Discrete quantum random walk

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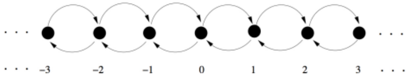
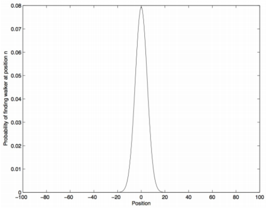
Random walks



$$\mathrm{pr}(Z_n = k | Z_0 = 0) = \begin{cases} \binom{n}{\frac{1}{2}(k+n)} p^{\frac{1}{2}(k+n)} q^{\frac{1}{2}(n-k)}, & \frac{1}{2}(k+n) \in \mathbb{N} \cup \{0\}; \\ 0, & \text{otherwise} \end{cases}$$



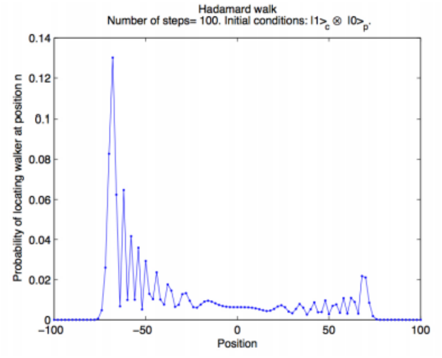
- Classical random walks(CRW) on a lattice - both lattice and time are treated discrete. Common discrete model for diffusion equation.
- In CRW, the walker tosses a coin at each time-step and takes a step forward(with prob p) or backward(prob. q) according to the outcome.
- After n steps, the probability of finding the walker at step k follows a binomial distribution as shown - with mean position $n(2p-1)$ and variance $4npq$

$$\mathbf{C}_2^{(\mathrm{H})} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} \qquad \hat{S} = |0\rangle_c\langle 0| \otimes \sum_i |i+1\rangle_p\langle i| + |1\rangle_c\langle 1| \otimes \sum_i |i-1\rangle_p\langle i|.$$

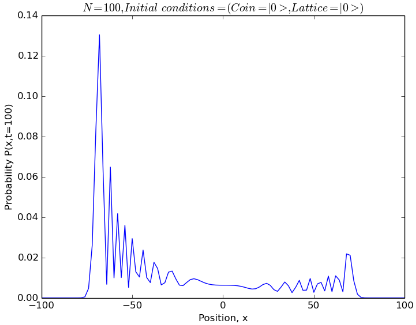
- The basic quantum random walk has two quantum systems - a 2-state quantum **coin**($\mathcal{H}_c$), and a walker on a **lattice**($\mathcal{H}_p$).
- State of system lies in direct product space ($\mathcal{H}_c \otimes \mathcal{H}_p$), most general state $|\Psi\rangle = \sum_{c=0}^{1} \sum_{x=-N}^{N} \alpha_{c,x} |c\rangle |x\rangle$
- Time-step involves two stages: 1) Toss of a coin, performed by a Hadamard($\hat{C}_c^H$) operator, 2) a conditional 'shift' operator($\hat{S}$) on the lattice-space. The operator $\hat{U} = (\hat{S})(\hat{C}_c^H \otimes \hat{I}_p)$ represents a time-step, giving $|\psi_{t+1}\rangle = \hat{U}|\psi_t\rangle$ for the time-evolution of the system.
- When implemented as arrays, dimensions of $|\Psi\rangle$, $\hat{U}$ are (2N+1) and (2N+1 $\times$ 2N+1), respectively.

$$|\Psi(t)\rangle = \begin{pmatrix} \Psi_L(x,t) \\ \Psi_R(x,t) \end{pmatrix}, \ x \in [-N, N] \qquad (1)$$

- $|\Psi(t)\rangle$ implemented as a 1d complex numpy array, $\hat{U} = \hat{S}\hat{T}$, where $\hat{T}$ is the TOSS operator, and $\hat{S}$ is the STEP operator, both 2d numpy arrays.
- $|\Psi(t+1)\rangle = \hat{U}|\Psi(t)\rangle$ is performed in each step, for three initial conditions: $|\Psi(0)\rangle = |0\rangle_c \otimes |0\rangle_p, |1\rangle_c \otimes |0\rangle_p, \frac{|0\rangle_c+|1\rangle_c}{\sqrt{2}} \otimes |0\rangle_p$. First two are biased, third case is symmetric.
- Probability of finding walker at 'x' in step 't' is $P(x,t) = |\Psi_L(x,t)|^2 + |\Psi_R(x,t)|^2$
- State is verified to be unitary at every step as a check against errors: $\sum_{x=-N}^{N} P(x,t) = 1, \ \forall t.$

