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Quantum Simulation of Schrödinger Equation using Qiskit Framework

Project

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Introduction

Why Quantum simulation?

- Initial idea was proposed by Feynman in his 1982 paper "Simulating Physics with Computers"
- Idea of a non-Turing machine that would simulate quantum systems (i.e., quantum computer)
- Simulation of quantum many-body problems on a classical computer is a difficult task.
- Size of the Hilbert space of the sytem grows exponentially with the no. of particles.

- For example, consider simulating a system of n spin-1/2 particles
- Size of the Hilbert space grows as 2^n
  - For classical simulation, no. of bits required $= 2^n$
  - For quantum simulation, no. of qubits required $= n$
- As noted by Feynman, growth in memory requirement is only linear on a quantum computer.
- Of course this is only true if we can design a quantum algorithm to extract information efficiently.
- In an actual quantum computer, we would need more than n qubits to account for noise and error correction.

Quantum Simulation: Approach and Software used

Software

- We have used IBM's Qiskit library for our project.
- Qiskit has many quantum computer simulators, two among them are:
  - Statevector simulator
  - Quantum Assembly Language Simulator (QASM)
- Statevector simulator assumes an ideal quantum computer with no noise, which gives an ideal output for a circuit.
- QASM, on the other hand, attempts to mimic a quantum computer by adding little noise to the result.
- QASM operates by running the circuit multiple times and storing the no. of times an outcome has occurred.

Approach

- We have used both the statevector simulator and QASM simulator for our project.
- The result for a given quantum circuit can be then visualized by plotting a histogram.
- We have performed 6-qubit simulations for a single particle quantum system in different exactly solvable potentials, namely:
  - Free particle
  - Infinite square well potential
  - Quantum tunneling across Barrier potential
  - Simple Harmonic Oscillator potential
- In addition to this, we have performed simulation of an interacting two-particle system in an infinite square well potential.

Quantum Simulation of Schrödinger Equation

Quantum simulations

- The goal is to model single-particle quantum systems using quantum computing.
- There are two primary parts to the simulation process:
  - Initializing the Wavefunction: The first stage is to initialize the wavefunction, which is the quantum system's initial state.
  - The second phase involves creating and putting into practice a time-evolution algorithm that can precisely evolve the wavefunction over time.
  - The noncommutativity of the Hamiltonian operators a feature of quantum systems must be handled by this technique.
- By changing V we have simulated for free particle, particle in a box, Quantum tunneling, SHO and two particle potential.

Schrödinger Equation

- The time dependent Schrödinger Equation is given by:

$$H|\psi(t)\rangle = i\hbar\frac{\partial}{\partial t}|\psi(t)\rangle$$

- Solving this differential equation yields:

$$|\psi(t)\rangle = e^{-iHt}|\psi_{\text{init}}\rangle$$

- Since the Hamiltonian encompasses the total energy of the system, it can be expressed as $H = K + V$, where K and V denote the operators for kinetic and potential energies, respectively. It's worth noting, however, that V and K do not commute, implying that $e^{V+K} \neq e^{V}e^{K}$, which complicates the simulation of the system.

Discretization of Variables

- We must first discretize the continuous variables x and t. Consider the motion inside a finite region $-d \leq x \leq d$. Then, we can decompose this region into 2^n intervals of length $\Delta = 2d/2^n$ and represent these intervals by means of the Hilbert space of an n-qubit quantum register.
- The wave function is approximated as follows:

$$\tilde{\psi}(t) = \frac{1}{\aleph} \sum_{i=0}^{2^n-1} \psi(x_i, t)|i\rangle$$

where

$$x_i = -d + (i + \frac{1}{2})\Delta$$

and

$$\aleph = \sqrt{\sum_{i=0}^{2^n-1} |\psi(x_i, t)|^2}$$

Trotter Decomposition

- The Schrödinger equation may be integrated by propagating the initial wave function for each time step ϵ as follows:

$$\psi(x, t+\epsilon) = e^{\frac{-i}{\hbar}[H_0+V(x)]\epsilon}\psi(x, t)$$

- The Lie-Trotter formula is given by:

$$\lim_{n\to\infty}\left(e^{A\frac{t}{n}}e^{B\frac{t}{n}}\right)^n = e^{(A+B)t}$$

- If the time step is small enough, we may write:

$$e^{\frac{-i}{\hbar}[H_0+V(x)]\epsilon} = e^{-\frac{i}{\hbar}H_0\epsilon}e^{-\frac{i}{\hbar}V(x)\epsilon}$$

Final Algorithm

- We now consider the momentum k, variable conjugate to x, i.e. $-i(d/dx) = F^{-1}kF$
- The first operator (kinetic energy part may be written as:

$$e^{-\frac{i}{\hbar}H_0\epsilon} = F^{-1}e^{\frac{i}{\hbar}(\frac{\hbar^2k^2}{2m})\epsilon}F$$

- Thus, the final wave function after time t=lϵ obtained from the initial wave function is given by applying the following unitary operator l times:

$$F^{-1}e^{\frac{i}{\hbar}(\frac{\hbar^2k^2}{2m})\epsilon}Fe^{-\frac{i}{\hbar}V(x)\epsilon}$$

Final Algorithm

Below is the final simulation algorithm we arrive at after combining everything discussed above. The time evolution operator is given by:

$$|\psi(t)\rangle = F^{-1} \exp\left(-\frac{i}{\hbar}\frac{p^2}{2m}\Delta t\right) F \exp\left(-\frac{i}{\hbar}V(x)\Delta t\right) |\psi_{\text{init}}\rangle$$

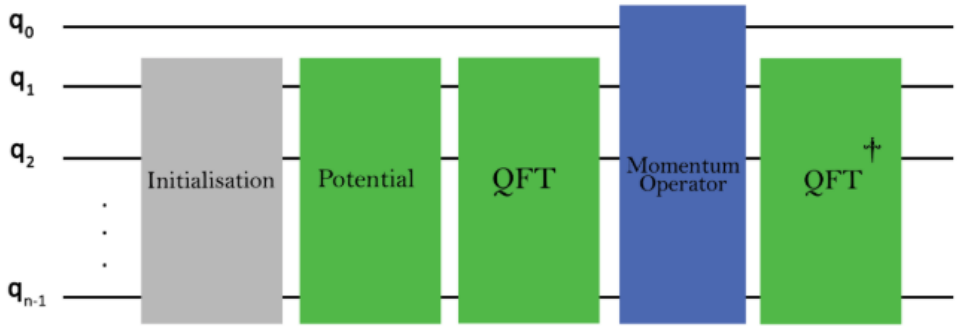


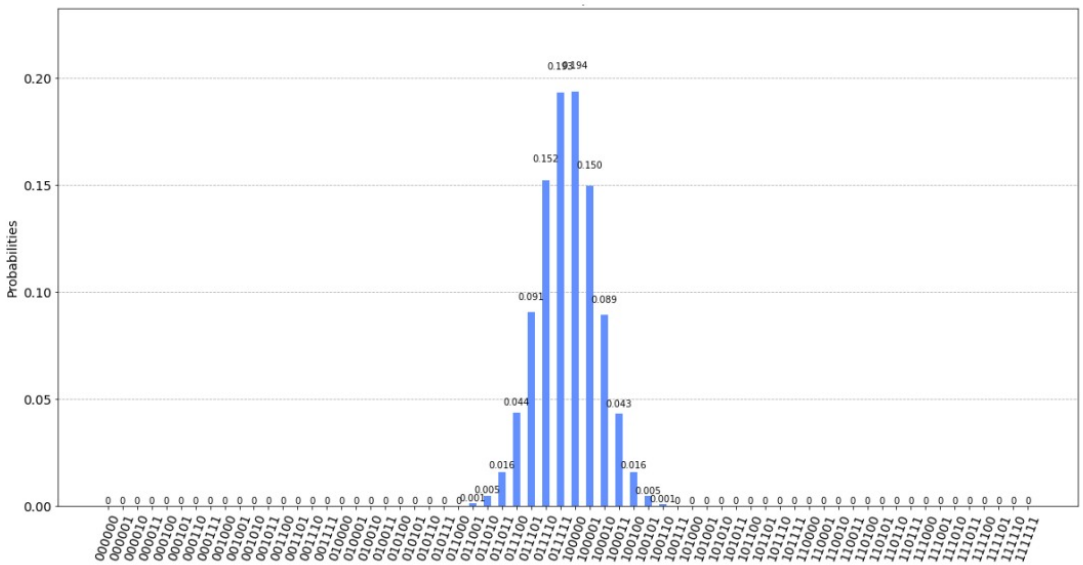
Figura 1: Quantum circuit representation of the time evolution operator for a single time step

