Random walk

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1 Classical random walk - CRW

Random walk is an ubiquitous process in physics. It can be used to model particles (eg: electrons) in a medium. The goal of this section is for the readers to get familiar with classical RW. The section is organized as following. We start with the simplest classical RW, a RW in one dimension. In particular, we will learn about discrete RW and how to transform it into a continuous RW using the Taylor's approximation. We then investigate the scaling limit of the RW, i.e the mean and variance. We will not go into detail of RW in higher dimension since there are not many new important insights for this project. Nevertheless, I must remark that RW in higher dimension is has some slightly different properties compared to 1D. Finally, we will see one application of RW in solving a problem outside of physics - namely the 2-SAT problem.

1.1 Discrete CRW in 1D

Let's play a simple game. Assuming that we have a particle centered at the origin. Each turn, the particle can move the the left by 1 unit with probability p_L, or 1 unit to the right with probability p_R (with $p_L + p_R = 1$). We denote $P(d, t)$ the probability of finding the particle $d \in \mathbb{Z}$ units away from the origin after $t \in \mathbb{N}$ turns. If $d < 0$, the particle is on the left side of the origin and vice versa. Based on the description of the RW, we can write down an update rule

$$P(d, t+1) = p_R P(d-1, t) + p_L P(d+1, t) \tag{1}$$

dictates how the the probability $P(d, t)$ evolves in time with the initial condition $P(0, 0) = 1, P(d \neq 0, 0) = 0$. In the other words, Eq. (1) is simply a mathematical description of the RW in which the particle has probability $p_L(p_R)$ moving left (right) each turn.

We now ask a simple question: could we derive an analytical expression for $P(d, t)$? The answer is yes! To this end, we introduce a method called "generating function", which easily gives us the number of possible paths and their corresponding probabilities. For the RW problem in 1D, we use two dummy variables χ_L and χ_R representing the particle moves left or right accordingly. We can find all the possible paths the particle has taken after $t = T$ turns by examining the polynomial

$$(p_L \chi_L + p_R \chi_R)^T. \tag{2}$$

Why would the above polynomial contains all the information we need? For simplicity, let's set $T = 2$ and explaining what each terms mean in the polynomial. If $T = 2$, the polynomial after expanding is

$$(p_L \chi_L + p_R \chi_R)^2 = (p_L^2)\chi_L^2 + (2p_L p_R)\chi_L \chi_R + (p_R^2)\chi_R^2. \tag{3}$$

The first term $(p_L^2)\chi_L^2$ tells us that there is one way for the particle to move left two steps (due to χ_L^2) with probability p_L^2. Similarly, the third term $(p_R^2)\chi_R^2$ tells us that there is one way for the particle to move right two steps with probability p_R^2. The interesting term is the second term $(2p_L p_R)\chi_L \chi_R$ which tells us that there are two ways the particle could take one step to the left and one step to the right (i.e stay at the origin). Each way has the corresponding probability $p_L p_R$, and thus $2p_L p_R$ is the total probability that the particle still stay at the origin after $T = 2$ turns. Additionally, we note that when T is even, the particle distance d is also even and vice versa.

With the knowledge of the generating function, i.e Eq. (2), we can calculate everything the random walk. If we denote n_L (n_R) the number of steps the particle takes to the left (right) after T turns, there are some constraints, namely:

$$n_R + n_L = T, \tag{4a}$$

$$n_R - n_L = d. \tag{4b}$$

The first constraint is that the total number of steps (whether left or right) must equal the turn number T. This is expected since the particle only takes one step in a turn. The second constraint is that the distance of the particle from the origin is simply the difference between the number of right steps and left steps taken. Therefore, we can easily calculate that

$$n_R = \frac{T+d}{2}, \quad n_L = \frac{T-d}{2}. \tag{5}$$

Consequently, the probability that the particle is at distance d from the origin after T turn is

$$P(d,T) = \binom{T}{n_R} p_R^{n_R} p_L^{n_L} = \binom{T}{\frac{T+d}{2}} p_R^{\frac{T+d}{2}} p_L^{\frac{T-d}{2}}, \tag{6}$$

where we have simply substitute n_R and n_L in the generating function expansion by d and T. For simplicity, we consider symmetric random walk, namely $p_L = p_R = 0.5$. The probability $P(d,T)$ then acquires a simple form

