparrow,\downarrow\}} \psi_c(k,t)\,|c\rangle = \begin{bmatrix} \psi_\uparrow(k,t) \\ \psi_\downarrow(k,t) \end{bmatrix}, \tag{5}$$

where $\psi_\uparrow(k,t)$ and $\psi_\downarrow(k,t)$ represent probability amplitudes of the particle at the site $k$ at time $t$, depending on the internal states $|\uparrow\rangle$ and $|\downarrow\rangle$, respectively.

At time $t$, the quantum state of the quantum walker is given by

$$|\psi(t)\rangle = \hat{U}^t\,|\psi(0)\rangle\,, \tag{6}$$

where $|\psi(0)\rangle = |\chi, m\rangle$ is the initial state of the coin $|\chi\rangle$ and the position $|m\rangle$ ($m \in \mathbb{Z}/K\mathbb{Z}$). Here, we define the density operator of the quantum walker as $\Phi(t) = |\psi(t)\rangle\langle\psi(t)|$. Then, the probability distribution of the walker at position $x$ at time $t$ can be calculated by

$$P(x,t) = \sum_{c\in\{\uparrow,\downarrow\}} \langle c, x|\,\Phi(t)\,|c, x\rangle \quad (x \in \mathbb{Z}/K\mathbb{Z}). \tag{7}$$

This can be rewritten as

$$P(x,t) = |\psi_\uparrow(x,t)|^2 + |\psi_\downarrow(x,t)|^2. \tag{8}$$

### *2.2. Multi-particle walk*

One can easily envision that multi-particle random walks can be more advantageous in search algorithms than single-particle ones. Indeed, recent experimental progress and theoretical studies favor the many-body random walk problem in both classical and quantum realms [37, 38]. As the general approach to this problem in terms of indistinguishable, correlated and interacting particles is too challenging to start with, we aim to comprehend the simplest scenario in this work and consider the complications in particular implementation settings in future studies. Let us assume that the walkers are non-interacting distinguishable particles and they are initially uncorrelated. For $N$ such walkers, the Hilbert space is given by a direct product of single walker spaces,

$$\mathcal{H} = \bigotimes_{i=1}^{N} (\mathcal{H}_C \otimes \mathcal{H}_P)_i, \tag{9}$$

with the particle label $i$. The particles walk independent of each other on the $K$-cycle so that the time evolution of the whole system is determined by

$$\hat{U}_{1,2,\ldots,N} := \hat{U}^{\otimes N}, \tag{10}$$

where $\hat{U}$ is given by equation (2) and is the same for all particles.

The initial state of $N$ walkers is given by a tensor product of the single walker initial states as

$$|\Psi(0)\rangle = \bigotimes_{i=1}^{N} |\chi, m_i\rangle_i\,, \tag{11}$$

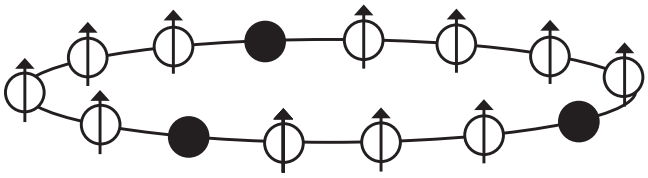


**Figure 1.** Schematic representation of multi-particle QW on the $K$-cycle for 11 walkers with the initial state $|\uparrow\rangle$ and three absorbing trapped sites (black color).

where $|\chi, m_i\rangle_i$ expresses the $i$th particle state with the chirality $|\chi\rangle$ and the position $m_i = 1, \ldots, K$. This is illustrated in figure 1. At time $t$, the quantum state of the system becomes

$$|\Psi(t)\rangle = \hat{U}^t_{1,2,\ldots,N} |\Psi(0)\rangle . \tag{12}$$

Using the reduced single-particle density matrix

$$\Phi_i(t) = \mathrm{Tr}_{j\neq i} |\Psi(t)\rangle \langle\Psi(t)| , \tag{13}$$

the probability distribution of a single walker at time $t$ can be evaluated by

$$P_i(x,t) = \sum_{c\in\{\uparrow,\downarrow\}} \langle c, x| \Phi_i(t) |c, x\rangle \quad (x \in \mathbb{Z}/K\mathbb{Z}). \tag{14}$$

This shows that $P_i(x,t)$ can be interpreted as a conditional probability to find a walker at site $x \in \mathbb{Z}/K\mathbb{Z}$ at time $t$ when the particle started to walk from site $m_i$ at $t = 0$. The complete set of $\{P_i(x,t)\}$ for all particles $i = 1, \ldots, N$ can be visualized as the set of transition probabilities from $\{m_i\}$ to $x$ of a single particle, so that the simplest multi-particle QW problem under study here is essentially a single particle problem that starts to walk at a set of different initial locations.

