Confined Quantum Walk

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1 Problem Statement

We have seen that for a classical random walk, the distance wrt (with respect to) time of a particle scales as $D \sim \sqrt{t}$. We can also define a quantum version of the classical random walk. We have seen that for a 1D quantum random walk, it turns out that the particle variance distance from the origin scales as $D \sim t$, corresponding to a quadratic speed up over a classical random walk. In this project, we will investigate a more interesting case, in which the quantum particle is entirely confined in a small region of space.

a) We consider a Creutz ladder that extends from $-\infty$ to ∞. By threading a magnetic field through the lattice, we can modify the hopping amplitude (up to a gauge transformation). The result lattice is given in Fig. 1. The Hamiltonian

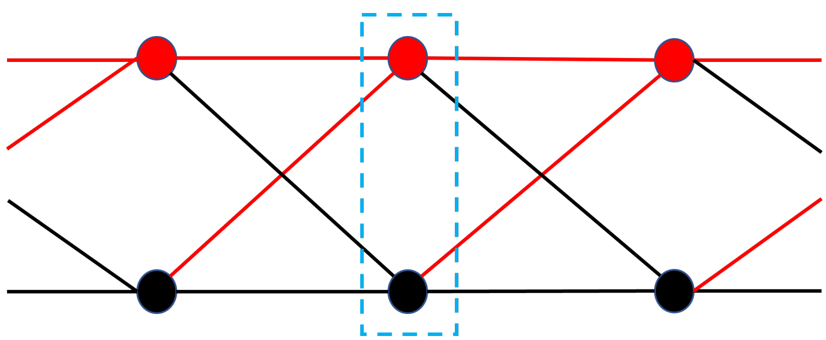

Figure 1: Creutz ladder with threading magnetic field with reduced flux per plaque $\Phi/\Phi_0 = 1/2$. The red edge has hopping amplitude -1 and the black edge has hopping amplitude 1. The blue-dashed square is a unit cell of the ladder. Each cell has two sites/orbitals (red site and black site)

of the system is given by

$$\hat{\mathcal{H}}_{\text{Creutz}} = \sum_j \left[\left(\hat{c}^\dagger_{j+1,r} \hat{c}_{j,r} - \hat{c}^\dagger_{j+1,b} \hat{c}_{j,b} \right) + \left(\hat{c}^\dagger_{j+1,r} \hat{c}_{j,b} - \hat{c}^\dagger_{j+1,b} \hat{c}_{j,r} \right) + \text{ H.c. } \right], \tag{1}$$

where H.c. means taking Hermitian conjugate of the previous written terms. Performing the Fourier Transform on the creation and annihilation operators

$$\hat{c}_{k,r/b} = \frac{1}{\sqrt{2\pi}} \sum_{j} e^{-ikj} \hat{c}_{j,r/b} \tag{2}$$

the Hamiltonian $\hat{H}_{Creutz}$ can be rewrite it as

$$\hat{H}_{Creutz} = \int_{-\pi}^{\pi} dk \begin{bmatrix} \hat{c}^{\dagger}_{k,r} & \hat{c}^{\dagger}_{k,b} \end{bmatrix} H(k) \begin{bmatrix} \hat{c}_{k,r} \\ \hat{c}_{k,b} \end{bmatrix}. \tag{3}$$

The 2×2 matrix $H(k)$ is called the Bloch-Hamiltonian. Could you find the analytical form of $H(k)$, its eigenvalues $\lambda_n(k)$ (n is the band index, which is just 1 or 2 since we only have two orbitals per unit sites) and the corresponding eigenfunctions $|g_n(k)\rangle$?

b) If you do the previous question correctly, you should find that the eigenvalues $\lambda_n(k)$ are independent of the momentum vector k. This property is called flat band energy, and it turns out to be critical. We can define the Wannier functions $|w_n(j)\rangle$ (j is the index of the unit cell) which are the Fourier Transform of the Bloch functions $|g_n(\boldsymbol{k})\rangle$ ($n = 1, 2$).

$$|w_n(j)\rangle = \frac{1}{\sqrt{2\pi}} \int_{-\pi}^{\pi} dk \ e^{ik.j} \, |g_n(k)\rangle \tag{4}$$

Is the Wannier function localized or extended over all the lattice? Is the Wannier function eigenstate of the Hamiltonian?

Comment: Since the energy band is flat, it means that the Wannier functions $|w_n(j)\rangle$ are also the eigenstates of the Hamiltonian. This property implies that if the Wannier function is localized, the electrons will also be localized on the Creutz ladder. In fact, the Creutz ladder is one of the toy model for topological insulator. For this project, we will see whether the localization property of the Creutz ladder still holds when we have a quantum walk particle on it.

c.1) To simulate the quantum random walk, we introduce a coin operator C (to simulate the coin toss) and a shifting operator S. Thus, the space of the quantum system consisting of the coin space and the lattice space. For the Creutz-ladder, we can model the coin space and lattice space as in the below figure (again it is extended from $-\infty$ to ∞).