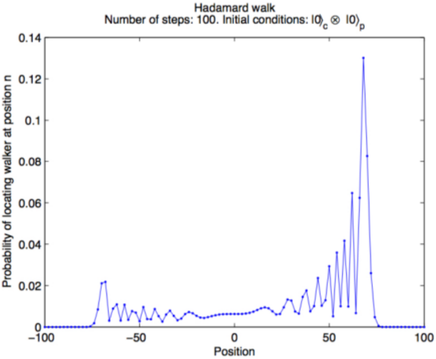


Venegas, Quant. Inf. Proc.**11**(5), (2012)



My results

Simulation results



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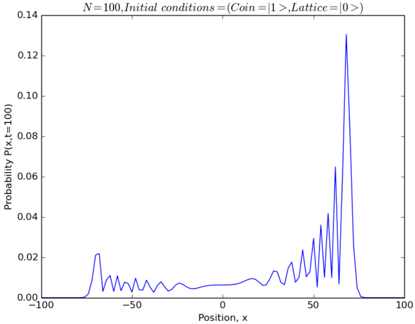

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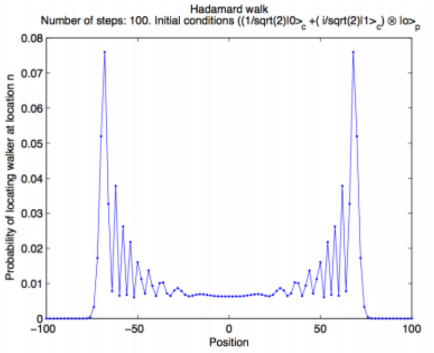
Simulation results



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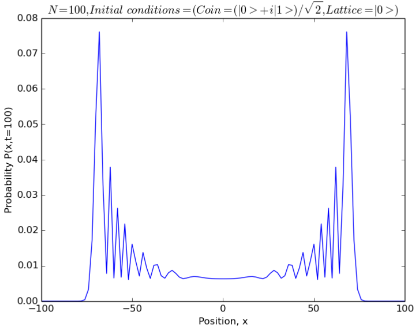


My results

- Original plan to treat Continuous Quantum Random Walk to model simulation results turned out to be too ambitious - topic not yet a closed problem.
- Followed up with a model that derives an analytic expression for P(x,t) on a discrete lattice, as discussed first in Nayak and Vishwanath, ACM-DL, Technical Report(2000).
- Start with the two-component state associated with position $|x\rangle$, $\Psi(x,t) = \begin{bmatrix} \Psi_L(x,t) \\ \Psi_R(x,t) \end{bmatrix}$, we can show that

$$\Psi(x, t+1) = \mathbf{M}_{+}\Psi(x-1, t) + \mathbf{M}_{-}\Psi(x+1, t). \tag{2}$$

- Here, $\mathbf{M}_{+} = \begin{bmatrix} 0 & 0 \\ \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} \end{bmatrix}$ and $\mathbf{M}_{-} = \begin{bmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ 0 & 0 \end{bmatrix}$ are derived from toss operator $\mathbf{C}$.

- Move to Fourier transform space for discrete spatial lattice, writing $\tilde{\Psi}(k,t) = \sum_x \Psi(x,t)e^{ikx}$. (Inverse transform would be $\Psi(x,t) = \frac{1}{2\pi}\int_{-\pi}^{\pi} \tilde{\Psi}(k,t)e^{-ikx}dk$, analogous to DTFT).
- For initial condition $\Psi(x, t=0) = \begin{bmatrix} \delta_{0x} \\ 0 \end{bmatrix}$, we require $\tilde{\Psi}(k,0) = \begin{bmatrix} 1 \\ 0 \end{bmatrix}$ $\forall k \in \mathbb{R}$.
- Applying Fourier transform in equation 2, we obtain

$$\tilde{\Psi}(k,t+1) = e^{ik}\mathbf{M}_+ \sum_x \Psi(x-1,t)e^{ik(x-1)} + e^{-ik}\mathbf{M}_- \sum_x \Psi(x+1,t)e^{ik(x+1)} \quad (3)$$

$$\tilde{\Psi}(k,t+1) = (e^{ik}\mathbf{M}_+ + e^{-ik}\mathbf{M}_-)\tilde{\Psi}(k,t) \quad (4)$$

- We obtain $\tilde{\Psi}(k,t+1) = \mathbf{M}_k\tilde{\Psi}(k,t)$, where $\mathbf{M}_k = \frac{1}{\sqrt{2}}\begin{bmatrix} e^{-ik} & e^{-ik} \\ e^{ik} & -e^{ik} \end{bmatrix}$.