## 3. Survival probability

We use the exact enumeration method for calculating the survival probability in CRW [25], which is suitable for the randomly distributed immobile traps on a 1D lattice. Initially, every untrapped site is occupied by a walker. At each step, $N$ walkers perform CRW on the 1D lattice, for which the probability of finding a walker at a particular site $P_i(x,t)$ is calculated with the sum of the corresponding probabilities at its nearest-neighbor sites divided by two. The survival probability at time $t$ is given by

$$P_r(t) = \frac{1}{N} \sum_{i=1}^{N} \sum_{x=1}^{K} P_i(x,t). \tag{15}$$

Here $r$ enumerates a particular independent initial configuration of the system. Note that we have the relation $N = K - n$ or $N = K(1-\rho)$, where $n$ is the number of traps on the lattice and $\rho = n/K$ is the concentration from our assumption. We take the lattice sites at $\{x : x = 1, \ldots, K\}$. Note that we assume non-overlapping, immobile, perfectly absorbing sites such that $P_i(x,t) = 0$ if the site $x$ is a trapping site; hence the sum is not restricted to the untrapped sites. Furthermore, in this paper, a single particle only occupies each untrapped site.

To account for random distribution of the traps, a statistical configurational average of mean survival probability is calculated over different independent realizations of the initial system via

$$\langle P\,(t)\rangle = \frac{1}{M}\sum_{r=1}^{M} P_r(t), \tag{16}$$

where $M$ denotes the number of different configurations.

Let us now examine the quantum analogue of the survival probability [32, 39, 41]. In QW, quantum states of the particles lead to non-trivial path interference effects. The quantum states can be initialized arbitrarily before the walk starts. At each time step, new positions and states of quantum walkers are determined with the unitary transformation $\hat{U}$ for each walker. If a state meets an immobile trap, it gets annihilated. In the previous section, we have seen that for our simplified case, the process is equivalent to a single-particle problem with an ensemble of initial configurations. Thus, we can use the classical definition of the survival probability by only making a quantum mechanical calculation of the single-particle probability distribution.

Let us briefly consider the experimental realization of this system. In the system of the 2D ion trap experiment [5], it seems possible to manipulate the QW on the ring. Localized ion losses can be effectively considered as the absorption traps. Also, in the system using the photon by the waveguide, the nonlinear phase gate is essentially used for realizing the QW on the circle [42]. Combining the waveguides, the absorption traps could be realized.

## 4. Results and discussions

### *4.1. Survival probability in a quantum walk on a finite one-dimensional trapped lattice*

We numerically analyze the dynamics of the survival probability in a QW for three different initializations of the system. In the first case, all quantum states at the untrapped sites are initialized as $|\uparrow\rangle$. In the second case, the initial states are randomly assigned either $|\uparrow\rangle$ or $|\downarrow\rangle$. In the last case, all states are chosen as superpositions $\frac{1}{\sqrt{2}}(|\uparrow\rangle + \mathrm{i}|\downarrow\rangle)$. We shall, respectively, call them up, mixed and symmetric initializations.

Typical simulation results are reported in figures 2(a)–(c), for the three cases of initialization of the QW, and for different trap densities, $\rho = 0.05$, $\rho = 0.1$, $\rho = 0.2$ and $\rho = 0.3$. The figures are plotted in a convenient double logarithmic scale. While the survival probability exhibits the expected behavior of decrease in time and being less at higher trap densities, it invites a closer look because of some non-trivial qualitative changes in its dynamics. All the different initializations lead to two qualitatively different dynamical regimes of survival probability. These two regimes make a crossover at a certain time point, $t_c$, whose location depends on the trap density. The crossover time $t_c$ appears at $t_c \approx 25/\rho$ for up and symmetric initializations and at $t_c \approx 8/\rho$ for mixed initialization. Figure 2 is plotted for $K = 101$ sites, but we also tried different lattice sizes and found results similar to figure 2.

As seen in figure 3, the 'mixed' initial configuration behaves dynamically different from the 'up' and 'symmetric' cases. This is due to the profound quantum character of pure states in contrast to the statistical mixture, evolving closer to a classical walk. Pure quantum states are more beneficial for the fast spread of the QW in the RS regime than a statistical mixture. Classical walks perform worst in this regime as we shall argue below.