Results

Free Particle

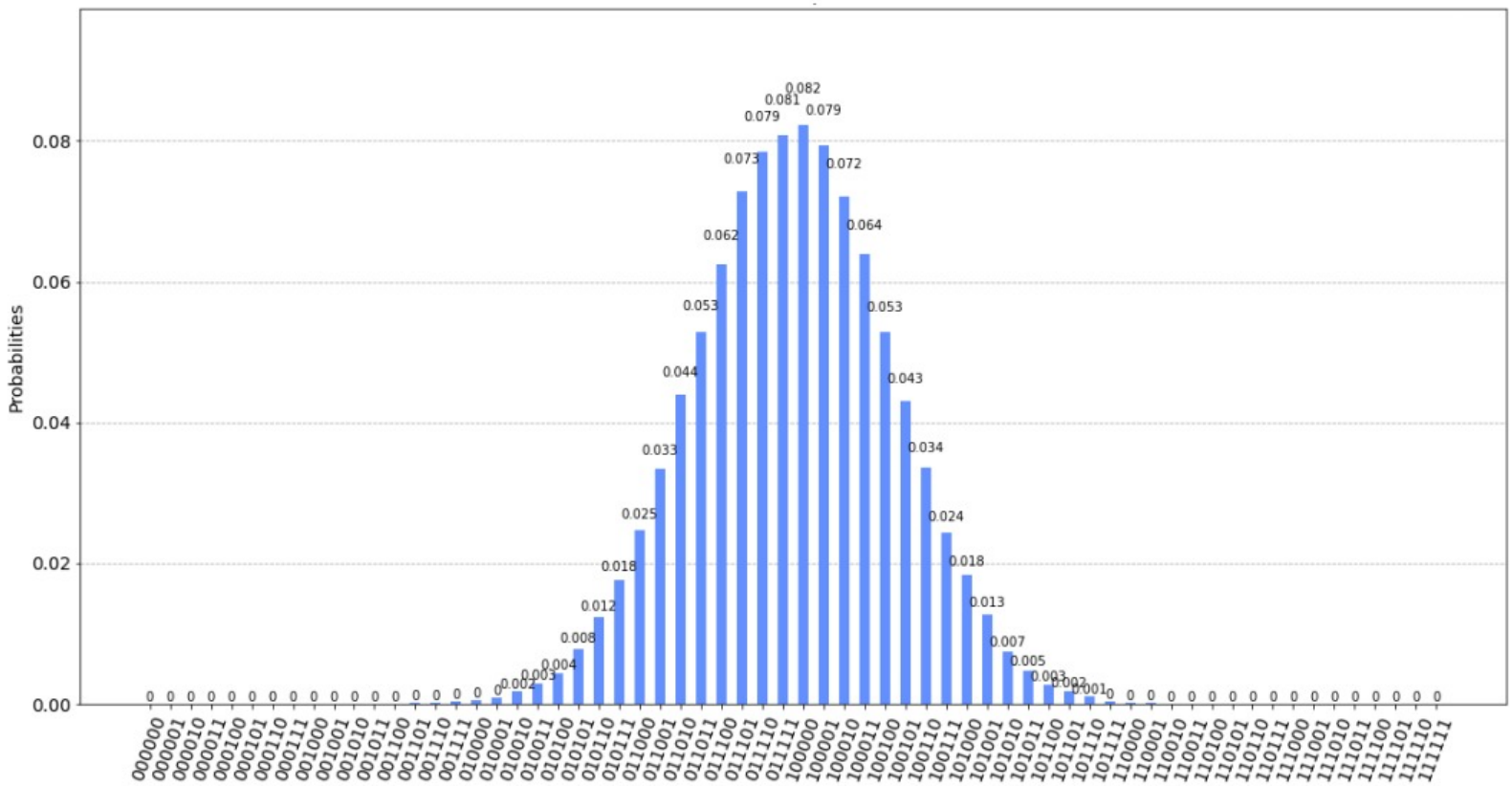
V = 0, We start by initializing Gaussian wave packet

$$|\psi(x)\rangle = \frac{1}{\sigma\sqrt{2\pi}} e^{-\frac{1}{2}\left(\frac{x-\mu}{\sigma}\right)^2},$$



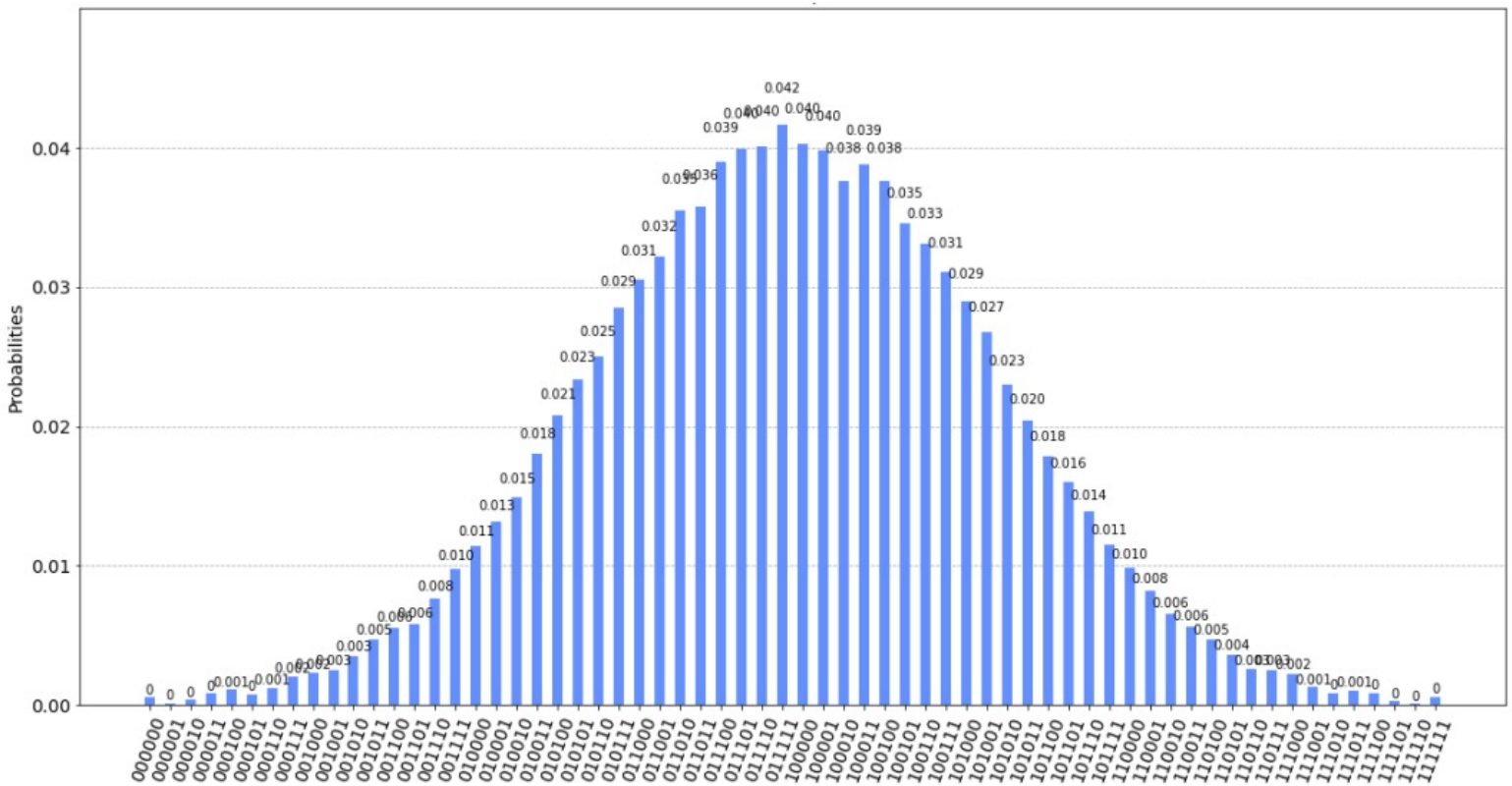
Initialisation, t=0 : Initial Wave packet

Free Particle



After 1st iteration, t=1 : Slightly Spread out

Free Particle



After 8th iteration, t=8 : Spread out increases with time as expected

Particle in Infinite potential well

We need to solve,

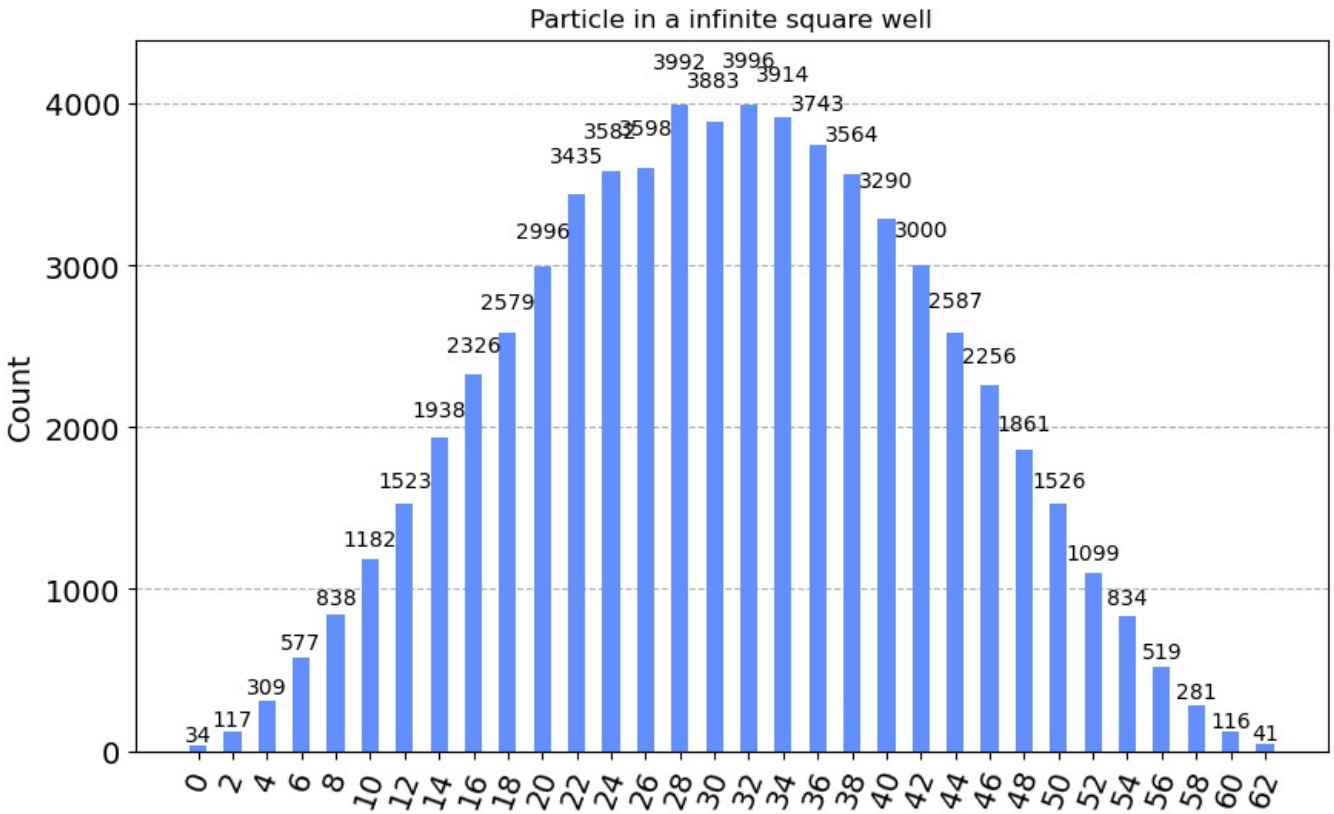
$$\left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}+V(x)\right)\varphi_E(x)=E\varphi_E(x),$$

