Quantum random walk with Rydberg atoms in an optical lattice

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\textbf{Abstract.} We study the implementation of quantum random walks (QRWs) in a realistic system, an optical lattice of ultracold Rydberg atoms. The power-law nature of the dipolar interaction between Rydberg atoms influences the behaviour of QRWs. We discuss the QRW with a short-range nearest-neighbour interaction for two types of power-law interactions, the dipole–dipole and the van der Waals interaction. A specific scheme to implement a QRW using Rydberg atoms in different sites of an optical lattice is described, in which the sites are prepared using a blockade mechanism to ensure a single Rydberg atom per site.

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1. Introduction

Recent advances in quantum information [1] indicate that computational devices based on fundamental quantum principles, such as interference and entanglement [2, 3], can perform certain tasks considerably more efficiently than any classical computer. As opposed to classical information, quantum information consists of superpositions of states which can be manipulated according to the laws of quantum mechanics to produce phenomena with no classical counterpart (e.g., entanglement). The potential ramifications of computing devices based on these principles have inspired a great deal of effort aimed at determining the information processing power of such devices and possible methods for physically realizing them.

A particularly promising direction of research has focused on the development of the quantum random walk (QRW) [4]. This is an algorithmic tool appearing in quantum algorithms for element uniqueness [5, 6]. It is an attractive candidate for realization, as it is significantly less complex than general-purpose quantum computation and still has interesting applications: in particular, a QRW has been featured in a simple recent oracle algorithm with provable exponential speedups [7, 8]. Schemes to implement QRW based on ion traps [9], microwave cavities [10], ground state atoms in optical lattices [11], and linear optics [12], have only recently been proposed. Of the many systems studied to manipulate quantum information [13], neutral atoms are particularly attractive because they can have very long coherence times, and techniques to cool and trap them are well developed [14]–[16]. In addition, optical lattices allow manipulation of internal and external (position/motion) degrees of freedom, while ultracold Rydberg atoms provide strong and controllable interactions [17, 18].

In this paper, we study QRWs and their implementation in a realistic system using optical lattices and ultracold Rydberg atoms. We first give an overview of QRWs, followed by a discussion of the impact of short-range versus power-law interactions on the QRWs. Finally, we describe a scheme to implement QRWs using ultracold Rydberg atoms in optical lattices.

2. QRW: an overview

A QRW is a variation on the classical notion of a random walk in which the location of the ‘particle’ evolves in a unitary, rather than stochastic, fashion. Recent articles have shown that
QRWs can disperse more quickly than their classical counterparts and can exhibit remarkable concentration properties. In particular, it is known that the QRWs on the line and the hypercube disperse faster than the associated classical walks [19, 20]; in the case of the line, the speed-up is in fact quadratic.

2.1. QRWs with short-range interactions

As in the case of classical walks, where both discrete-time walks (such as the coin-flipping example below) and continuous-time walks (such as Brownian motion and Chapman–Kolmogorov walks) occur, QRWs come in two flavours: discrete-time QRWs and continuous-time QRWs. The first, introduced by [4, 20, 21], studies the behaviour of a ‘directed particle’, while the second, introduced in [22, 23], defines the dynamics by treating the adjacency matrix (or Laplacian) of the graph as a Hamiltonian. While the exact relationship between these models is unknown, in several important cases the walks behave similarly [19].

To illustrate the differences between classical and quantum walks, let us consider a natural discrete walk on the line. In a classical random walk (CRW), a ‘walker’ initially located at the origin flips a coin; if the result is heads, the walker steps to the right; if it is tails, to the left (assume a fair coin with equal probabilities 1/2). After repeating this procedure \( n \) times, the probability that the walker is at the position \( d \) is given by

\[
P_n(d) = 2^{-n} \binom{n}{d + n}.
\]

with the convention that this binomial coefficient is zero when \( d + n \) is not even; the standard deviation is \( \sigma_{\text{cl}} = \Theta(\sqrt{n}) \).