$$P(d,T) = \binom{T}{\frac{T+d}{2}} \left(\frac{1}{2}\right)^T. \tag{7}$$

With this simple form, we can see that the mean distance of the particle from the origin after T turns is

$$\langle d \rangle = \sum_{d=-T,-T+2,\ldots}^{T} d \; P(d,T) = 0 \tag{8}$$

since d is an odd function and $P(d,T)$ is an even function (due to symmetric walk). We remind that the summation is from $-T$ to T with step size 2 since the distance d must have the same parity as T (even or odd). The mean distance $\langle d \rangle$ is zero since the particle has equal chance to move left or right each turn. Therefore, the interesting quantity is the variance $\langle d^2 \rangle$, which tells us about the dispersion of the particle

$$\langle d^2 \rangle = \sum_{d=-T,-T+2,\ldots}^{T} d^2 \; P(d,T) = T. \tag{9}$$

The meaning of this variance is that particle will mostly be in $\sqrt{\langle d^2 \rangle} = \sqrt{T}$ unit distance away. We see that the scaling of the variance $\langle d^2 \rangle$ is T (diffusive regime) instead of T^2 (ballistic regime). That is, for a random walk particle to cover the same distance as a normal particle moving in one direction, the random walk particle need T^2 time instead of T.

We have just solved the discrete version of symmetric CRW. However, we see that to solve the discrete version, we need to find $P(d,T)$ using combinatorics, which is generally difficult. However, we can translate the discrete version into continuous version and use tools such as calculus to understand behavior of the random walk. This will be done in the next subsection. However, this subsection will be presented as a control question where the readers are encouraged to solve it step by step.

1.2 Continuous CRW in 1D (controlled question)

In the continuous version, instead of advancing one unit of time and one unit of distance each turn, we advance time in dt unit and distance in dx unit. Furthermore, since we will take the limit $dx \to 0$ and $dt \to 0$, it is approriate to work with the probability density function (pdf) $\rho(x,t)$ instead of the probability $P(x,t)$ itself. They are related by the relation that the probability $P(x,t)$ of finding a particle at near position x at time t is simply $\rho(x,t)dx$. From Eq. (1), the evolution equation for the pdf is

$$\rho(x, t+dt) = p_R \; \rho(x-dx, t) + p_L \; \rho(x+dx, t). \tag{10}$$

For simplicity, we consider again the symmetric random walk ($p_L = p_R = 1/2$).

***Question**: Using the Taylor's approximation, expand $P(x,t)$ to first order in time and second order in position. We will obtain the diffusion equation*

$$\frac{\partial \rho(x,t)}{\partial t} = D\frac{\partial^2 \rho(x,t)}{\partial x^2}. \tag{11}$$

What is the diffusion constant D here in term of dx and dt?.

This is a second order PDE which can be easily solved. In the following questions, we will show how to compute the basis solution for the PDE in which the general solution (with initial condition) can be constructed from.

***Question**: Using the separation of variable ansatz, solve all possible solutions of Eq. (11).*

***Question**: Assume that originally the particle is at the origin, i.e $\rho(x,0) = \delta(x)$ where $\delta(x)$ is the dirac-delta function. Using the basis solutions found from the previous question, construct the pdf $\rho(x,t)$ at later time with the given initial condition. If everything went correctly, you should obtain that the pdf is given by a Gaussian distribution*

$$\rho(x,t) = \frac{1}{\sqrt{4\pi Dt}}\exp\Big(-\frac{x^2}{4Dt}\Big). \tag{12}$$

***Question**: From the above pdf, what is the mean $\langle d(t)\rangle$ and variance $\langle d^2(t)\rangle$ with respect to time of the particle.*

***Question**: Numerically simulate the symmetric discrete RW in 1D, where the time unit and distance unit are dt and dx correspondingly. Compare the plot with Eq. (12). Does the numerical solution of discrete RW agree with Eq. (12)? If not, could you explain why?*

1.3 One application of RW outside of physics

RW has many applications in physics. For example, it could be used to model the movement of electrons in nano-structure with impurities. or the movement of a heavy particle in fluid. However, I want to introduce an interesting application of RW outside of physics, namely the 2-SAT problem. This example is used to show the universal of RW as well as the interdisciplinary nature of science.