$$V(x)=\begin{cases}\infty, & x<0\\ 0, & 0<x<L\\ \infty, & x>L.\end{cases}$$

Solution is

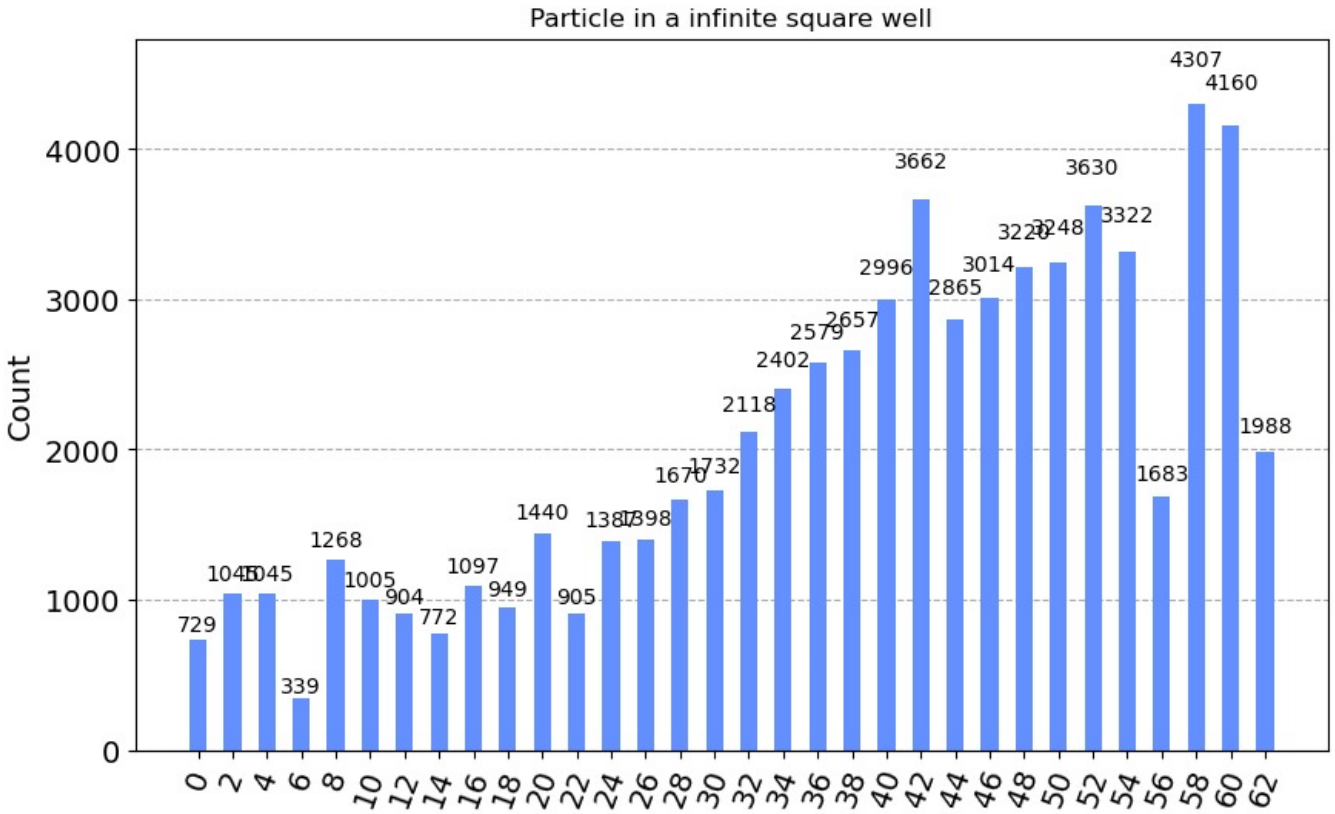
$$\varphi(x)=\sqrt{\frac{2}{L}}sin(\frac{n\pi x}{L}), \qquad n=1,2,3,...$$

Particle in Infinite potential well



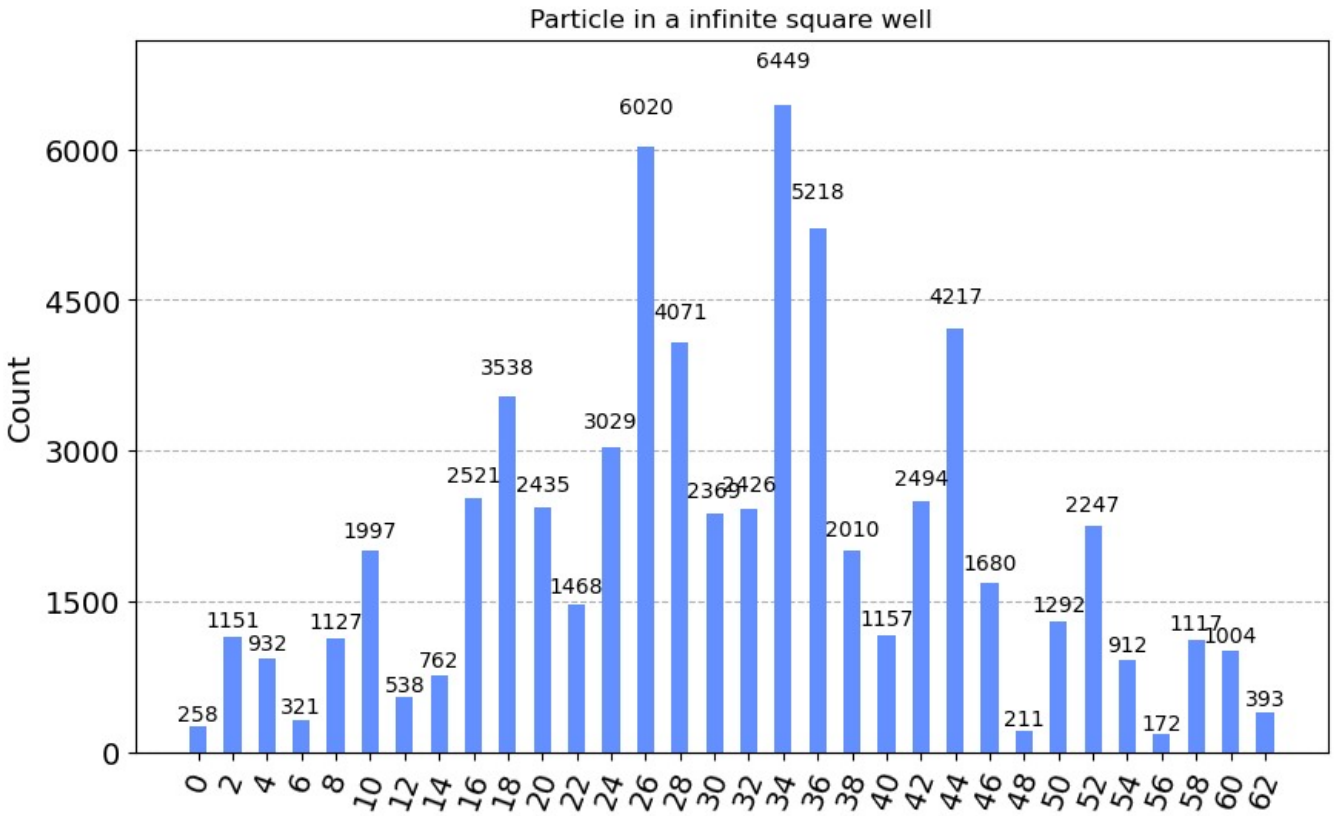
Initialisation, t=0 : Initial Wave packet