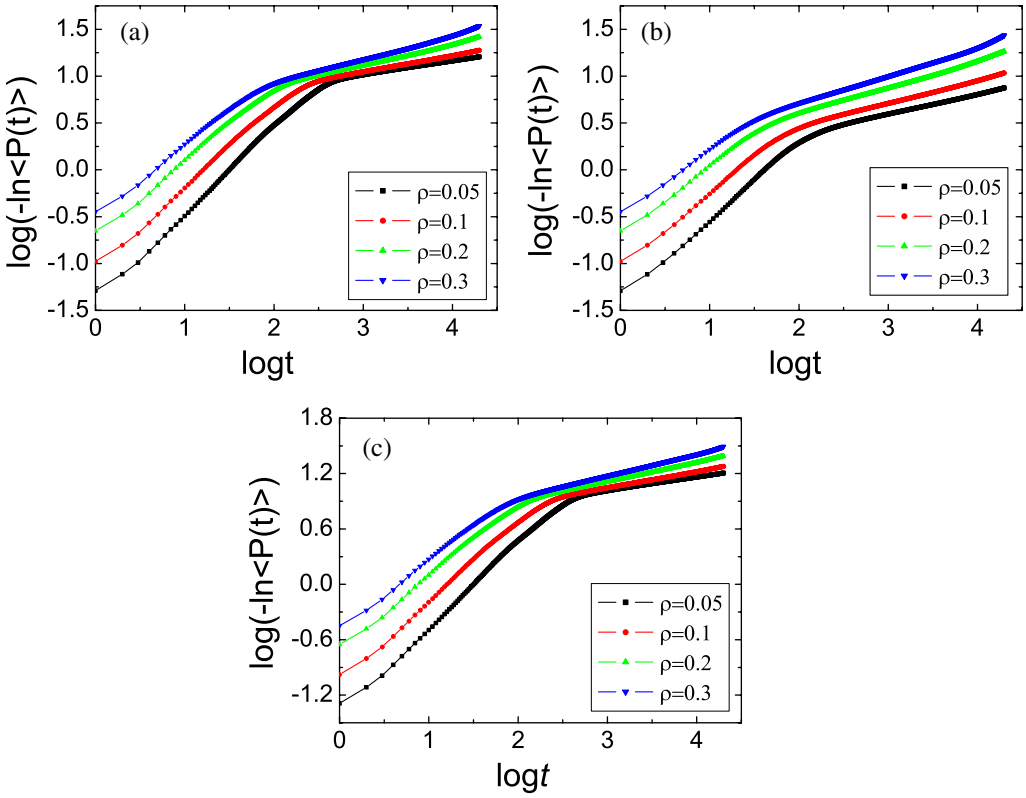



**Figure 2.** (a) The time dependence of the survival probability in the QW on a lattice of $K = 101$ sites for $T = 20\,000$, $M = 10\,000$, $\rho = 0.05$, $\rho = 0.1$, $\rho = 0.2$ and $\rho = 0.3$ with the initializations (a) $|\uparrow\rangle$ (up), (b) randomly distributed $|\uparrow\rangle$ or $|\downarrow\rangle$ (mixed) and (c) $\frac{1}{\sqrt{2}}(|\uparrow\rangle + \mathrm{i}|\downarrow\rangle)$ (symmetric).

Before and after the crossover point, the survival probability exhibits a linear dependence on time in the double logarithmic scale. By increasing $M$ the linear behavior becomes more evident, including the end and the beginning times. After that, it is simple to make linear fits to the curves in the regimes from $t = 1$ to $t = t_c$ and from $t = t_c$ to $t = T$, the end of the walk. The line fits yield the Kohlrausch–Williams–Watts stretched exponential function [40] description of the survival probabilities, given by

$$\langle P\,(t)\rangle \sim \exp[-t^{\beta}], \tag{17}$$

where the stretching exponent $0 < \beta < 1$ determines the decay rate of $\langle P(t)\rangle$. It gets different values, $\beta_1$ and $\beta_2$, before and after $t_c$, respectively. Their dependence on the trap density $\rho$ is shown in figure 4. $\beta_1$ decreases monotonically with increasing $\rho$, whereas $\beta_2$ increases with increasing $\rho$.

The value of $\beta_1$ at low $\rho$ can be understood following the classical RS approximation method. When $s_t$ is the number of distinct sites visited at time $t$, the probability of being not absorbed for a single walker can be written as $p_t = (1-\rho)^{s_t}$. Formally the mean probability can be expressed in the form $P(t) = \langle p_t\rangle = \langle \exp(-\lambda s_t)\rangle$ with $\lambda = -\ln(1-\rho)$. Employing the RS approximation for short times and small $\rho$, we obtain $P(t) \approx \exp(-\lambda\langle s_t\rangle)$. For the CRW, $\langle s_t\rangle \sim \sqrt{t}$ gives the usual RS scaling form. For the QW, however, the ballistic spread of the

