Full-Stack Quantum Computing

1 Quantum Tunneling

Quantum tunneling refers to the effect that microscopic particles have a chance of going through a region with higher potentials. In this problem, we are going to explore the mathematical formalism that makes quantum tunneling possible.

(a) Consider the 1D time independent Schrodinger's Equation

$$-\frac{\hbar}{2m}\frac{d^2\psi(x)}{dx^2} + V(x)\psi(x) = E\psi(x)$$

Show that the ansatz $\psi(x) = Ae^{-ikx} + Be^{ikx}$ is a solution to this equation. What's k? You can think of the two components as the parts of the wave moving to the right vs moving to the left.

(b) Consider a potential where

$$V(x) = \begin{cases} V_0, & \text{if } 0 < x < L \\ 0, & \text{if } x < 0 \text{ or } L < x \end{cases} \tag{1}$$

Sketch the potential, and write down the generalized wave functions for the following:

i. $x < 0$

ii. $0 < x < L$

iii. $L < x$

Hint: it should look like $Ae^{ik_1x} + Be^{-ik_1x}$ for region i, and $Ce^{k_2x} + De^{-k_2x}$ for region ii.

(c) Consider now that we are shooting a particle from left to right (x is increasing). In this case, you can set the coefficient of the left moving component to be 0 in region 3. Consider the fact that wave functions need to be continuous. Write down boundary conditions at 0 and L.

(d) Use the boundary conditions at L to determine the relationship between C and D. In particular, find $\frac{|C|}{|D|}$, and discuss under what kind of condition can we get $|C| >> |D|$ and approximate D to 0.

(e) Take the approximation that D is 0, and find the reflection coefficient defined as $\frac{|B|^2}{|A|^2}$. In classical cases, we would expect the reflection coefficient to be 1, since when we throw a ball at the wall, it's always going to bounce back. Show that in this case, the reflection coefficient is less than 1. Explain what's happening.

(f) Sketch qualitatively the wave function in all three regions.

2 Hermitian and Unitary

In class we covered that a Hermitian H and a Unitary U are defined as

$$H = H^\dagger \qquad UU^\dagger = I$$

Where dagger $A^\dagger$ denotes the complex conjugate transpose of a matrix

$$A^\dagger = \overline{A^\top}$$

(a) Show the following matrices are Hermitian and Unitary using the definitions above

$$X = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \qquad Y = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix} \qquad Z = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} \qquad H = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}$$

(b) Compute the eigenvalue decomposition of $X = V \Lambda V^{-1}$. Can you represent the decomposition components V and Λ using only matrices we defined above?