Particle in Infinite potential well



After 3rd iteration, t=3 : Wave bounces of the boundary as expected

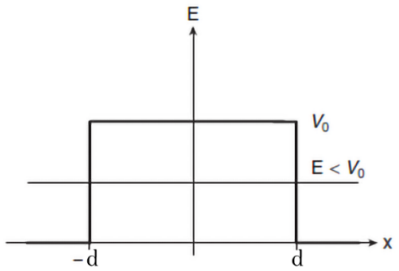
Particle in Infinite potential well

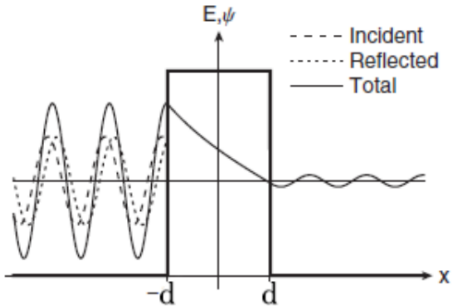


After 7th iteration, t=7

Quantum Tunneling

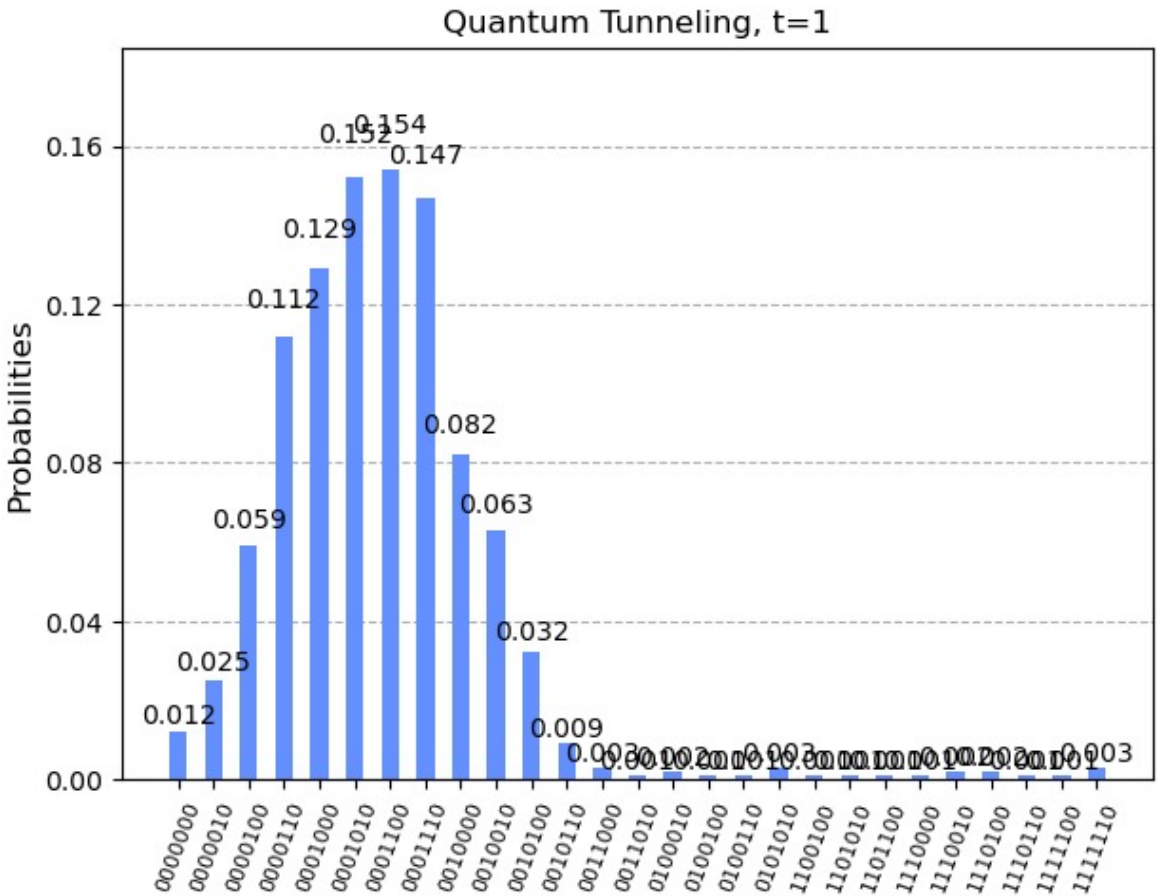
A potential barrier with the incident particle energy below the potential barrier height.





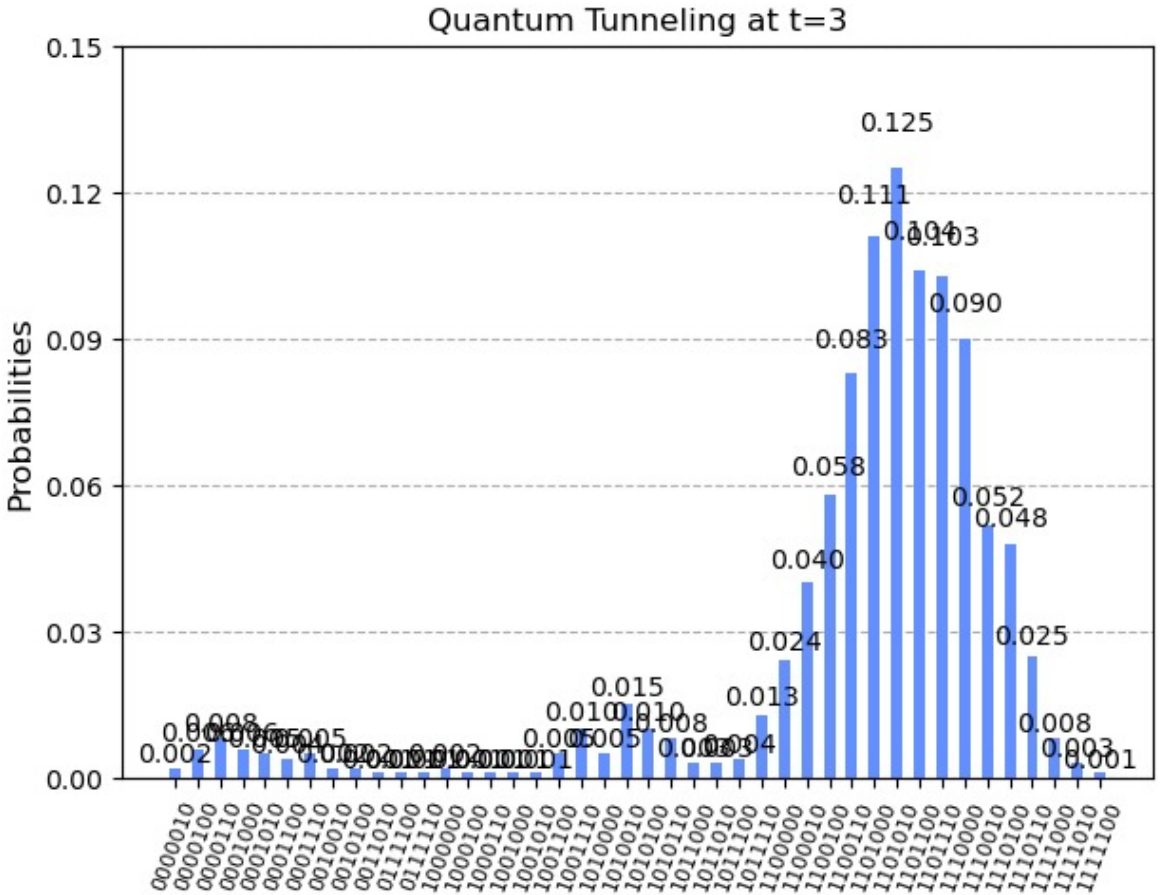
An incident sinusoidal wavefunciton quantum tunneling through a barrier. The wavefunciton exponentially decays within the potential barrier.

Quantum Tunneling



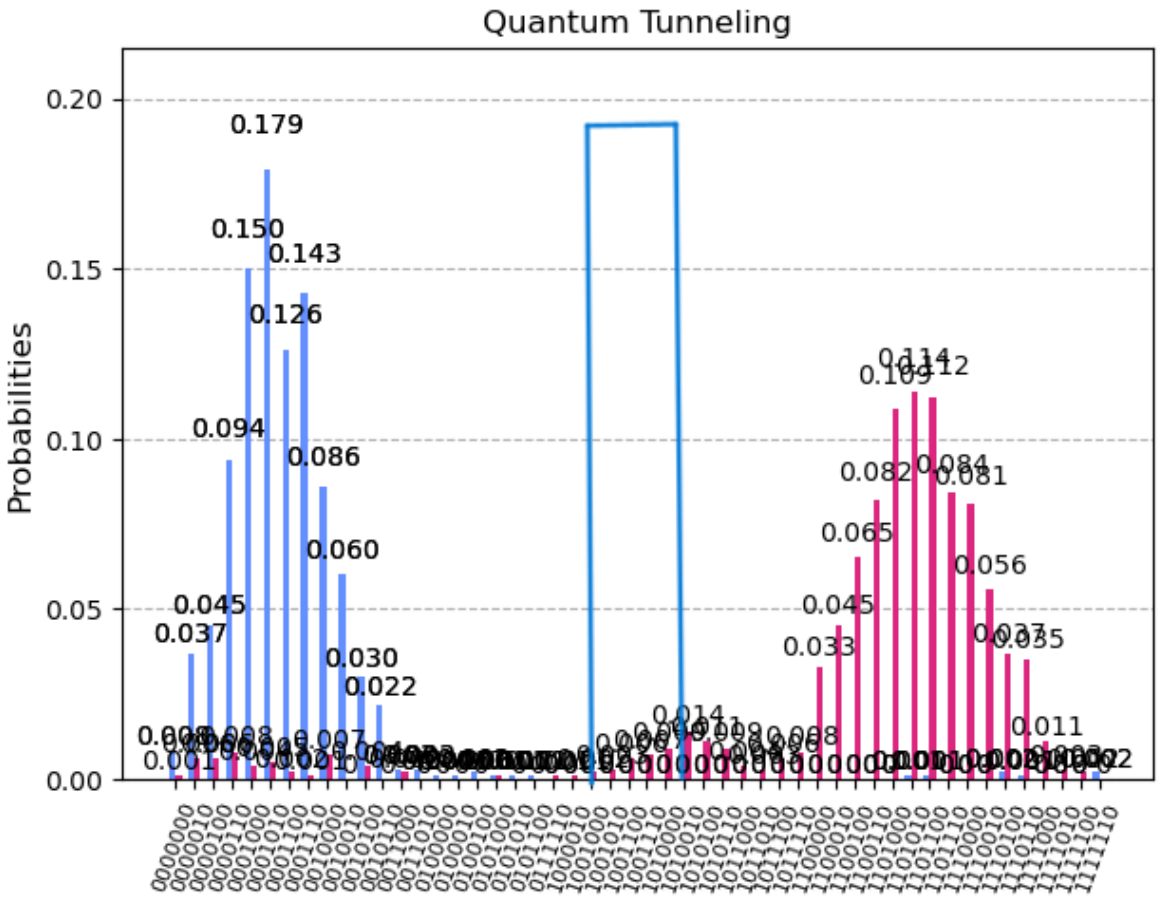
Initialisation, t=1 : Wave packet just before interacting with the potential barrier