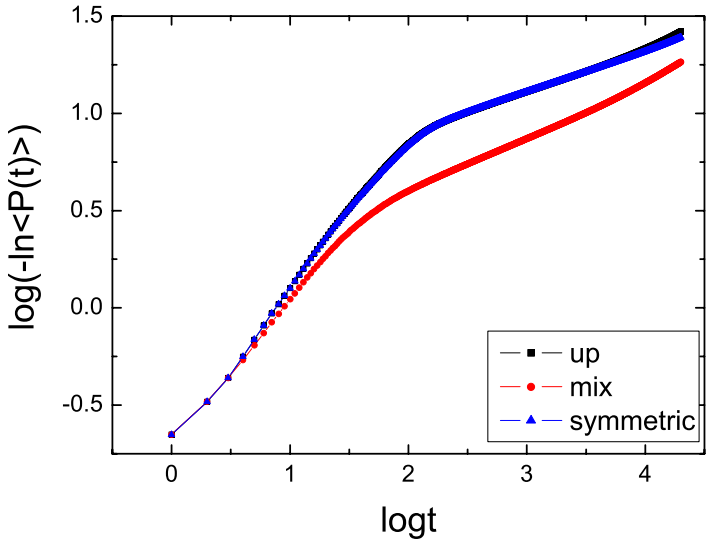



**Figure 3.** The time dependence of the survival probability in the QW on a lattice of $K = 101$ sites for $T = 20\,000$, $M = 10\,000$ and $\rho = 0.2$ with the initializations $|\uparrow\rangle$ (up), randomly distributed $|\uparrow\rangle$ or $|\downarrow\rangle$ (mixed) and $\frac{1}{\sqrt{2}}(|\uparrow\rangle + \mathrm{i}|\downarrow\rangle)$ (symmetric).

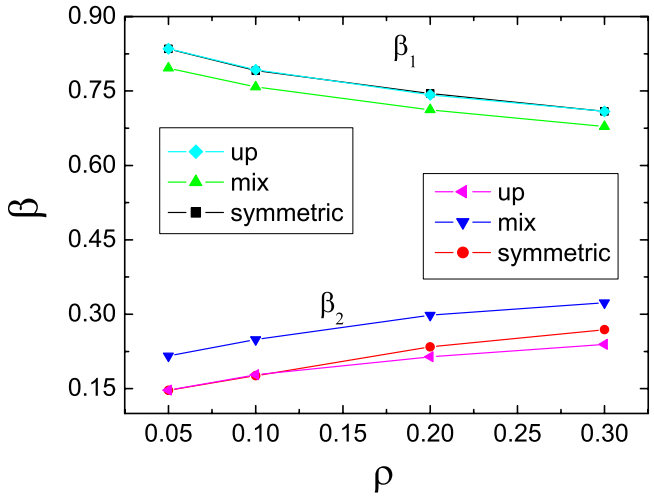



**Figure 4.** Dependence of the decay parameters $\beta_{1,2}$ on the low trap density $\rho$ in a lattice of $K = 101$ sites, in the cases of the up, mixed and symmetric initializations.

quantum walkers allows for $\langle s_t \rangle \sim t$ [43, 44] so that the equivalent rate of survival is enhanced to $\beta_1 \sim 1$ in the quantum analogue of the RS regime.

The maximal value of $\langle s_t \rangle$ is associated with the screening or penetration length that measures the distance between the starting and the trapping site of the walkers. Quantum walkers have larger penetration lengths than classical ones and as such can survive at asymptotic times provided that they start in larger clusters. The probability of such configurations is

exponentially rare with the size of the segment, while the quantum spreading is a power-law (quadratic) gain relative to classical walk. Hence, it is necessary to find indeed large voids (relatively larger than their classical counterparts) to ensure that quantum walkers can survive. In the quantum analogue of the DV regime, the size of the dominating, remaining clusters with quantum walkers would therefore be larger than the classical DV regime. Averaging over such slowly decaying large voids would then lead to the survival probability decaying slower than the DV regime of classical diffusion. A similar observation for the case of continuous-time quantum transport gives $-\ln\langle P(t)\rangle = t^{1/4}$ [32]. In our case, $\beta_2$ is close to this value up to $\rho < 0.3$ as demonstrated in figure 4.

The Flory-type heuristic arguments for $\beta_2$ and RS approximation for $\beta_1$ justify that the numerically observed crossover in figure 2 is indeed the quantum analogue of the classical RS-to-DV transition. It is known that such a crossover can happen only at long times and is hard to observe in the CRW. In classical systems, $t_c$ can be decreased either by increasing $\rho$, which is especially efficient for one dimension [31] or by using systems with large diffusive constants [31]. Remarkably, decrease of $t_c$ with $\rho$ is also observed in figure 2 for QW. Increase of $\rho$, however, would mean to lose the benefits of quantum coherence in QW due to the quantum-to-classical transition that happens at high $\rho$ [11, 14, 15]. On the other hand, a strong de-localization of quantum walkers contributes significantly to further reduction of $t_c$ in the QW. As such, we expect that the quantum analogue of the RS-to-DV crossover can occur earlier than CRW. As the decay of survival probability of QW is even slower than classical diffusion in the quantum DV regime, this makes the quantum RS-to-DV crossover a serious limitation to implement QW-based quantum search algorithms even for a relatively small number of traps (or targets). The usual limitation factor of quantum-to-classical transition is an issue only for high $\rho$. In the next section, we shall verify our predictions and investigate the effect of large trap concentrations. Furthermore, we will analytically show the crossover in the thermodynamic limit.