  $\implies \tilde{\Psi}(k,t) = {\mathbf{M}_k}^t\tilde{\Psi}(k,0)$.
- We can compute ${\mathbf{M}_k}^t$ by diagonalizing $\mathbf{M}_k$ and thus calculate the two components $\tilde{\Psi}_L(k,t), \tilde{\Psi}_R(k,t)$.

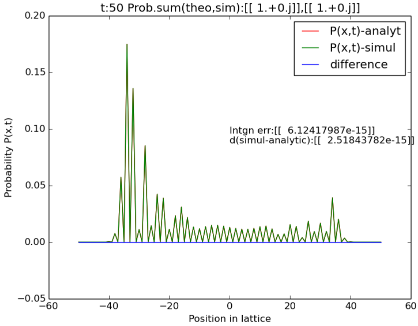
- Analytic expressions in position-space obtained by inverse Fourier transform, giving

$$\begin{aligned}\Psi_L(x,t) &= \frac{1}{2\pi}\int_{-\pi}^{\pi}\tilde{\Psi}_L(k,t)dk \\ &= (\frac{1+(-1)^{x+t}}{4\pi})\int_{-\pi}^{\pi}(1+\frac{cos(k)}{\sqrt{1+cos^2(k)}})e^{-i(\omega_k t+kx)}dk\end{aligned} \tag{5}$$

$$\begin{aligned}\Psi_R(x,t) &= \frac{1}{2\pi}\int_{-\pi}^{\pi}\tilde{\Psi}_R(k,t)dk \\ &= (\frac{1+(-1)^{x+t}}{4\pi})\int_{-\pi}^{\pi}\frac{e^{ik}}{\sqrt{1+cos^2(k)}}e^{-i(\omega_k t+kx)}dk\end{aligned} \tag{6}$$

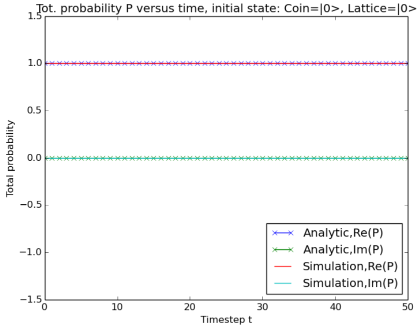
with $\omega_k \in [-\frac{\pi}{2}, \frac{\pi}{2}]$, such that $sin(\omega_k) = \frac{sin(k)}{\sqrt{2}}$.

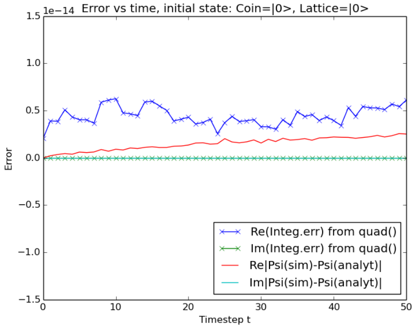
Results for the analytical treatment



- The two complex integrals 5 and 6 were split into their real and imaginary parts and integrated using numpy.quad() at each step (x,t) to obtain $|\Psi(t)\rangle$. The error of the integral output is ensured to be at the limit of precision $\approx 10^{-15}$.
- Furthermore, completeness of the state is verified at every timestep, $\sum_{x=-N}^{N} |\Psi_L(x,t)|^2 + |\Psi_R(x,t)|^2 = 1, \ \forall t.$
- The plots obtained at t=50 for an N=50 walk, with initial state $|0\rangle_c \otimes |0\rangle_p$ are shown above, along with error values.