A possible quantum version of this walk can be obtained by replacing the coin by a qubit with internal states, say \( |0\rangle \) and \( |1\rangle \). These internal states of the walker determine the direction of movement; if it is \( |0\rangle \) (\( |1\rangle \)), the walker moves to the left (right). Consider now the Hadamard operation \( \hat{H} \) so that

\[
\hat{H}|0\rangle = \frac{1}{\sqrt{2}}|0\rangle + \frac{1}{\sqrt{2}}|1\rangle,
\]

\[
\hat{H}|1\rangle = \frac{1}{\sqrt{2}}|0\rangle - \frac{1}{\sqrt{2}}|1\rangle.
\]

Application of this operation to the qubit will serve as the quantum analogue of ‘flipping’ the coin. Note that if we apply the Hadamard operation, measure the qubit, and move accordingly, we recover the classical walk described above. If instead the system is permitted to proceed without measurement, the result is quite different. In particular, consider that at each iteration, \( \hat{H} \) is applied and then the walker shifts left and right according to the qubit, i.e., one applies the operator \( \hat{U} \equiv \hat{S}\hat{H} \), where the shift operator \( \hat{S} = e^{i\hat{P}\hat{\sigma}_z} \) is unitary, with \( \hat{P} \) and \( \hat{\sigma}_z \) being the 1-D momentum operator and the Pauli-z operator, respectively. The initial state of the system \( |\Psi_0\rangle \) becomes, after \( n \) iterations, \( |\Psi_n\rangle = (\hat{S}\hat{H})^n|\Psi_0\rangle \). Choosing \( |\Psi_0\rangle = \frac{1}{\sqrt{2}}|0\rangle + \frac{1}{\sqrt{2}}|1\rangle \) determines a distribution with a mean of zero. The main difference with the CRW resides in the standard deviation. Various analytic and numerical results reveal that it is almost independent of the choice of \( |\Psi_0\rangle \), and is approximately linear with \( n \): \( \sigma_{\text{qw}} \simeq (3/5)n \) (i.e. it disperses quadratically faster than the classical case).
The implementation framework described in section 3 relies on a continuous-time rather than discrete-time QRW. In a simple example of such a QRW on a line, the walker jumps between adjacent sites at a rate $\gamma$. Then, the Hamiltonian can simply be written as $H = -\gamma$ between adjacent sites, and zero otherwise. The time evolution follows the Schrödinger equation: $U^t = e^{itH}$ (where $U^t$ is unitary since $H$ is real and symmetric). Then, if we measure the position of the particle at time $t$, the probability of observing the walker at site $v$ is

$$P_t(v) = |\langle U^t \psi_0 | \delta_v \rangle|^2,$$

where $|\delta_v \rangle$ describes the site $v$.

### 2.2. QRWs with power-law interactions

As the physical systems we explore typically exhibit power-law couplings between distant particles, we here record the predicted behaviour of (continuous-time) QRWs on the line with power-law interactions. In particular, we consider the continuous quantum walk on the line defined by the dynamics $\psi_t = e^{-itH} \psi_0$, where $H$ is a suitable Hamiltonian and $\psi_0$ is a unit length vector in $L^2(\mathbb{Z})$. Here $L^2(\mathbb{Z})$ is the family of all functions $f: \mathbb{Z} \rightarrow \mathbb{C}$ for which $\sum_i |f(i)|^2 \leq \infty$; these functions, when $\sum_i |f(i)|^2 = 1$, are the states of the system. Thus the ‘measured distribution’ of such a walk is given by $P_t(n) = |\langle e_n, e^{-iHt} \psi_0 \rangle|^2$, where $e_n$ is the basis function $e_n(m) = \delta_{mn}$. If we make the reasonable assumption that $H$ is translation invariant, then we may represent it as an infinite matrix