### *4.2. Survival probability in classical random walk versus quantum walk*

Short- and long-time behavior of the survival probability in the CRW and evidence of RS-to-DV crossover are shown in figure 5. In short-time behavior, the survival probability at low trap densities complies with RS behavior and fits well to $\beta = 1/2$ in figure 5(a). If the trap density is increased, the slope decreases and approaches $1/3$ for large values of $\rho$. DV behavior emerges in figure 5(b). These analytical values are strictly valid for a thermodynamically large system. Convergence to the asymptotic DV scaling form is faster in the case of higher trap concentrations.

To compare the CRW and QW, we consider a lattice of $K = 101$ sites and take $T = 1000$. The time dependence of survival probability is shown in figure 6(a) for the CRW and in figure 6(b) for the QW. We choose the initialization that gives the longest $t_c$, to consider the worst situation for the QW. Even for this case, we see that quantum RS-to-DV crossover happens while the CRW is still in the classical RS regime. In particular for low $\rho$, a highly distinct and clear crossover can be observed in the QW.

From the plots of survival probability in figure 6, the influence of $\rho$ on the scaling forms can be systematically investigated by using figure 7, in which the stretching exponents are plotted as functions of trap density $\rho$. As the trap concentration increases, $\beta_1$ and $\beta_{cl}$ decrease. In contrast, $\beta_2$ increases with $\rho$. As noted earlier, the sharpest transition between the quantum RS and DV

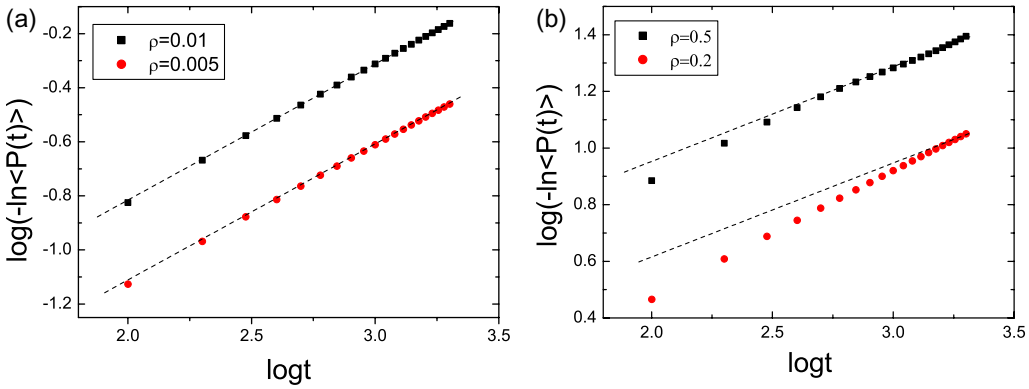



**Figure 5.** Time dependence of the survival probability in the CRW on a lattice of $K = 50\,000$ sites for (a) $T = 2000$, $M = 100$ and $\rho = 0.01$, $\rho = 0.005$, where the broken lines represent the slope of $\beta = 1/2$; and (b) $T = 2000$, $M = 100$ and $\rho = 0.2$, $\rho = 0.5$, where the broken lines represent the slope of $\beta = 1/3$.

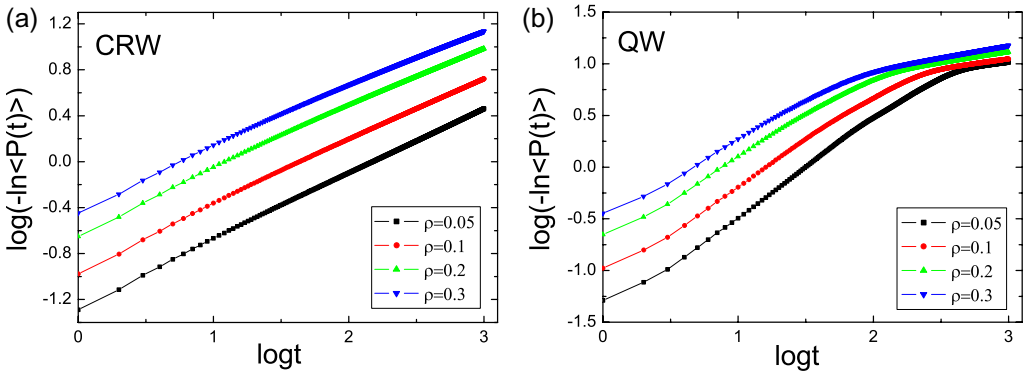



**Figure 6.** Time dependence of the survival probability for a lattice of $K = 101$ sites, $T = 1000$, $M = 100\,000$ in (a) the CRW and (b) the QW with the initial state $|\uparrow\rangle$.

regimes happens at low $\rho$. At high trap densities, their separation shrinks and both $\beta_{1,2}$ converge to the classical exponent $\beta_{\mathrm{cl}}$. This is in accordance with the expectation that for such high $\rho$, decoherence transition of QW to CRW should occur. Figure 7 gives strong and clear evidence that the dynamical transition in figure 6(b), between early and longer time scaling forms of QW, is not a quantum-to-classical transition, but the true quantum analogue of the classical RS-to-DV crossover.