Quantum Tunneling



After 3rd iteration, t=3 : Tunneled wave

Quantum Tunneling



initial state and 4th iteration: Better visualization of tunneling

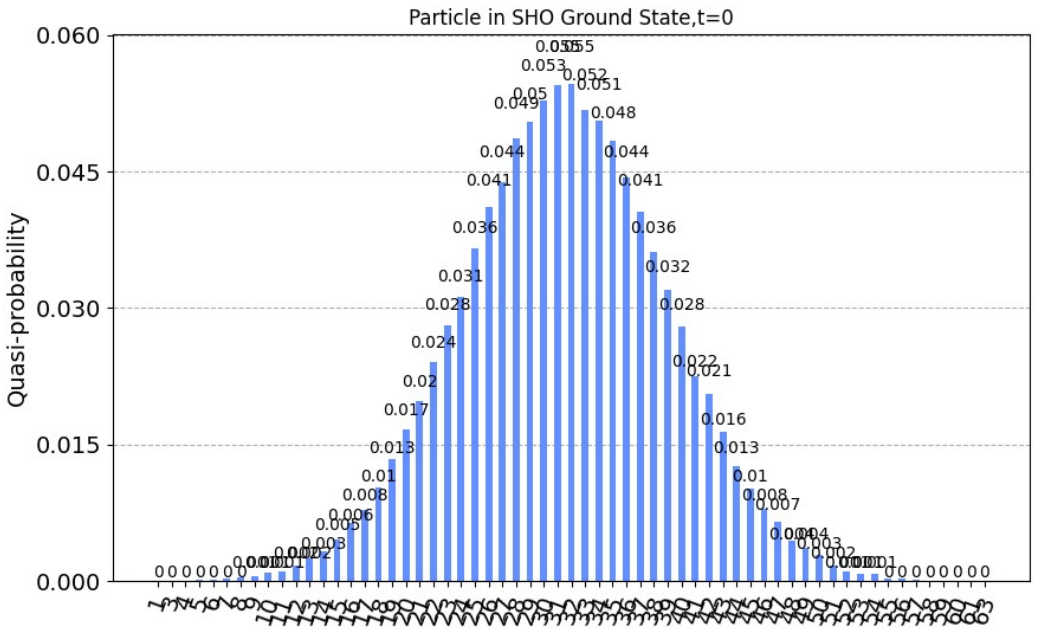
Simple Harmonic Potential

Hamiltonian: $\hat{H} = \frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega^2\hat{x}^2$
Time-independent Shrodinger Eqn: $\hat{H}\psi_n(x) = E_n\psi_n(x)$
The wave functions of the harmonic oscillator are given by the Hermite polynomials multiplied by a Gaussian factor:

$$\psi_n(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} \frac{1}{\sqrt{2^n n!}} H_n\left(\sqrt{\frac{m\omega}{\hbar}}x\right) e^{-\frac{m\omega x^2}{2\hbar}}$$

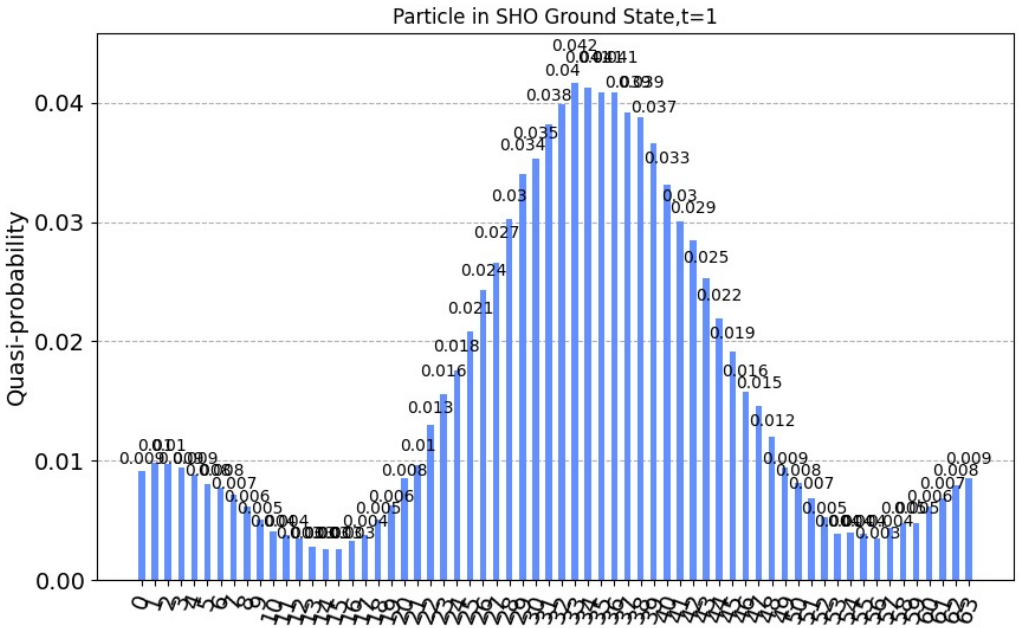
where $H_n(x)$ are the Hermite polynomials, and $\hbar$ is the reduced Planck constant.
Energy eigenvalues: $E_n = \left(n + \frac{1}{2}\right)\hbar\omega$, where $n = 0, 1, 2, \ldots$ represents the quantum number associated with the energy levels.

Simple Harmonic Potential



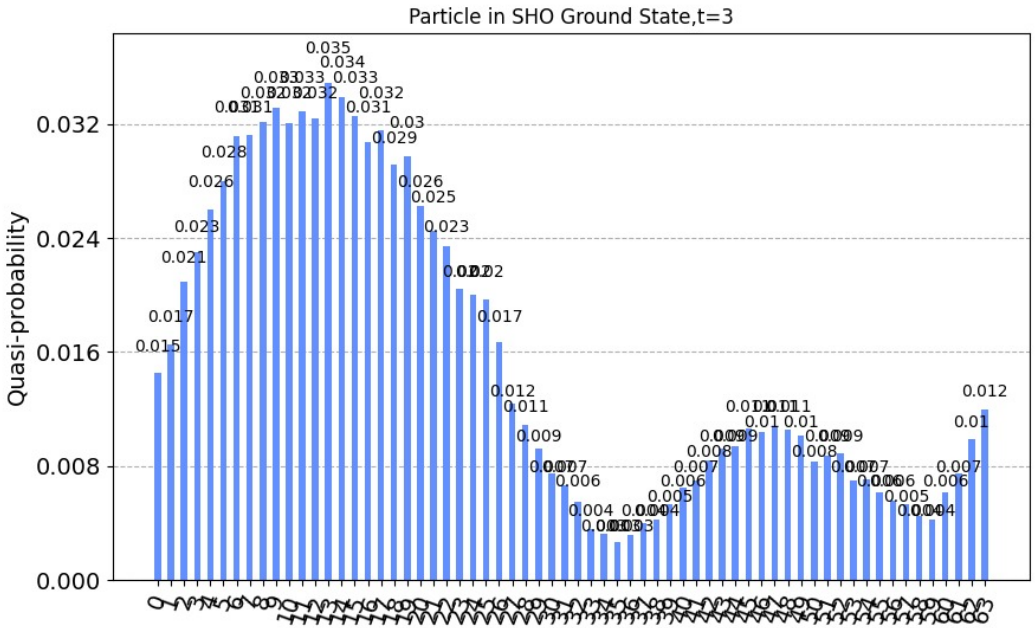
Initialisation, t=0 : Initial Wave packet