As you probably have learnt, there are problems that are easy to compute, and there are problems that are hard to compute. One of the classic example is the boolean satisfiability (SAT) which belongs to the set of NP-hard problems. A satisfiability formula is given by any logic gate or combination of gates that takes n bits to 1 bit. A formula is said to be satisfiable if there exists a truth assignment—a set of bit values assigned to each variable—such that the entire statement evaluates to one. The SAT problem is then deciding a formula can be satisfied. A subset of SAT formulas are those that can be written in k conjunctive normal form (k-CNF). A formula in k-CNF consists of literals defined as one of n variables or their negation, of which groups of k are combined by OR to form clauses, with m clauses combined by AND. For instance, the following example is in conjunctive normal form

$$(a \text{ OR } \neg b \text{ OR } c) \text{ AND } (\neg a \text{ OR } b \text{ OR } d). \tag{13}$$

The problem of k-satisfiability (k-SAT) consists of all SAT formulas in k-CNF. As it turns out, k-SAT is also NP-complete for $k \geq 3$. However, the 2-SAT is actually easy. In fact, it is in the problem class P. We will prove this fact by presenting a simple random walk algorithm due to Christos Papadimitriou. The algorithm is as following

- Assign an initial random values to the bits.
- While the SAT formula is unsatisfied:
- 1. Choose an unsatisfied clause at random.
- 2. Flip the value of the variable associated with a random literal in that clause

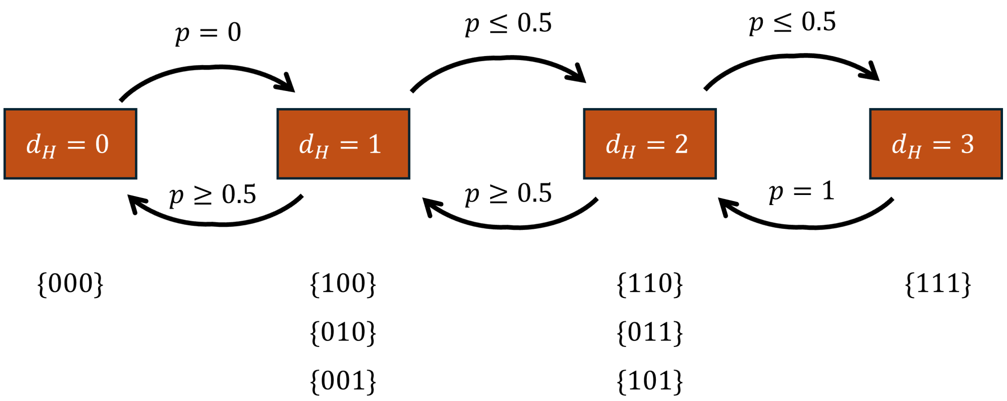

Figure 1:

To see that this algorithm is a disguised random walk, we can imagine a bit string such as $(1, 0, 1, 1)$ to be the coordinate of hypercube vertices in high dimension. As we flip one bit per turn in the algorithm, we are moving along the edges of the hybercube from one vertice to another. In fact, this is a random walk on a directed graph where the weight of each edge is dependent on the problem structure. However, in the following theorem, we will show that this algorithms will take at most $O(n^2)$ steps to complete where n is the number of bits.

Theorem: *If its formula is satisfiable, the 2-SAT algorithm given above terminates in $O(n^2)$ steps.*

Proof. In this proof, we will introduce a concept of Hamming distance. The Hamming distance between two bit strings is simply the number of places they are different. For example, the Hamming distance between the bit 101 and 110 is two. Let us say the true solution is x_0, say $x_0 = 000$. There could be multiple true solutions, but let us keep the discussion simple for now. We then group the bit strings into group according to their distances from the true solution x_0. One can visualize it as a random walk along a line in Fig. 1.

The key point is that in each turn, we have probability of at least 1/2 to move closer to the true solution. Why do we know it is at least 1/2? Because when a clause is wrong, one of its literal must have the wrong values, and there are only 2 literals per clause in the 2-SAT problem. Therefore, the probability of moving closer must be at least 1/2. We simply remark that this random walk also have some boundary condition, namely the walk will terminate if it reachs the true solution or it will be reflect perfectly if the Hamming distance is already maximum.