$$H = \begin{pmatrix} \ddots & \ddots & \ddots & \ddots & \ddots \\ \ddots & a_0 & a_{-1} & a_{-2} & a_{-3} & \ddots \\ \ddots & a_1 & a_0 & a_{-1} & a_{-2} & \ddots \\ \ddots & a_2 & a_1 & a_0 & a_{-1} & \ddots \\ \ddots & a_3 & a_2 & a_1 & a_0 & \ddots \\ \ddots & \ddots & \ddots & \ddots & \ddots & \ddots \end{pmatrix} \tag{5}$$

with $a_{-n} = a_n$ for all $n \in \mathbb{Z}$. Recent works [24, 25] have analysed the limiting distribution of these walks, viewed on scales inversely proportional to time $t$. For the nearest neighbour walk defined by setting $a_i = \delta_{i1}$ and $\psi_0 = e_0$, Konno [24] found that, essentially, this limiting distribution is $(\pi \sqrt{1 - x^2})^{-1}$, where $x \in (-1, 1)$. Gottlieb [25] extended Konno’s result significantly, proving a convergence theorem for walks whose Hamiltonian is equal to the Fourier transform of multiplication by a differentiable function $\alpha \in \ell^2(T)$. His theorem states that, for such a walk, the distributions

$$P_t(dx) = \sum_{n \in \mathbb{Z}} P_t(n) \delta(x - n/t) \tag{6}$$

converge weakly to the distribution $P$, defined on measurable sets $X \subset \mathbb{R}$ by

$$P(X) = \frac{1}{2\pi} \int_{[\theta, -\alpha(\theta) \in X]} |\mathcal{F}_x \psi_0(\theta)|^2 \, d\theta. \tag{7}$$
Figure 1. A plot of $-\alpha'$ for $k = 3$ and $k = 6$. Also shown is the result for short-range interactions ($k \to \infty$).

Here $\delta$ denotes the Dirac distribution, and $\mathcal{F}^*$ the inverse Fourier transform. A sufficient condition for the application of this theorem is that $\sum_{n=1}^{\infty} n |a_n| < \infty$, since this implies that

$$\alpha'(\theta) = -i \sum_{n \in \mathbb{Z}} n \cdot a_n e^{i n \theta}$$

(8)

converges absolutely. We can thus, for example, apply the theorem to the walk described by letting $a_0 = 0$, $a_n = |n|^{-k}$ for constant $k > 2$, and $\psi_0 = \psi_0$. In this situation, the theorem states that the convergence distribution is defined, on measurable $X \subset \mathbb{R}$, by

$$P(X) = \frac{1}{2\pi} \left| \sum_{n \in \mathbb{Z}} e_0(n) e^{i n \theta} \right|^2 d\theta = \lambda \{ \theta : -\alpha'(\theta) \in X \},$$

(9)

where $\lambda$ is the (normalized) Lebesgue measure on the unit circle $T$. We also have

$$\alpha'(\theta) = -i \sum_{n=1}^{\infty} \frac{e^{i n \theta} - e^{-i n \theta}}{n^{k-1}} = 2 \sum_{n=1}^{\infty} \frac{\sin(n\theta)}{n^{k-1}}.$$ (10)

Using the triangle inequality, we can immediately conclude that $P$ is zero outside the finite interval $[-2\zeta(k-1), 2\zeta(k-1)]$, where $\zeta$ is the Riemann zeta-function. For $k = 3$, for example, this is the interval $[-\pi^2/3, \pi^2/3]$. As one would expect, as $k$ grows larger (and, accordingly, as the coupling between vertices decreases), the interval decays, converging in the limit to $[-2, 2]$. More information about this distribution can also be gleaned from the plots of $-\alpha'$, shown in figure 1 for $k = 3$ and $k = 6$. Observe that for the ‘nearest neighbour’ walk corresponding to short-range interactions, the Fourier transform is precisely $2 \sin \theta$, agreeing with the leading term of the sums above (i.e. for $k \to \infty$).
3. Implementation

