One-dimensional discrete-time quantum walk

1 Introduction

Quantum walk (QW) is the quantum analog of the classical random walk (CRW). QW is an integral part of the development of numerous quantum algorithms. Hence, an in-depth understanding of QW helps us grasp quantum algorithms. In this repository, three MATLAB codes are provided that generate the probability distribution of a CRW, QW, and QW under decoherence.

In one-dimensional QW, synonymously known as QW on a line, there are typically two degrees of freedom: the position of the walker and the coin state. The coin degree of freedom represents the internal state of the walker, often conceptualized as a quantum coin that can be in a superposition of two states (e.g., spin up and spin down). Just like with the walker's position, coherence between different states of the coin is crucial for the quantum walk to exhibit quantum behavior, such as quantum interference.

Dephasing in the coin degree of freedom can occur due to interactions with the environment or imperfections in the experimental setup. When dephasing occurs, the coherence between different coin states is lost, and the quantum behavior of the walk may degrade, resembling that of a CRW.

2 Mathematical Framework

At a given time, a particle moving in a CRW has a specific position on the integer line and a specific coin outcome. To define the quantum version of it, we attach the position and the coin outcome of the quantum particle with two suitable Hilbert spaces. Let $\mathcal{H}_{\boldsymbol{x}}$ be the Hilbert space spanned by the basis set $\{|\boldsymbol{x}\rangle\}_{x\in\mathbb{Z}}$. Further, the coin outcome has only two possible outcomes (head and tail). Hence, we can attach the outcome of the coin to a Hilbert space that spans from a basis set containing two elements. Let $\mathcal{H}_{\boldsymbol{c}}$ be the Hilbert space spanned by the basis set $\{|\mathbf{H}\rangle, |\mathbf{T}\rangle\}$. Note that the coin has two states.

By attaching the coin state and the position state of the quantum walker, to $\mathcal{H}_{\boldsymbol{c}}$ and $\mathcal{H}_{\boldsymbol{x}}$, one can represent the wave function or state $|\psi(\boldsymbol{x}, t)\rangle \in \mathcal{H}_{\boldsymbol{c}} \otimes \mathcal{H}_{\boldsymbol{x}}$ of the quantum walker at position $\boldsymbol{x}$ and time t as

$$|\boldsymbol{\psi}(\boldsymbol{x}, t)\rangle = \Big(\alpha_{\boldsymbol{x}}(t)|\mathbf{H}\rangle + \beta_{\boldsymbol{x}}(t)|\mathbf{T}\rangle\Big) \otimes |\boldsymbol{x}\rangle \tag{1}$$

where the positions state is represented by $|\boldsymbol{x}\rangle$ and the coin state is represented by the superposition of two basis states of $|\mathbf{H}\rangle$ and $|\mathbf{T}\rangle$ as

$$\alpha_{\boldsymbol{x}}(t)|\mathbf{H}\rangle + \beta_{\boldsymbol{x}}(t)|\mathbf{T}\rangle \tag{2}$$

where $\alpha_{\boldsymbol{x}}(t)$ and $\beta_{\boldsymbol{x}}(t)$ are some complex numbers known as probability amplitudes at time t. The mathematical operation $\otimes$ is known as the tensor product. Then the probability of finding the quantum walker at position $\boldsymbol{x}$ at time t can be calculated as

$$P(\boldsymbol{x}, t) = \langle \boldsymbol{\psi}(\boldsymbol{x}, t)|\boldsymbol{\psi}(\boldsymbol{x}, t)\rangle = |\alpha_{\boldsymbol{x}}(t)|^2 + |\beta_{\boldsymbol{x}}(t)|^2 \tag{3}$$

under the condition $P(\boldsymbol{x}, t) \leq 1$. Further, by adding each wave function given in Eq. (1) over the entire number line, we can find the total wave function or full state $|\boldsymbol{\psi}_t\rangle$ of the quantum walker at time t. The corresponding expression can be written as

$$|\boldsymbol{\psi}_t\rangle = \sum_{\boldsymbol{x}=-\infty}^{\infty} |\boldsymbol{\psi}(\boldsymbol{x}, t)\rangle = \sum_{\boldsymbol{x}=-\infty}^{\infty} (\alpha_{\boldsymbol{x}}(t)|\mathbf{H}\rangle + \beta_{\boldsymbol{x}}(t)|\mathbf{T}\rangle) \otimes |\boldsymbol{x}\rangle \tag{4}$$