***Question**: Before reading the following paragraph, could you come up with an explanation for the $O(n^2)$ scaling.*

At this point, we can already intuitively the $O(n^2)$ scaling. In the worst case scenario, our initial random bit string assignment is the furthest away in term of the Hamming distance, say $x = 111$. Since this is a random walk, to travel back to the origin which is n distance away from our initial location, we need the time scale of $O(n^2)$ since we know that the (symmetric) random walk has diffusive scaling.

However, the above argument is a little bit hand-waving. We can make the above argument more concrete as following. Let's denote E_d the expected number of steps needed to reach the true solution when our current bit string x is d Hamming distance away from the true solution. Then, we can write down a recurrence relation for E_d, namely

$$E_d = \frac{E_{d-1}}{2} + \frac{E_{d+1}}{2} + 1, \quad \forall\ 0 < d < n. \tag{14}$$

and the boundary conditions

$$E_0 = 0 \tag{15a}$$

$$E_n = E_{n-1} + 1. \tag{15b}$$

***Question**: Could you explain how do we obtain the recurrence relation and the boundary conditions?*

Without going into much detail, the solution to this recurrence equation is

$$E_d = n^2 - (n-d)^2. \tag{16}$$

In the worst case, we start with a bit string x which has $d = n$ distance away from x_0, so algorithm is expected to terminate in n^2 steps. By repeating this algorithm some constant number of times, we can make the probability of failure in the case that a satisfying solution exists arbitrarily small. Then if after $O(n^2)$ steps the algorithm does not terminate, with arbitrary certainty the formula is unsatisfiable. □

The above algorithm also partly explains why the 3-SAT problem is hard. This is due to that in each turn, the probability of coming closer to the true solution is only 1/3 (instead of 1/2) where are the probability of moving further away is 2/3. Therefore, this algorithms will fail most of the time since there is a tendency to move away from the true solution. Although the above random walk algorithm for the 2-SAT problem is extremely simple, it is very efficient and many faster (and more complicated algorithms) take inspiration from this random walk algorithms. We see that the number of steps in this algorithms is the diffusive scaling limit of the symmetric classical random walk. The interesting question arise, could we have a quantum random walk that has a better scaling, i.e $O(n)$. If we do, it means that there is potentially a faster quantum algorithms that can solve this problem. This is a motivation for why quantum computer is interesting - solving some problems much faster.

2 Quantum random walk

In this section, we start with a simple example why quantum algorithms could be faster due to interference. From the example, we show how classical world and quantum world can coincide, namely due to randomized of phase. We then properly define a quantum walk in 1D. For simplicity, we will only consider the case of Hadamard quantum coin. We shall see how to solve the 1D random quantum walk using Fourier Transform. Finally, you will have the chance to read a paper discussing how we can recover classical random walk from quantum random walk.

2.1 Phase interference

In this subsection, we look back at the wave interference effect in the double slit experiment. Assume that we have two wave functions $A_1 e^{i\phi_1}$ and $A_2 e^{i\phi_2}$, where $A_i > 0$ and ϕ_i are the real-valued wave amplitudes and phases accordingly. The quantity of interest is the intensity, which is the square absolute of the wave functions. Since the two wave functions intefering with each other, the total intensity is

$$|A_1 e^{i\phi_1} + A_2 e^{i\phi_2}|^2 = |A_1|^2 + |A_2|^2 + 2A_1A_2\cos(\phi_1 - \phi_2). \tag{17}$$

Let's denote $\delta\phi = \phi_1 - \phi_2$ the phase difference between the two wave functions. If $\delta\phi = 0$ the waves constructively interference. If $\delta\phi = \pi$ the waves destructively interference. On the other hand, if light (or photon to be specific) is particle, there would be no wave interference and the total intensity is simply sum of each wave intensity, i.e

$$|A_1|^2 + |A_2|^2. \tag{18}$$

In some sense, Eq. (17) would be more "quantum"-like while Eq. (18) would be more classical-like. Although we see that quantum mechanic governs everything on the microscopic levels, why do classical mechanic still hold on larger scales? This question is interesting by itself, but we will solve a much easier question: "when do Eq. (17) and Eq. (18) coincide?". Let's say that originally, the phases of two waves are identical $\phi_1 = \phi_2$ (i.e $\delta\phi = 0$). However, due to noise from the environment or whatever other factors, the phase difference is now randomized and follows a distribution. For simplicity, we assume that the phase difference $\delta\phi$ follows the Gaussian distribution with the pdf:

$$\rho(\delta\phi) = \frac{1}{\sigma}\exp\Big[-\frac{\pi}{\sigma^2}(\delta\phi)^2\Big]. \tag{19}$$