Simple Harmonic Potential



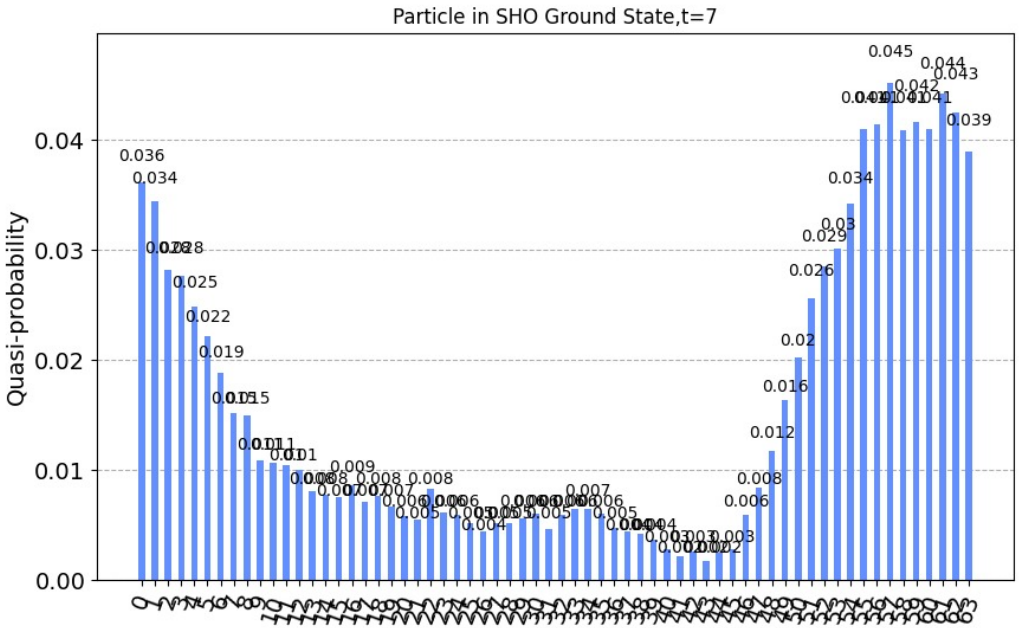
After 1st iteration, t=1

Simple Harmonic Potential



After 3rd iteration, t=3

Simple Harmonic Potential



After 7th iteration, t=7

Two particle Shcrödinger Equation

- Hamiltonian of two interacting particle:

$$H = (H_{0A} + H_{0B} + V_A(x_A) + V_B(x_B) + V_{AB}(x_A - x_B)) \quad (1)$$

  where x_A and x_B represent the position coordinates of the first and second particle, respectively.

- The operators $H_{0i} = \frac{p_A^2}{2m_i} = -\frac{\hbar^2}{2m_i}\frac{\partial^2}{\partial x_i^2}$ is the the standard free Hamiltonians for the particles.
- Schrödinger equation:

$$i\hbar\frac{d}{dt}\psi_{AB}(x_A, x_B, t) = H|\psi_{AB}(x_A, x_B, t), \quad (2)$$

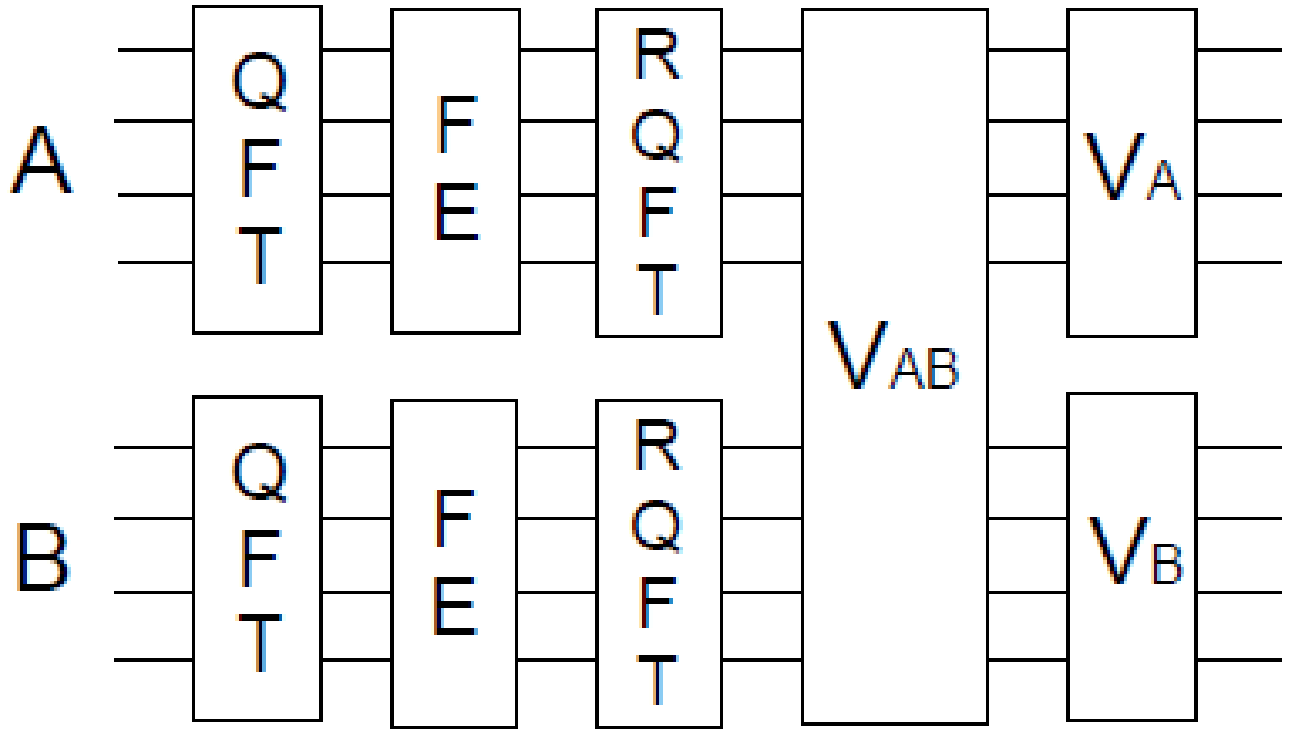
Two Particle Potential

- $V_A(x_A)$ and $V_B(x_B)$ are external potentials affecting particles A and B respectively.
- V_{AB}: Interaction potential
  Ddepends on the relative distance $x_A - x_B$.
- For our case, $V_{AB}(x_A - x_B) = v_0\delta(x_A - x_B)$,
  v_0 is a constant.
- System evolution from an initial state at time t_0 to a state at $t_1 = t_0 + \Delta t$ is given by:

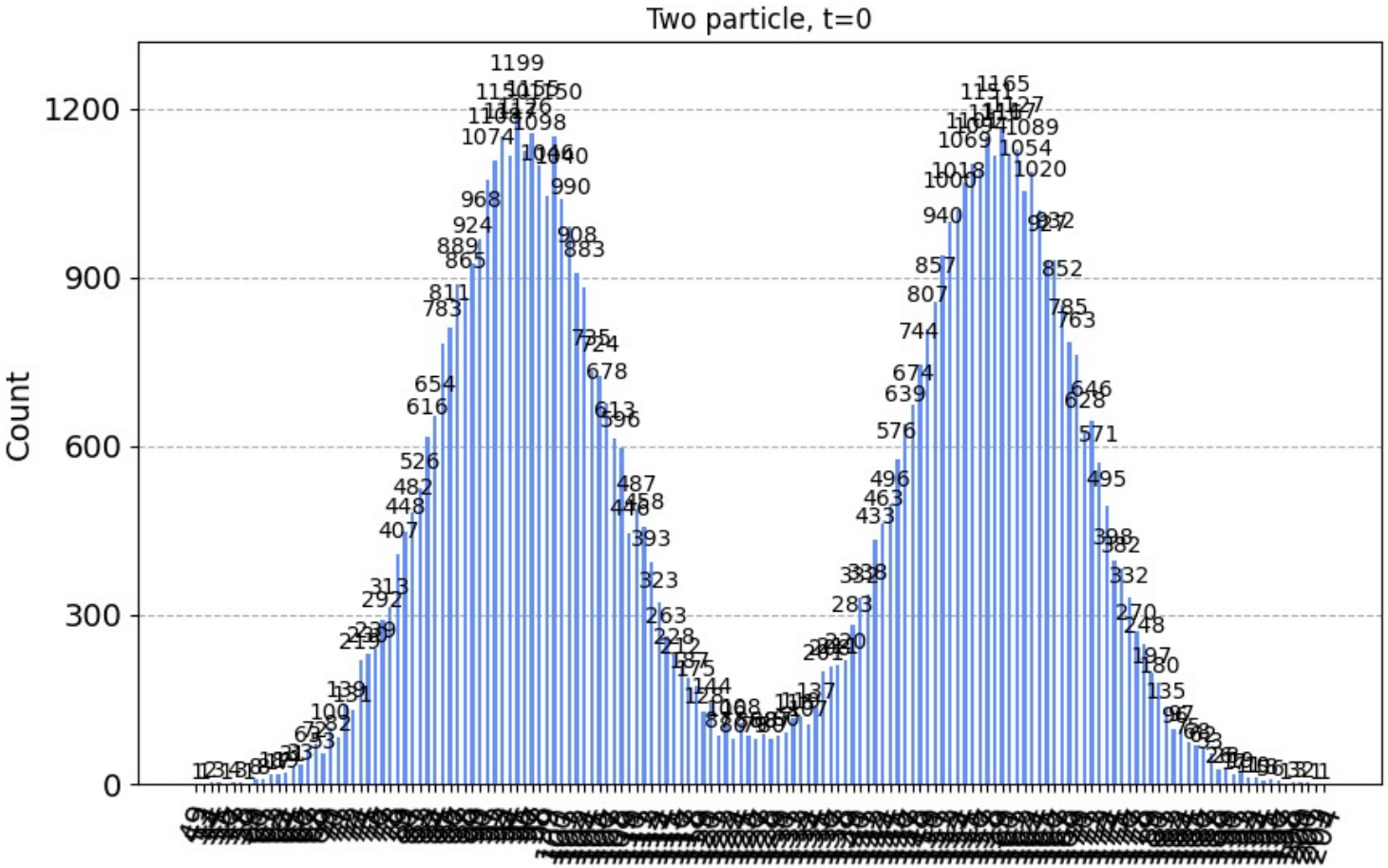
$$\psi_{AB}(x_A, x_B, t_1) = e^{\left(-\frac{i}{\hbar}(H)\Delta t\right)}\psi_{AB}(x_A, x_B, t_0),$$