Despite the attention by the theoretical community, the relationship between the mathematical models under current scrutiny and the behaviour of actual physical quantum diffusion processes remains largely speculative. Physical schemes to implement QRWs have only recently been proposed. They use ion traps [9], microwave cavities [10], ground state atoms in optical lattices [11], and linear optics [12]. Here, we describe a realistic scheme based on ultracold Rydberg atoms in an optical lattice. While optical lattices allow manipulation of internal and external (position/motion) degrees of freedom, ultracold Rydberg atoms provide strong and controllable interactions [17, 18].

3.1. Rydberg atoms and the blockade mechanism

Rydberg atoms are highly excited atoms that resemble hydrogen. The energy levels can be written approximately as $-1/2(n - \delta)\ell^2$, with the core electrons taken into account by the quantum defects $\delta$, where $n$ is the principal quantum number and $\ell$ is the electron orbital angular momentum. They have exaggerated properties: their radius and dipole moment $\vec{\mu}$ scale as $n^2$, while their long lifetimes $\tau_R$ scale as $n^3$ [26]. For the rubidium (Rb) 50 p ($l = 1$) state, $\tau_R = 238 \mu$s, compared to $0.026 \mu$s for the 5p state [27].

At large inter-atomic separations $R$, the interaction energy between two identical atoms depends on their states. For example, in the $ns + n'p$ or $np + n'p$ systems, it takes the form [28, 29]

$$V_{ns+n'p}(R) = -\frac{C_3}{R^3} - \frac{C_6}{R^6} - \cdots$$
$$V_{np+n'p}(R) = -\frac{C_5}{R^5} - \frac{C_6}{R^6} - \cdots$$

(11)

The coefficients depend on various multipole moments (dipole, quadrupole, etc) and on the energy differences involved [30]. If $\Delta n \equiv |n - n'| \approx 0$, then $C_3 \propto n^4$, $C_5 \propto n^8$, and $C_6 \propto n^{11}$. However, the coefficients rapidly become small as $\Delta n$ grows (the wavefunction overlap becomes negligible). Their signs and magnitudes vary substantially, and long-range potential wells or avoided crossings may exist [30, 31].

Because of their large polarizability, it is easy to Stark mix states of other $\ell$ character into a given Rydberg state with an electric field $F$. For example, the 49p state acquires one-third 49s character at $F = 3 \text{ V cm}^{-1}$ [32, 33]. Hence, two atoms $A$ and $B$, both initially in the state $np$, will acquire $ns$ character and interact to first order via dipolar interactions: $V_{\text{dip}}(R) = \mu_A \mu_B / R^3 \simeq C(F) \mu_{\text{sp}}^2 / R^3$, where $\mu_{\text{sp}} = \langle np|er|ns \rangle \propto n^2$ and $C(F)$ depends on the $\ell$-mixing. These very large $\mu$’s lead to exceptionally strong interactions, even over many tens of microns. On the other hand, interactions between Rydberg and ground-state atoms are much weaker, since $\Delta n$ is large. Similarly, interactions between two ground state atoms can be neglected. These constitute conditional interactions: atoms interact strongly only when they are both in Rydberg states.

The strong interactions between Rydberg atoms lead to the so-called blockade mechanism; in an ensemble containing many atoms and under the right conditions, no more than one can be excited into a Rydberg state. We have identified two types of blockade, namely the dipole blockade [17]), and the van der Waals (vdW) blockade [34]. The underlying principle of both mechanisms is the same; strong Rydberg–Rydberg interactions shift the energy levels. So, one atom can be resonantly excited into a Rydberg state, but additional Rydberg excitations of nearby atoms are prevented by the large shifts.