Therefore, the expected total intensity in Eq. (17) average over the Gaussian distribution is

$$|A_1|^2 + |A_2|^2 + 2\exp\left[-\frac{\sigma^2}{4\pi}\right] A_1 A_2. \tag{20}$$

Question*: Could you derive Eq. (20)?*
Question*: Instead of a Gaussian distribution, numerically simulate other distributions that you want to try. Does the interference term decay for these new distributions?*

We see that if the phase difference $\delta\phi$ is partially randomized (or equivalently that we d o not know the phase difference with certainty), the interference term in Eq. (20) decays (exponentially). In the extreme case that the phase difference is totally randomized (the limit $\sigma \to \infty$), the interference term vanishes and Eq. (20) and Eq. (18) coincide. Physically, this means that if the phase information is unknown to us, we would see the total intensity as having no interference on average.
To recap, we see that with interference, the intensity could increase compared to the case without wave interference. The important quantity in wave interference is the phase. If the information about the phase is lost, the expected intensity result with wave interference and without wave interference are the same. We shall see soon that due to wave interference, quantum random walk could achieve the ballistic regime instead of only the diffusive regime as in classical random walk. Furthermore, if the phase information is scrambled, the quantum walk and the classical walk coincide.

2.2 Quantum random walk (QRW) in 1D

In this subsection, we will define a quantum walk in 1D. In specific, the introduced quantum walk is the coined quantum walk, which is analogous to the discrete classical walk. In the CRW, we have a classical coin to dictate how the particle will move each turn. Analogously, in the QRW, we have a quantum coin to control the movement of the particle.
To be specific, the Hilbert space of the QRW is $\mathcal{H}_d \otimes \mathcal{H}_c$, which is the tensor product between the position Hilbert space $\mathcal{H}_d$ with discrete states $\{|n\rangle\}$ ($n \in \mathbb{Z}$) and the two dimensional coin space $\mathcal{H}_c$ with state $\{|h\rangle, |t\rangle\}$ representing head and tail respectively. Therefore, the state $|\psi\rangle \in \mathcal{H}_d \otimes \mathcal{H}_c$ of the particle is spanned by

$$|\psi\rangle \in \text{span}(\{|n,h\rangle, |n,t\rangle\}). \tag{21}$$

The discrete time Schrodinger evolution equation of the particle is given by two operators $\hat{C}$ and $\hat{S}$, i.e

$$|\psi_{t+1}\rangle = \hat{S}\hat{C}|\psi_t\rangle. \tag{22}$$

The coin flip operator $\hat{C}$ acts solely on the coin space $\mathcal{H}_c$ and its action is tossing the quantum coin. The matrix representation of $\hat{C}$ in the basis $\{|h\rangle, |t\rangle\}$ is

$$\hat{C} = \begin{bmatrix} a & b \\ c & d \end{bmatrix} \tag{23}$$

where a, b, c, d are chosen such that $\hat{C}$ is a unitary operator. As a result, the actions of $\hat{C}$ on the basis states $\{|h\rangle, |t\rangle\}$ are

$$\hat{C}|h\rangle = a|h\rangle + c|t\rangle, \tag{24a}$$

$$\hat{C}|t\rangle = b|h\rangle + d|t\rangle. \tag{24b}$$

Question*: Could you explain why $\hat{C}$ need to be unitary?*
One of the common coin operator is the Hadamard coin, which is given by

$$\hat{C} = \hat{H} = \frac{1}{\sqrt{2}}\begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}. \tag{25}$$