(3)

Two Particle Quantum circuit

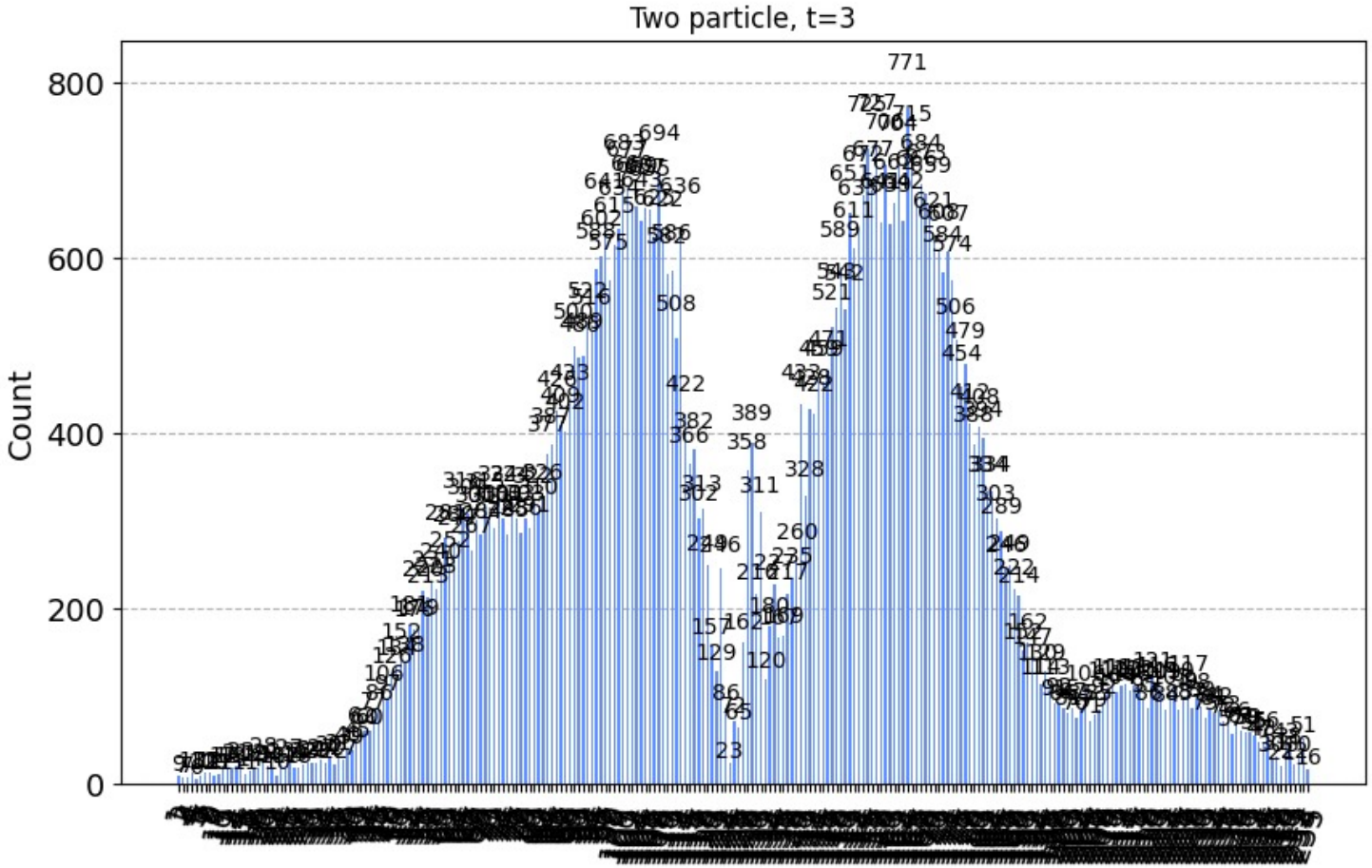


Two Particle



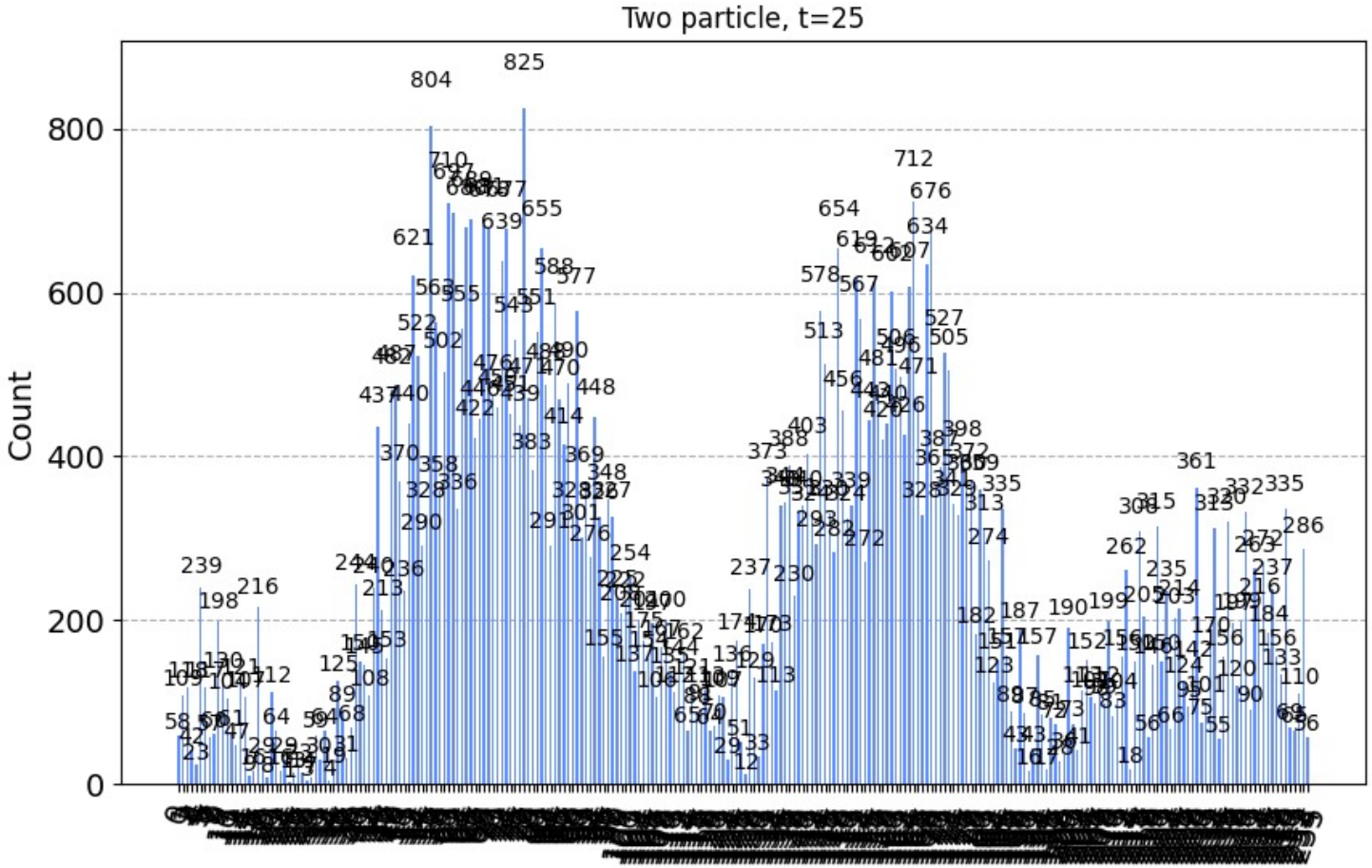
Initialisation of two particle wave packet, t=0 : Initial Wave packet

Two Particle



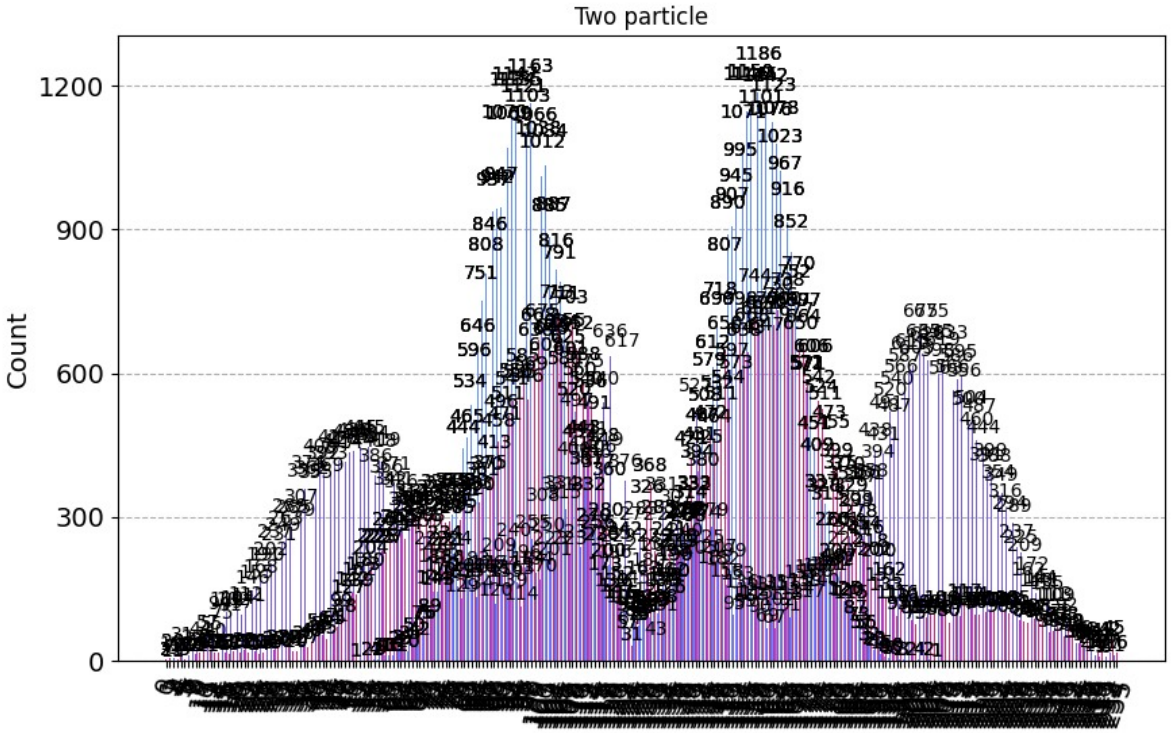
Two particle wave packet after 3rd iteration, t=3