Results for the analytical treatment





2D Quantum Walks

- Coin Hilbert-space ($\mathcal{H}_c$)now has $2 \times 2 = 4$ dimensions, basis $\{|j,k\rangle_c, j,k \in \{0,1\}\}$. Lattice Hilbert-space($\mathcal{H}_r$) has $N \times N = (2n+1)^2$ dimensions, and basis $\{|x,y\rangle_r, x,y \in \{-n,-n+1,...n-1,n\}\}$ the total problem is now $4(2n+1)^2$-dimensional.
- The state of the system at time 't' can be written as

$$|\Psi(t)\rangle = \sum_{x,y} \sum_{j,k} A_{j,k;x,y} |j,k\rangle_c |x,y\rangle_r \tag{7}$$

- The coin toss operator $\hat{C}$ can depend on the multiple ways of generating a unitary operator in 4 complex dimensions. In general, we can write its form as

$$\hat{C} = \sum_{j,k=0}^{1} \sum_{j',k'=0}^{1} C_{j,k;j',k'} |j,k\rangle_c \langle j',k'| \tag{8}$$

- The step operator $\hat{S}$ now has the action

$$\hat{S}|j,k\rangle_c |x,y\rangle_r = \hat{S}|j,k\rangle_c |x+(-1)^j, y+(-1)^k\rangle_r \tag{9}$$

on the basis of the system state.
- In order to reduce clutter and improve code readability, I abandon my approach of performing matrix products for the 2D case, using multidimensional complex numpy arrays to store states and operators instead.

2D Quantum Walks

- By using the knowledge that the Toss operator $\hat{T} = \hat{C} \otimes \hat{I}_r$, and the time-evolution operator $\hat{U} = \hat{S}\hat{T}$, we can write the probability amplitudes of the system state at time 't+1' as

$$A_{j,k,x,y}(t+1) = \sum_{j',k'=0}^{1} C_{j,k;j',k'} A_{j',k';x-(-1)^j,y-(-1)^k}(t) \tag{10}$$

- The observable of interest is once again, the occupation probability of the walker on the lattice, which is now measued as

$$P(x,y,t) = \sum_{j,k=0}^{1} |A_{j,k;x,y}(t)|^2 \tag{11}$$

In addition, we require completeness to be satisfied during system evolution, which functions as a check on the numerical accuracy of the output -

$$P_{net}(t) = \sum_{x,y=-n}^{n} \sum_{j,k=0}^{1} |A_{j,k;x,y}(t)|^2 = 1 \tag{12}$$

- We consider the classical worst-case scenario in this set of simulations too, and run the simulation only upto a maximum time of $t = n$.

- The simplest 2D coin that we can consider is the direct product of two Hadamard coins, $\hat{C}_{H,2d} = \hat{C}_{H,1d} \otimes \hat{C}_{H,1d}$, giving

$$\hat{C}_{H,2d} = \frac{1}{2}\begin{bmatrix} 1 & 1 & 1 & 1 \\ 1 & -1 & 1 & -1 \\ 1 & 1 & -1 & -1 \\ 1 & -1 & -1 & 1 \end{bmatrix} \tag{13}$$

  (Basis cycles through $|0,0\rangle_c, |0,1\rangle_c, |1,0\rangle_c, |1,1\rangle_c$ in order.)
- Since this coin can be factorized into the constituent dimensions, we expect no mixing to occur between the two coordinates during the quantum walk. The results seem to agree with our intuition.
- Initial states considered include the completely asymmetric states $|\Phi(t=0)\rangle = |0,0\rangle_c|0,0\rangle_r$(left/down), and $|1,1\rangle_c|0,0\rangle_r$(right/up), which lead to singly-peaked distributions on the lattice, which resemble 1D quantum walks at the periphery. For $n = 40$, the peaks are at $x = 26$ at $t = 40$.

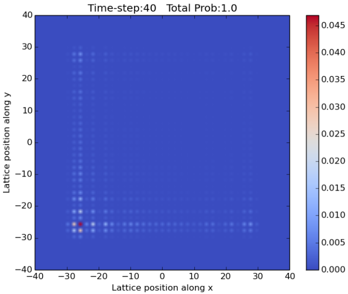
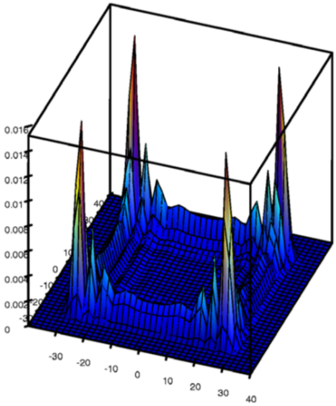


Figure : Probability distribution of a walker performing a 2D quantum Hadamard walk on a lattice of $n = 40$ at $t = 40$, for asymmetric initial conditions $|0,0\rangle_c|0,0\rangle_r(\mathit{left})$ and $|1,1\rangle_c|0,0\rangle_r(\mathit{right})$.