However, the Hadamard coin operator is not unique and we can equally choosing other coins. The Hadamard coin operator is "fair" in a sense that if the initial coin state is $|h\rangle$ or $|t\rangle$, we have equal chance of measuring head or tail after an application of the Hadamard coin operator. Nevertheless, we note that, without measurement, the coin will generally be in superposition of head and tail after applications of the coin operators. It is due to the coin being in superposition that will lead to ballistic growth instead of diffusive growth as we shall see soon. On the other hand, the action of the shift operator $\hat{S}$ is

$$\hat{S}\left|n,h\right\rangle = \left|n+1,h\right\rangle, \tag{26a}$$

$$\hat{S}\left|n,t\right\rangle = \left|n-1,t\right\rangle. \tag{26b}$$

In other words, if the coin state is head, we move right by one step and vice versa. We now analyzing the asymptomatic behaviors of the quantum random walk in the large time limit. To this end, we will first convert Eq. (22) into an update rule similar to Eq. (1). Afterward, we will solve the update rule of QRW using the discrete Fourier transform. We now define the local state

$$\left|\psi(n,t)\right\rangle = \begin{pmatrix}\psi_H(n,t)\\ \psi_T(n,t)\end{pmatrix} = \psi_H(n,t)\left|H\right\rangle + \psi_T(n,t)\left|T\right\rangle \tag{27}$$

encoding the wave function of the particle at position n and time t where the coin is in the head state (through $\psi_H(n,t)$) or tail state $\psi_T(n,t)$. Therefore, after application of the Hadamard coin, the local state $\left|\psi(n,t)\right\rangle$ becomes

$$H\left|\psi(n,t)\right\rangle = \frac{1}{\sqrt{2}}\begin{bmatrix}\psi_H(n,t)+\psi_T(n,t)\\ \psi_H(n,t)-\psi_T(n,t)\end{bmatrix}. \tag{28}$$

Plugging in the shift operator, we obtain the update rule for the wave function $\psi(n,t)$, i.e

$$\psi(n,t+1) = M_+\psi(n-1,t) + M_-\psi(n+1,t), \tag{29}$$

where

$$M_+ = \begin{pmatrix}\frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}}\\ 0 & 0\end{pmatrix}, \quad M_- = \begin{pmatrix}0 & 0\\ \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}}\end{pmatrix} \tag{30}$$

are the right-moving and left moving operators accordingly. To solve this update rule, we will use the discrete Fourier transform. To motivate the usage of the discrete Fourier transform, we remember that the free wave functions $\{e^{ikx}\}$ are solutions to the spatial ODE after using the separation of variable ansatz. In the discrete Fourier transform, we define

$$\tilde{\psi}(k,t) = \frac{1}{\sqrt{2\pi}}\sum_n \psi(n,t)e^{-ink} \tag{31}$$

and the corresponding inverse transformation

$$\psi(n,t) = \frac{1}{\sqrt{2\pi}}\int_{-\pi}^{\pi}\tilde{\psi}(k,t)e^{ikn}dk. \tag{32}$$

Question: *Verify that Eq. (32) is indeed the inverse transformation of Eq. (31).*

Under the discrete Fourier transform, the update rule transform as

$$\begin{aligned}\tilde{\psi}(k,t+1) &= \frac{1}{\sqrt{2\pi}}\sum_n\Big(M_+\psi(n-1,t)+M_-\psi(n+1,t)\Big)e^{-ink}\\ &= \Big(M_+e^{-ik}+M_-e^{ik}\Big)\psi(k,t) = M_k\ \tilde{\psi}(k,t).\end{aligned} \tag{33}$$

Physically, it means that M_k is the evolution operator in the frequency space. We see that in the frequency space, the update rule of wave function is particularly simple. We can immediete read out how the wave function $\psi(k,t)$ after t turns depending on the initial conditions

$$\tilde{\psi}(k,t) = (M_k)^t\ \tilde{\psi}(k,0), \tag{34}$$

where $\tilde{\psi}(k,0)$ can be determined from the initial real space wave function $\psi(n,0)$ through Fourier transform. Hence, we only need to calculate M_k to some power and we know everything about the random quantum walk. This task can be achieved through the eigenvalue decomposition of M_k:

$$M_k = \lambda_{1,k}\left|\phi_{1,k}\right\rangle\left\langle\phi_{1,k}\right| + \lambda_{2,k}\left|\phi_{2,k}\right\rangle\left\langle\phi_{2,k}\right|, \tag{35}$$

such that

$$M_k^t = \lambda_{1,k}^t \left|\phi_{1,k}\right\rangle \left\langle\phi_{1,k}\right| + \lambda_{2,k}^t \left|\phi_{2,k}\right\rangle \left\langle\phi_{2,k}\right| \tag{36}$$