In quantum mechanics, the time evolution of any physical process in a closed system is defined in terms of a unitary transformation that alters a given initial state $|\boldsymbol{\psi}_i\rangle$ of the system to a final state $|\boldsymbol{\psi}_f\rangle$ in a reversible manner. Thus, one needs to utilize unitary operators in describing how the state of a quantum mechanical system changes with time. Therefore, when implementing a QW, it is essential to define unitary operators that mimic the sequential processes of coin toss and shifting. The most general unitary operator that can mimic the coin toss operation for a one-dimensional QW is defined as follows

$$\mathcal{C} = \cos\theta|\mathbf{H}\rangle\langle\mathbf{H}| + e^{i\phi_1}\sin\theta|\mathbf{H}\rangle\langle\mathbf{T}| + e^{i\phi_2}\sin\theta|\mathbf{T}\rangle\langle\mathbf{H}| - e^{i(\phi_1+\phi_2)}\cos\theta|\mathbf{T}\rangle\langle\mathbf{T}| \tag{5}$$

where $\theta \in [0, 2\pi)$ and $\phi_1, \phi_2 \in [0, \pi)$. In block matrix representation, the coin operator is given by

$$\mathcal{C} = \begin{pmatrix} \cos\theta & e^{i\phi_1}\sin\theta \\ e^{i\phi_2}\sin\theta & -e^{i(\phi_1+\phi_2)}\cos\theta \end{pmatrix} \tag{6}$$

Now, let us define the unitary operator that perform the shift operation as

$$\mathcal{S} = |\mathbf{H}\rangle\langle\mathbf{H}| \otimes \left(\sum_{x=-\infty}^{\infty} |\boldsymbol{x}+\mathbf{1}\rangle\langle\boldsymbol{x}|\right) + |\mathbf{T}\rangle\langle\mathbf{T}| \otimes \left(\sum_{x=-\infty}^{\infty} |\boldsymbol{x}-\mathbf{1}\rangle\langle\boldsymbol{x}|\right) \tag{7}$$

The mathematical operation $\otimes$ is termed as a tensor product. In layman's terms, the meaning of tensor products is that the operations on each space are executed separately. An single step evolution of the QW can be written as

$$|\boldsymbol{\psi}_{t+1}\rangle = \mathcal{S}\mathcal{C}|\boldsymbol{\psi}_t\rangle \tag{8}$$

Moreover, considering (4) we can also write the state at time $t+1$ as

$$|\boldsymbol{\psi}_{t+1}\rangle = \sum_{\boldsymbol{x}=-\infty}^{\infty} \Big(\alpha_{\boldsymbol{x}}(t+1)|\mathbf{H}\rangle + \beta_{\boldsymbol{x}}(t+1)|\mathbf{T}\rangle\Big) \otimes |\boldsymbol{x}\rangle \tag{9}$$

By applying $\mathcal{S}$ and $\mathcal{C}$ on $|\boldsymbol{\psi}_t\rangle$ and comparing the coefficients with (9) we can write

$$\begin{aligned} \alpha_{\boldsymbol{x}}(k+1) &= \alpha_{\boldsymbol{x-1}}(k)\cos\theta + \beta_{\boldsymbol{x-1}}(k)e^{i\phi_1}\sin\theta \\ \beta_{\boldsymbol{x}}(k+1) &= \alpha_{\boldsymbol{x+1}}(k)e^{i\phi_2}\sin\theta - \beta_{\boldsymbol{x+1}}(k)e^{i\phi_1+\phi_2}\cos\theta \end{aligned} \tag{10}$$

The recurrence formulas in (10) are used in MATLAB codes to calculate the probability distribution of the quantum walker. In the MATLAB codes, the initial state of the quantum walker is taken as

$$|\boldsymbol{\psi}_0\rangle = |0\rangle \otimes \left(\frac{1}{\sqrt{2}}|\mathbf{H}\rangle + \frac{1}{\sqrt{2}}|\mathbf{T}\rangle\right) \tag{11}$$

Hence, $\alpha_0 = \beta_0 = \frac{1}{\sqrt{2}}$.

3 Decoherence in QWs

In this scenario, a phase retarder is applied to the coin degree of freedom of the quantum walker for sometime steps. Initially, the QW evolves for some time steps without decoherence. Afterwards, a phase retarder is applied to the coin degree of freedom. The phase retarder is given by

$$\mathcal{R} = \begin{pmatrix} e^{i\gamma} & 0 \\ 0 & e^{-i\gamma} \end{pmatrix} \tag{12}$$

where $\gamma \in [0, 2\pi]$ is a random number. The evolution of the QW is governed by

$$\begin{cases} \mathcal{SC}|\boldsymbol{\psi}_t\rangle & \text{if } 0 < t \leq step1 \\ \mathcal{SRC}|\boldsymbol{\psi}_t\rangle & \text{if } step1 < t \leq step2 \end{cases} \tag{13}$$

Note that, *total time* $= step1 + step2$.