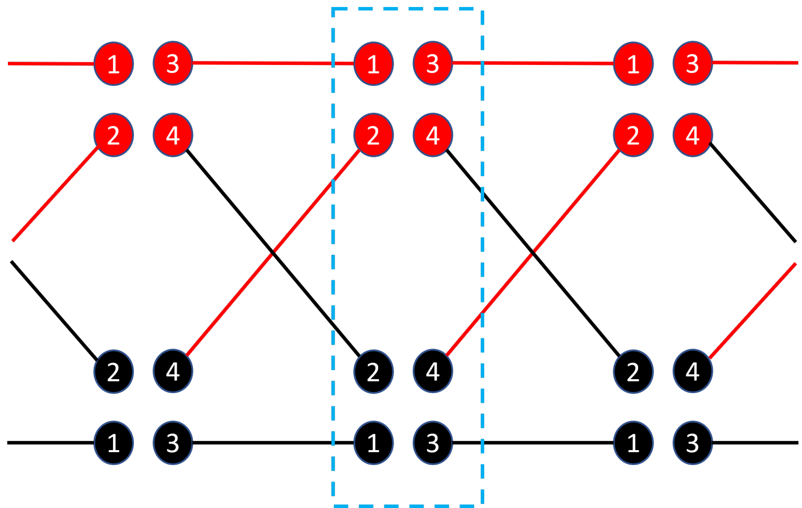

Figure 2: We incorporate the coin space into the lattice space by introducing additional sites/orbitals per unit cell. Since each red/black site in the original Creutz-ladder has 4 edges, the dimension of the coin space for each red/black site is 4. Again, the blue square depicting a unit cell in the coin-lattice space.

Given an initial state $|\psi_0\rangle$, the state of the system after T time steps is given by

$$|\psi_T\rangle = W^T |\psi_0\rangle , \quad W = SC \tag{5}$$

For this problem, we model the coin flip opreator C using the Grover G_4 coin since it is symmetric wrt to all coin states

$$G_4 = \frac{1}{2}\begin{bmatrix} -1 & 1 & 1 & 1 \\ 1 & -1 & 1 & 1 \\ 1 & 1 & -1 & 1 \\ 1 & 1 & 1 & -1 \end{bmatrix}, \quad C = \mathrm{Id} \otimes \mathrm{G}_4 \tag{6}$$

where the first subspace corresponds to the real space lattice and G_4 corresponds to the coin space. The shifting operator is given by

$$\begin{aligned} S = \sum_i \Big(& - |i-1, 3R\rangle \langle i, 1R| - |i+1, 1R\rangle \langle i, 3R| - |i-1, 4B\rangle \langle i, 2R| \\ & + |i+1, 2B\rangle \langle i, 4R| + |i-1, 3B\rangle \langle i, 1B| + |i+1, 1B\rangle \langle i, 3B| \\ & + |i-1, 4R\rangle \langle i, 2B| - |i+1, 2R\rangle \langle i, 4B| \Big). \end{aligned} \tag{7}$$

where, for instance, the state $|i, 3R\rangle$ describing that the drunkard walker is located at the red orbital of the i-th unit cell, and the coin state is 3. Following part a) + b), we want to see if the "Bloch energy" of the operator W is flat or not. Performing Fourier transform of operator W and find the eigenvalues of it

(also called quasi-energy).
c.2) The existence of flat bands does not guarantee that the particle will be localized. Numerically check that if the particle is at the origin at $T = 0$, the particle will never be 3 unit cells away from the origin.
d) We will now prove the above fact analytically using a combinatorial approach. Denoting $|\psi_n, t\rangle$ the amplitude vector of finding the particle in n-th unit cell at time t, we can write a master equation for the time evolution of the particle

$$|\psi_n, t+1\rangle = F\,|\psi_{n-1}, t\rangle + B\,|\psi_{n+1}, t\rangle \tag{8}$$

Find the expression of the forward and the backward operator F and B. If the particle is initially in the unit cell 0 at time t=0, how do you calculate the local wave function $|\psi_3, t = 3\rangle$ of the particle at 3-th unit cell at time step $t = 3$?
e) To analyze the property of operators F and B, we can use Jordan decomposition since

$$F^m \sim J_F^m \quad B^n \sim J_B^n. \tag{9}$$

Finding the Jordan matrices J_F and J_B. Are they equal? What does that imply? Show that $J_F^4 = J_B^F = J^4 = 0$.
f) If we have $J^4 = 0$, it implies that $J^{m \geq 4} = 0$ or equivalently $F^{m \geq 4} = B^{n \geq 4} = 0$. This properties hints that the particle can never be more than 3 unit-cell away from the origin. We will now focus on only even time step T. For even time step, the master equation can be generated from the set

$$\{FF, FB, BF, BB\} \tag{10}$$

As we have seen before $(FF)(FF) = (BB)(BB) = 0$, thus we should investigate the algebra between these generators. Form a table of product between the above generators, what products are vanishing?
g) Now, consider $t \geq 4$. A possible generator sequence could be

$$(FF)(FB)(BF)(FF)\ldots \tag{11}$$

We denote n_F the total power of the F operator and n_B the total power of the B operator. For example for the sequence $(FF)(BF)$ has $n_F = 3$ and $n_B = 1$. We focus on a sequence in which $n_F - n_B \geq 4$, i.e. the electron is more than 4 unit cells from the origin on the right-hand side. Prove that any sequence with $n_F - n_B \geq 4$ equals zero using the table above. What does this result mean?