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For the vdW blockade, the shift arises mainly from the $C_6/\ell^6$ interaction scaling as $n^{11}/\ell^6$. Because of its short-range character, the blockade is effective in a limited volume which depends on $n$ and the laser bandwidth $\gamma_L$. For $n = 80$ and $\gamma_L = 1$ MHz, we conservatively estimate a blockaded volume 4.6 $\mu$m in diameter [34], sufficient to include a single site of a CO$_2$ optical lattice. Naturally, higher $n$ values will give larger volumes [34, 35].

A similar effect can be obtained using resonant interactions tuned by electric fields to produce a dipole blockade [17]; if the field is chosen to match the frequency difference between two transitions originating and terminating in levels $|np\rangle$, dipolar interactions cause a rapid ‘hopping’ of the excitation between the energy levels of two atoms. Associated with this rapid hopping (Föster process [36]) is an effective splitting of this doubly excited state: $\Delta = \sqrt{2V(R)/\hbar}$ (figure 2). When the splitting is sufficiently large, the components are shifted far away from the unperturbed atomic resonance, effectively eliminating the transition to this doubly excited state. Note that unshifted states (so-called dark states) may exist [18, 37], and that resonant interactions have been studied experimentally [38]–[40].

Both mechanisms offer advantages: the vdW blockade is always on and requires no electric field, while the dipole blockade relies on the longer range $R^{-3}$ interactions and can be turned on and off with an electric field.

3.2. QRW with Rydberg atoms

The strong interactions between Rydberg atoms could be used to study the diffusion of a given excitation (say $np$) among many sites (say all in $ns$). Contrary to the scheme of Sanders et al [10] which utilizes a single Rydberg atom, QRW in our scheme takes place in position space.
and multiple steps may take place. Furthermore, as opposed to Dür et al [11], who employ a single ground state atom and optical lattices, we use mesoscopic ensembles localized by an optical lattice. Figure 3 illustrates the principle: using the blockade mechanism, one atom in each ensemble (each containing many atoms) but one is promoted to a Rydberg state $n_s$. In the remaining ensemble, one atom is pumped into $n_p$. The $n_p$ excitation will rapidly transfer from site to site by resonant transfer, $n_A s + n_B p \rightarrow n_A p + n_B s$: the timescale will be $\tau_{\text{hop}} \sim \hbar / 4V_{\text{dip}}$ with $V_{\text{dip}} \sim n^4 / R^3$ (for $n = 70$ and $R = 25 \mu m$, $\tau_{\text{hop}} \sim 170 \text{ ns}$). After a period such that many steps have occurred, the location of the $n_p$ state is measured. By repeating this sequence, one can determine the QRW distribution function. Such implementation could verify the linear scaling of the spread with the walk duration $t$ (versus $t^{1/2}$ for a classical walk).

Consider a sample of cold $^{87}$Rb atoms loaded from a MOT (magneto-optical trap) into a 1D CO2 optical lattice, for which the trapping sites are separated by $5.3 \mu m$ [41]. Assuming that about 5 atoms can be loaded per site (all in the upper $F = 2$ hyperfine level of $^{87}$Rb), if the atom number distribution is Poissonian, only 0.7% of the sites would be unoccupied. After loading the lattice trap and turning off the MOT, untrapped atoms will fall away. For a better fractional definition of the atom separation, a more practical timescale for the steps in the quantum walk, and an easier site-selective state preparation and detection, we would then eliminate the atoms except in every fifth site (spacing $\sim 25 \mu m$). This can be accomplished with a mask (or holographic phase plate) imaged onto the lattice [42], illuminating the selected sites to transfer the atoms into $F = 1$. Atoms in all other sites could be ‘blown away’ using the cycling transition ($F = 2 \rightarrow F' = 3$). Finally, a selected single site would be transferred back into $F = 2$ (using another mask). At this point ($t_0$ in figure 3(b)), we will have a regular array of sites spaced by $26.5 \mu m$, each containing 5 atoms on average. All of the atoms will be in $F = 1$, except those at the selected site (where the ‘walker’ will start), which will be in $F = 2$.