### *4.3. Single-particle quantum walk with position measurement and survival probability in multi-particle quantum walk*

In this subsection, we analytically show the relationship between the survival probability and the QW with position measurement on the line.

Let us recapitulate the QW with position measurement on the line [13, 45, 46]. Here, we replace the position Hilbert space by $\tilde{\mathcal{H}}_{\mathrm{P}} = \{|z\rangle : z \in \mathbb{Z}\}$. The one-step dynamics is

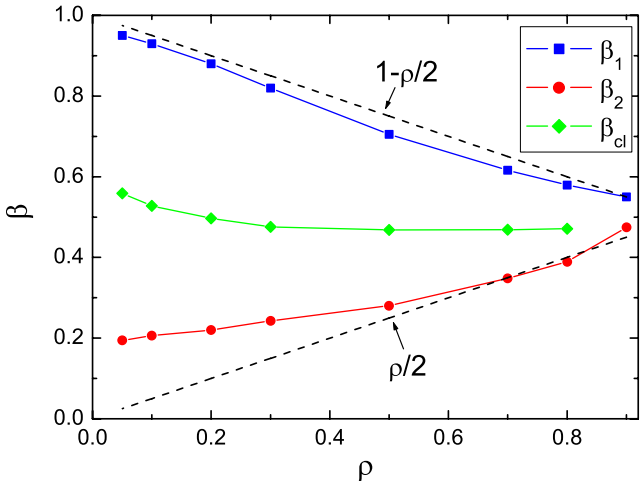



**Figure 7.** Dependence of the decay parameter $\beta$ on the trap density $\rho$ for a lattice of $K = 101$ sites and $t = 1000$ time steps in the CRW and the QW with the initial state $|\uparrow\rangle$. Dashed lines represent analytical fitting results.

given by

$$\Phi(t+1) = (1-p)U\Phi(t)U^{\dagger} + p\,|\chi\rangle\langle\chi| \otimes \left[\mathrm{Tr}_C \sum_{z,z' \in \mathbb{Z}} \left[(\hat{I} \otimes |z\rangle\langle z|)\hat{U}\Phi(t)\hat{U}^{\dagger}(\hat{I} \otimes |z'\rangle\langle z'|)\right]\right], \tag{18}$$

where $\Phi(0) = |\tilde{\psi}(0)\rangle\langle\tilde{\psi}(0)|$ with $|\tilde{\psi}(0)\rangle = |\chi, 0\rangle$ and $p \in [0, 1]$. This model can be taken as the position measurement of the 1D QW with probability $p$. When $p = 1/t^{\gamma}(0 \leqslant \gamma \leqslant 1)$, the asymptotic behavior of the QW with position measurement is $\langle s_t^{(D)}\rangle \sim t^{(1+\gamma)/2}$ [13, 45].

In the case of the thermodynamic limit, $K \to \infty$ with fixed $\rho$, and sufficiently large $t$, many-particle QW on the $K$-cycle can be reduced to the single-particle QW on the line as follows. For uncorrelated quantum walkers and quantum coin in our model of multi-particle QW, the event of annihilation of the walker reaching a trap site is equivalent to a position measurement. The mean probability that the particle reaches the trapped site at time $t$ is $p = t^{\rho}/t = (1/t)^{(1-\rho)}$. Therefore, it is possible to apply the result for the QW with position measurement on the line to this system to obtain the asymptotic behavior of the QW to arrive at the trapped site as $\langle s_t^{(T)}\rangle \sim t^{1-(\rho/2)}$. This can be taken as the mean free path. In the thermodynamic limit, we can apply the central limit theorem to obtain that the survival probability is the exponential decay for the mean free path as

$$\langle P(t)\rangle \sim \exp\left[-\frac{\langle s_t^{(NT)}\rangle}{\langle s_t^{(T)}\rangle}\right] \sim \exp[-t^{\rho/2}], \tag{19}$$

where $\langle s_t^{(NT)}\rangle \sim t$ is the mean free path without the trap site, i.e. the QW behavior without position measurement.