- The symmetric case in 2D Hadamard walk uses the initial state $|\Psi(t=0)_H\rangle = \frac{1}{2}(|0\rangle_{cx} + i|1\rangle_{cx}) \otimes (|0\rangle_{cy} + i|1\rangle_{cy}) \otimes |0,0\rangle_{r}$., and leads to a distribution with four peaks.



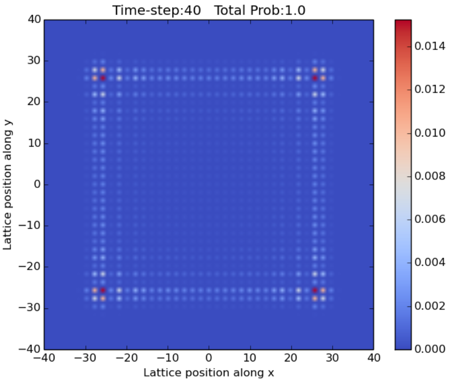


Figure : Probability distribution of a walker performing a 2D quantum Hadamard walk on a lattice of $n = 40$ at $t = 40$, for symmetric initial conditions. The first figure(left) is reproduced from Tregenna et al.[4], and the second figure is generated by the Python code.

Other 2D coin operators

- For the 1D walk, Tregenna et al[4] showed that the 1D Hadamard operator is sufficient to generate full range of unbiased evolutions in the lattice, which can be chosen by choosing different initial states.
- In the 2D case, there are many more unbiased coin operators possible, due to the SU(4) group nature of the coin operator. Choosing only unbiased coins with $+1/2$ as the leading diagonal term would lead to 640 possible unitary operators.
- Out of these, there are only 10 unique operators whose outcomes are uniquely determined with respect to all possible rotations or reflections. We have already considered one of these cases in the 2D Hadamard coin.
- Two significant other cases of interest include the Grover coin(which borrows from Grover's search algorithm) and the Fourier coin(which borrows its structure from the Discrete Fourier Transform).

- The 2D Fourier coin has the following structure -

$$\hat{C}_{F,2d} = \frac{1}{2}\begin{bmatrix} 1 & 1 & 1 & 1 \\ 1 & i & -1 & -i \\ 1 & -1 & 1 & -1 \\ 1 & -i & -1 & i \end{bmatrix} \tag{14}$$

- The symmetric case in 2D Fourier walk uses the initial state $|\Psi(t=0)_F\rangle = \frac{1}{2}\Big(|0,0\rangle_c + \frac{1-i}{2}|0,1\rangle_c + |1,0\rangle_c - \frac{1-i}{2}|1,1\rangle_c\Big) \otimes |0,0\rangle_r$., which leads to a distribution which is maximally spread along one axis, and a tad less spread on the other axis.
- The 2D Grover coin has the following structure -

$$\hat{C}_{G,2d} = \frac{1}{2}\begin{bmatrix} 1- & 1 & 1 & 1 \\ 1 & -1 & 1 & 1 \\ 1 & 1 & -1 & 1 \\ 1 & 1 & 1 & -1 \end{bmatrix} \tag{15}$$

- The maximally symmetric case in 2D Grover walk uses the initial state $|\Psi(t=0)_G\rangle = \frac{1}{2}\Big(|0,0\rangle_c - |0,1\rangle_c - |1,0\rangle_c + |1,1\rangle_c\Big) \otimes |0,0\rangle_r$., which leads to a distribution which is maximally spread along both the axes.

- The Fourier walk hits the lattice boundary along one of the axes! Position varies roughly as $\mathbb{O}(t)$ along this axis.
- Rotation symmetry of 180^o about the lattice center.