Without going too much details, the eigenvalues $\lambda_{1,k}$ and $\lambda_{2,k}$ are

$$\lambda_{1,k} = e^{i\omega_k},\ \lambda_{2,k} = e^{i(\pi-\omega_k)}, \qquad \text{where } \omega_k \in [-\frac{\pi}{2}, \frac{\pi}{2}] \text{ and } \sin(\omega_k) = \frac{\sin(k)}{\sqrt{2}}. \tag{37}$$

and their corresponding (normalized) eigenvectors

$$\phi_{1,k} = \frac{1}{\sqrt{2[(1+\cos^2(k)) + \cos(k)\sqrt{1+\cos^2(k)}]}} \begin{pmatrix} \sqrt{2}e^{i\omega_k} + e^{ik} \\ e^{ik} \end{pmatrix}, \tag{38a}$$

$$\phi_{2,k} = \frac{1}{\sqrt{2[(1+\cos^2(\pi-k)) + \cos(\pi-k)\sqrt{1+\cos^2(\pi-k)}]}} \begin{pmatrix} -\sqrt{2}e^{-i\omega_k} + e^{ik} \\ e^{ik} \end{pmatrix}. \tag{38b}$$

If we assume that the coin is initially at origin and the coin state was tail, i.e

$$\psi(0,0) = \begin{pmatrix} 0 \\ 1 \end{pmatrix}. \tag{39}$$

Consequently, the initial state $\tilde{\psi}$ in the frequency space is

$$\tilde{\psi}(k,0) = \begin{pmatrix} 0 \\ 1 \end{pmatrix}, \tag{40}$$

and we obtain the wave function in frequency space after t turns

$$\tilde{\psi}_H(k,t) = \frac{ie^{ik}}{2\sqrt{1+\cos^2 k}}(e^{-i\omega_k t} - (-1)^t e^{i\omega_k t}), \tag{41a}$$

$$\tilde{\psi}_T(k,t) = \frac{1}{2}(1 + \frac{\cos k}{\sqrt{1+\cos^2 k}})e^{-i\omega_k t} + \frac{(-1)^t}{2}(1 - \frac{\cos k}{\sqrt{1+\cos^2 k}})e^{i\omega_k t}. \tag{41b}$$

If we now inverse the Fourier transform to the real space, we will run into integral of the form

$$\psi_H(n,t) = \frac{1+(-1)^{n+t}}{2} \int_{-\pi}^{\pi} \frac{dk}{2\pi} \frac{e^{ik}}{\sqrt{1+\cos^2 k}} e^{-i(\omega_k t - kn)}, \tag{42a}$$

$$\psi_T(n,t) = \frac{1+(-1)^{n+t}}{2} \int_{-\pi}^{\pi} \frac{dk}{2\pi} (1 + \frac{\cos k}{\sqrt{1+\cos^2 k}}) e^{-i(\omega_k t - kn)}. \tag{42b}$$

These kind of integrals can be done using complex theory or the stationary phase approximation. However, for the sake of time, we will not solving these kind of integrals. The most important detail is that if we calculate the variance of the walk in the long time limit, we will see that it scales as $O(t^2)$ instead of $O(t)$ as in the classical walk.

Question: *Whew, that was a lot of analytical calculations. As we have said, calculating these integrals are tedious and not very illuminating. However, we can numerically simulate the quantum random walk. Firstly, numerically verify that the scaling of variance in quantum random walk is indeed $O(t^2)$ instead of $O(t)$. Secondly, try to change the initial coin state and see how it affects the time evolution of the random walk.*

2.3 Make a quantum walk into a classical walk: decoherence

At the start of this section, we have learnt that one of the reason of the quantum speed up is due to constructive phase interference. Furthermore, if the phase information is lost due to decoherence, we lose all the "quantumness" and everything agree with the classical calculations. This is our way to make a quantum walk into a classical walk, namely phase decoherence in the coin space.

For this subsection, we will not derive the results ourselves. Your task is to read the following paper https://journals.aps.org/pra/pdf/10.1103/PhysRevA.67.032304. Your goal is to understand the main result and how to derive it.