Let us reconsider the thermodynamic limit with the fixed $\rho$ for the two types: $t \ll K$ and $t \sim K$. In the first case, i.e. before the crossover time, the survival probability can be

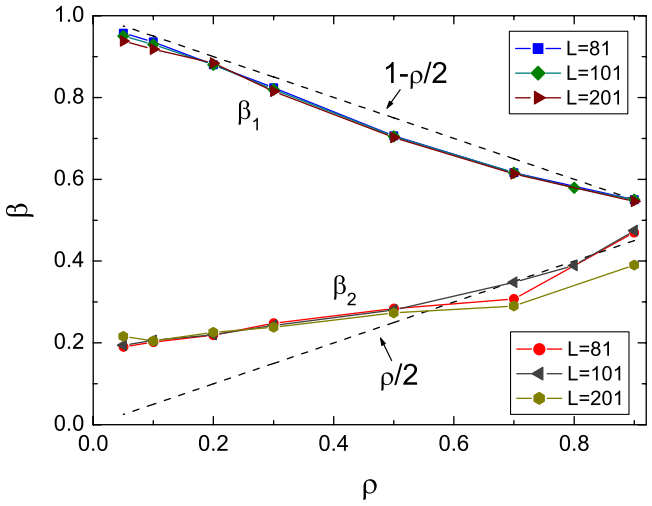



**Figure 8.** Dependence of the decay parameter $\beta$ on the trap density $\rho$ for a lattice of $K = 81$, $K = 101$ and $K = 201$ sites, $t = 1000$ time steps in the QW with the initial state $|\uparrow\rangle$.

approximately taken as the small $t$. That is, it is impossible to directly apply equation (19). Analogous to the discussion in the above section, the survival probability can be rewritten as

$$\langle P(t)\rangle \approx 1 - \langle s_t^{(T)}\rangle \sim 1 - t^{(1-(\rho/2))}. \tag{20}$$

From $\langle P(t)\rangle \sim \exp[-t^{\beta_1}] \approx 1 - t^{\beta_1}$, we obtain

$$\beta_1 = 1 - \frac{\rho}{2}. \tag{21}$$

In the second case, i.e. after the crossover time, on the other hand, equation (19) can express the exponential decay. Therefore, we directly obtain

$$\beta_2 = \frac{\rho}{2}. \tag{22}$$

These analytical results can be compared with the numerical results of figure 7. While these show good agreement, we cannot see the finite-size effects as seen in figure 8. Also, our numerical calculation is used in the same and specific chirality state for the multi-particle QW and the Hadamard coin. When we remove these conditions, our analytical observation is unchanged in the thermodynamic limit because the essential part of the proof of the limit distribution is to use the identical distribution for the single particle [45].

## 5. Conclusion and outlook

We have investigated the time dependence of the survival probability in discrete Hadamard QW on a $K$-cycle with random, static, perfect traps. We found that the survival probability exhibits a piecewise stretched exponential character. In the early time regime, it decays faster than that of CRW, whereas in the late time regime it decays slower. The crossover time

between two regimes decreases with trap density $\rho$. By analytical and heuristic arguments, we have identified the dynamical transition between two regimes as the quantum analogue of the RS-to-DV crossover in classical diffusion. We have shown that the quantum RS-to-DV crossover can happen earlier than its classical counterpart. At high trap concentrations, quantum-to-classical transition happens. At low trap concentrations, even though quantum-to-classical transition does not play a role, quantum RS-to-DV crossover is found to be a serious limitation on the benefits of quantum coherence, such as quadratic speeding up in implementations of QW-based quantum search algorithms.

As an outlook on the present work, consideration of larger dimensional systems with probabilistic or state-dependent traps and interacting walkers could make the results more suitable for applications and experimental realizations [47]. From a more fundamental point of view, further investigations of the quantum RS–DV scaling transitions can be performed in terms of the quantum Zeno effect in QW [48] or in relation to random quenched disorder [49]. A more direct and rigorous generalization of the Flory mean field theory to the trapped QW can also be pursued. An extension of our work to the question of quantum RS-to-DV transition in the case of continuous QW would be of interest in the light of recent realizations of multi-agent continuous QW [50].

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## References

[1] Barber M N and Ninham B W 1970 *Random and Restricted Walks: Theory and Applications* (New York: Gordon and Breach)
[2] Ambainis A, Bach E, Nayak A, Vishwanath A and Watrous J 2001 *Proc. 33rd Annu. ACM Symp. on the Theory of Computing* (New York: ACM) p 37
[3] Kempe J 2003 *Contemp. Phys.* **44** 307
[4] Shenvi N, Kempe J and Birgitta W K 2003 *Phys. Rev.* A **67** 052307
[5] Zähringer F, Kirchmair G, Gerritsma R, Solano E, Blatt R and Roos C F 2010 *Phys. Rev. Lett.* **104** 100503
[6] Schmitz H, Matjeschk R, Schneider Ch, Glueckert J, Enderlein M, Huber T and Schaetz T 2009 *Phys. Rev. Lett.* **103** 090504
[7] Schreiber A, Cassemiro K N, Potoček V, Gábris A, Mosley P J, Andersson E, Jex I and Silberhorn Ch 2010 *Phys. Rev. Lett.* **104** 050502
[8] Lu D, Zhu J, Zou P, Peng X, Yu Y, Zhang S, Chen Q and Du J 2010 *Phys. Rev.* A **81** 022308
[9] Broome M A, Fedrizzi A, Lanyon B P, Kassal I, Aspuru-Guzik A and White A G 2010 *Phys. Rev. Lett.* **104** 153602