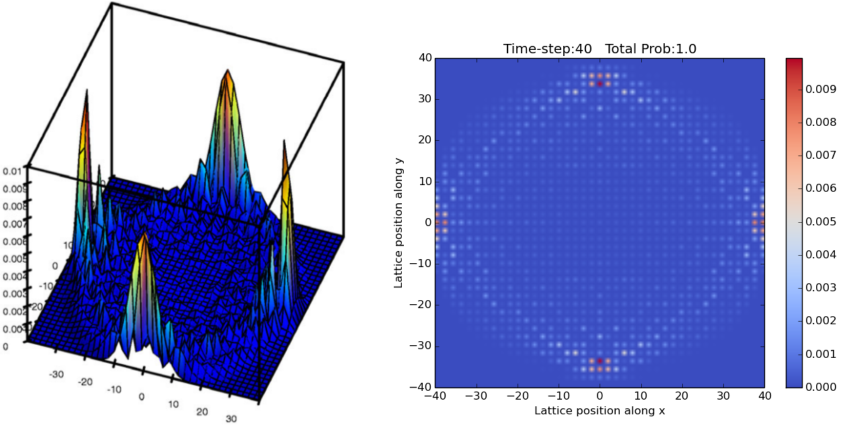
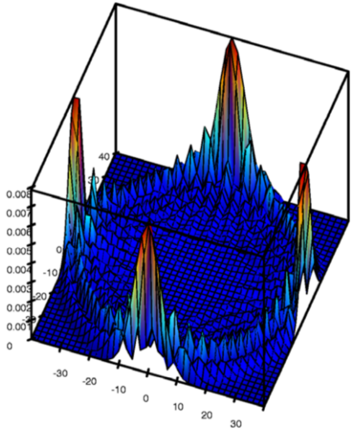


Figure : Probability distribution of a walker performing a 2D quantum Fourier walk on a lattice of $n = 40$ at $t = 40$, for symmetric initial conditions. The first figure(left) is reproduced from Tregenna et al.[4], and the second figure is generated by the Python code.

- The Grover walk hits the lattice boundary along both the axes, position $\approx \mathbb{O}(t)$.
- Rotation symmetry of 90^o about the lattice center.



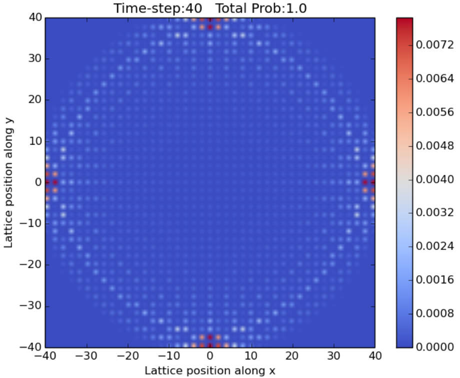


Figure : Probability distribution of a walker performing a 2D quantum Grover walk on a lattice of $n = 40$ at $t = 40$, for symmetric initial conditions. The first figure(left) is reproduced from Tregenna et al.[4], and the second figure is generated by the Python code.

2D Grover Walk with Hadamard initial conditions

- The Grover walk with $|\Psi(t=0)_H\rangle$ has a distribution sharply peaked at the origin, with $P(x=0, y=0) > 0.3$ even at $t = 40$, minimal spreading along the lattice.
- Grover walk is very customizable depending on the initial state chosen.

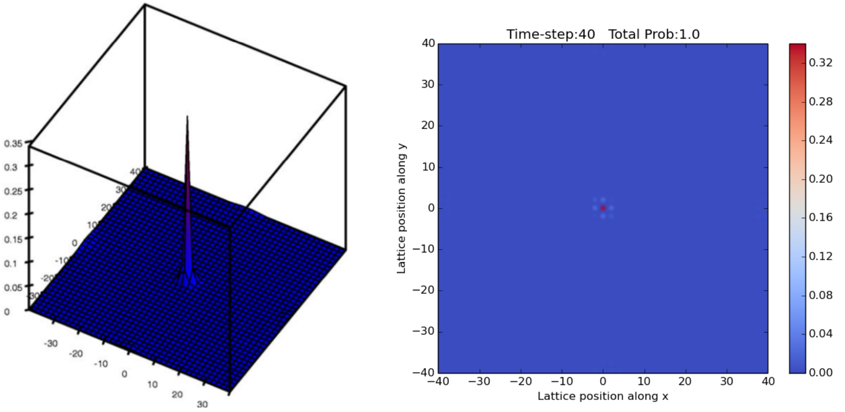


Figure : Probability distribution of a walker performing a 2D quantum Grover walk on a lattice of $n = 40$ at $t = 40$, for Hadamard-symmetric initial conditions. The first figure(left) is reproduced from Tregenna et al.[4], and the second figure is generated by the Python code.

References

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