The next step ($t_1$ in figure 3(b)) is excitation to the Rydberg states. Starting in the 5s ground state, a transition to $n_s$ requires two photons, while $n_p$ requires one (see figure 3(a)).

Figure 3. (a) Energy levels for the excitation sequence. (b) Scheme for the QRW with Rydberg atoms.
The combined requirements of rapid (<10 ns), efficient (∼100%), and high resolution (<100 MHz) excitation, could be met by using pulse-amplified, single-frequency cw light. Transform-limited pulses of light at 780 and 480 nm (near-resonant with the 5s → 5p and 5p → ns transitions, respectively) could drive the two-photon transition to ns, while light at the sum frequency (297 nm), generated by nonlinear mixing of the 780 and 480 nm pulses, could drive the one-photon transition to the np state. A key requirement for the lattice is that each of the N sites has exactly one excited atom: one in np and (N − 1) in ns. The vdW blockade mechanism will prevent multiple excitations at a given site. For example, assurance of one 70s excitation per site could be accomplished by adiabatic transfer using appropriately timed pulses [43]. This has the advantage of being very robust with respect to parameters such as intensity, pulse width, etc. For the 70p excitation, the blockade may not work perfectly. If this is the case, sites with zero or multiple excitations can be detected, and the run rejected by an error rejecting procedure described below. With the Rydberg atom array in place, the quantum walk begins. When the desired walk time τ has elapsed, we must detect where the walker ended up. Since each step will take ∼170 ns, typical walk times will be a few µs, short enough to avoid the disruptive influences of blackbody radiation and radiative decay. Redundant detection would allow error rejection. During the walk, the lattice trap must be turned off because this low-frequency radiation is actually an anti-trap for Rydberg atoms. However, the motion of the cold atoms is negligible on the timescale of the walk.

Detection commences by applying laser light at 1013 nm to selectively dump the 70s population to the 6p3/2 level, which rapidly decays (in ∼100 ns) to the 5s ground state. The 70p atom is then ionized by a ramped electric field and the ion is detected with a position-sensitive microchannel plate detector (quantum efficiency ∼50%). Ion optics magnification by a factor of 10 will allow individual sites to be resolved. Temporal resolution will allow free ions (e.g., those produced by autoionization if a multiple 70p excitation occurs) to be identified. After the 70s atoms have returned to the ground state, the lattice is turned back on and near-resonant light (with repumping) illuminates the entire sample. The resulting resonance fluorescence will allow imaging of the individual lattice sites [44]. Since the walker will have been ionized, its final location will show up as a vacancy. Meanwhile, while the walk is taking place, the ground state atoms left behind after the Rydberg excitation must be removed from the lattice. This will be accomplished by an intense standing wave at 780 nm which will rapidly transfer enough momentum to these nonparticipating atoms to cause them to leave their site. With the lattice turned back on, the imaging can be delayed to allow their exit. An important aspect of our detection scheme is that imperfect runs can be rejected. Only those runs where a single ion is detected and a single vacancy is imaged in the lattice will be considered legitimate.

4. Conclusion

We have described some of the details of a proposed experimental implementation of QRWs. In addition to the intrinsic importance of realizing QRWs for future application in quantum algorithms, the proposed scheme will also allow a study of how the long-range nature of the interaction between sites affects the characteristics of QRWs.

Several issues relevant to QRWs still need to be explored, such as the importance of sources of decoherence [45, 46] (e.g., the effect of imperfect walk lattices, of unintentional partial measurements, of non-uniform site–site interactions), or the effect of multiple walkers (e.g., two
or more $np$ atoms). Finally, the proposed scheme could be generalized to other geometries, such as 1D loops or 2D lattices, which might prove relevant to new quantum algorithms.

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