[10] Konno N 2009 *Stoch. Models* **25** 28
[11] Gonulol M, Aydiner E and Mustecaplioglu O E 2009 *Phys. Rev.* A **80** 022336
[12] Kendon V 2007 *Math. Struct. Comput. Sci.* **17** 1169
[13] Shikano Y, Chisaki K, Segawa E and Konno N 2010 *Phys. Rev.* A **81** 062129
[14] Romanelli A, Siri R, Abal G, Auyuanet A and Donangelo R 2005 *Physica* A **347** 137
[15] Chandrashekar C M, Srikanth R and Banerjee S 2007 *Phys. Rev.* A **76** 022316
[16] Kendon V and Tregenna B 2003 *Phys. Rev.* A **67** 042315
[17] Whitfield J D, Rodríguez-Rosario C A and Aspuru-Guzik A 2010 *Phys. Rev.* A **81** 022323
[18] Havlin S and Ben-Avraham D 1987 *Adv. Phys.* **36** 696
[19] Weiss G H 1999 *Aspects and Applications of the Random Walk* (Amsterdam: North-Holland)
[20] Gallos L K and Argyrakis P 2001 *Phys. Rev.* E **64** 051111
[21] Anlauf J K 1984 *Phys. Rev. Lett.* **52** 1845
[22] Rosenstock H B 1970 *J. Math. Phys.* **11** 487
[23] Barkema G T, Biswas P and van Beijeren H 2001 *Phys. Rev. Lett.* **87** 170601
[24] Donsker M and Varadhan S R S 1979 *Commun. Pure Appl. Math.* **32** 721
[25] Havlin S, Weiss G H, Kiefer J E and Dishon M 1984 *J. Phys. A: Math. Gen.* **17** L347
[26] Grassberger P and Procaccia I 1982 *J. Chem. Phys.* **77** 6281
[27] Haus J W and Kehr K W 1987 *Phys. Rep.* **150** 263
[28] Lifshitz I M 1964 *Adv. Phys.* **13** 483
[29] Jayannavar A M and Köhler J 1990 *Phys. Rev.* A **41** 3391
[30] Nieuwenhuizen Th M 1989 *Phys. Rev. Lett.* **62** 357
[31] Schotland J 1988 *J. Chem. Phys.* **88** 907
[32] Parris P E 1989 *Phys. Rev.* B **40** 4928
[33] Mülken O, Blumen A, Amthor T, Giese C, Reetz-Lamour M and Weidemüler M 2007 *Phys. Rev. Lett.* **99** 090601
[34] Agliari E, Mülken O and Blumen A 2010 *Int. J. Bifurcation Chaos* **20** 271
[35] Flory P J 1971 *Principles of Polymer Chemistry* (Ithaca, NY: Cornell University Press)
[36] Aharonov D, Ambainis A, Kempe J and Vazirani U 2001 *Proc. 33rd ACM Symp. on Theory of Computing* (New York: ACM) p 50
[37] Omar Y, Paunkovic N, Sheridan L and Bose S 2006 *Phys. Rev.* A **74** 042304
[38] Goyal S K and Chandrashekar C M 2010 *J. Phys. A: Math. Theor.* **43** 235303
[39] Parris P E 1989 *Phys. Rev. Lett.* **62** 1392
[40] Phillips J C 1996 *Rep. Prog. Phys.* **59** 1133
[41] Jayannavar A M 1991 *Solid State Commun.* **77** 457
[42] Linjordet T 2009 *PhD Dissertation* Department of Physics and Engineering, Macquarie University (arXiv:1010.3784)
[43] Konno N 2002 *Quantum Inf. Proc.* **1** 345
[44] Konno N 2005 *J. Math. Soc. Japan* **57** 1179
[45] Chisaki K, Konno N, Segawa E and Shikano Y 2010 arXiv:1009.2131
[46] Shikano Y 2011 *AIP Conf. Proc.* **1327** 487
[47] Mayer K, Tichy M C, Mintert F, Konrad T and Buchleitner A 2010 arXiv:1009.5241
[48] Chandrashekar C M 2010 *Phys. Rev.* A **82** 052108
[49] Schreiber A, Cassemiro K N, Potoček V, Gábris A, Jex I and Silberhorn Ch 2011 arXiv:1101.2638
[50] Peruzzo A *et al* 2010 *Science* **329** 1500