Two Particle



Two particle wave packet after 25th iteration, t=25

Two Particle



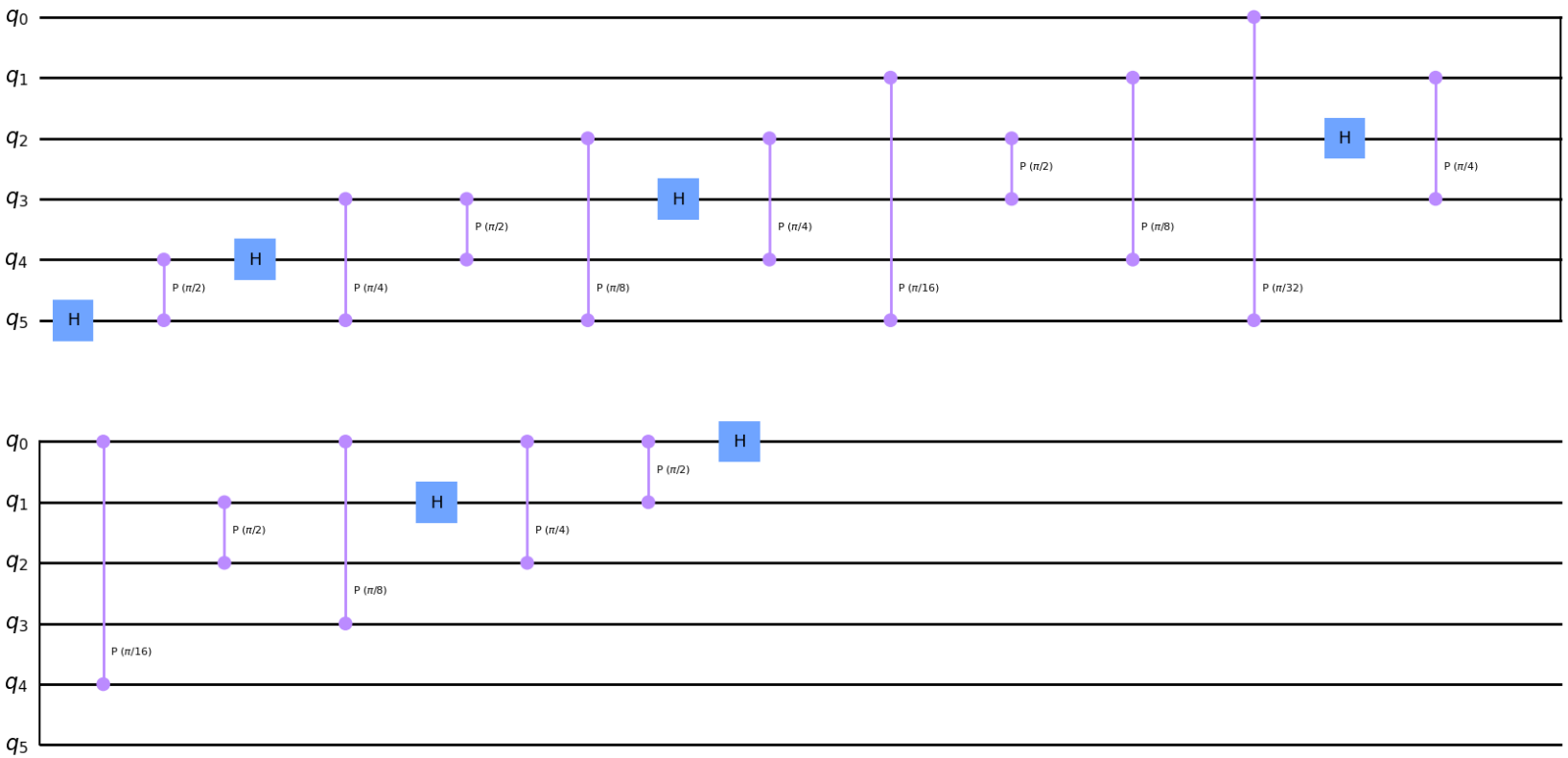
Visualization of time evolution of two-particle wavefunction(blue:t=0,Pink:t=3,violet:t=7)

References

1. I. N. Michael Chuang, "Quantum computation and quantum information," 2005.
2. M. Ostrowski, "Quantum simulation of two interacting schrödinger particles,"
3. S. Beneti Casati, "Principles of quantum computation and information," vol. 1,
4. M. Abouelela, "Quantum simulation of the Schrodinger equation using IBM's quantum computers,"

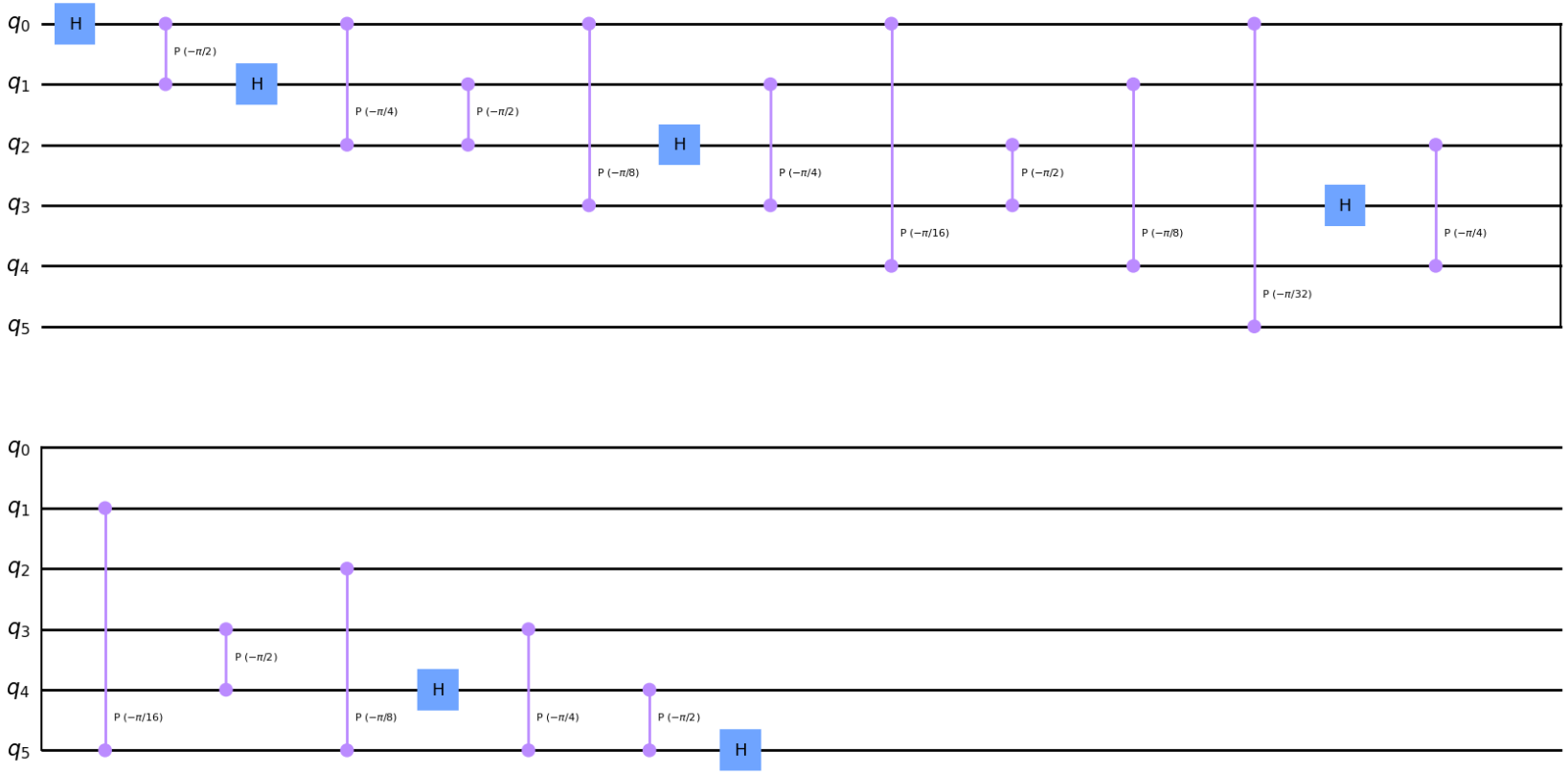
Appendix

1. Quantum circuit for Quantum Fourier Transform for 6-qubit system



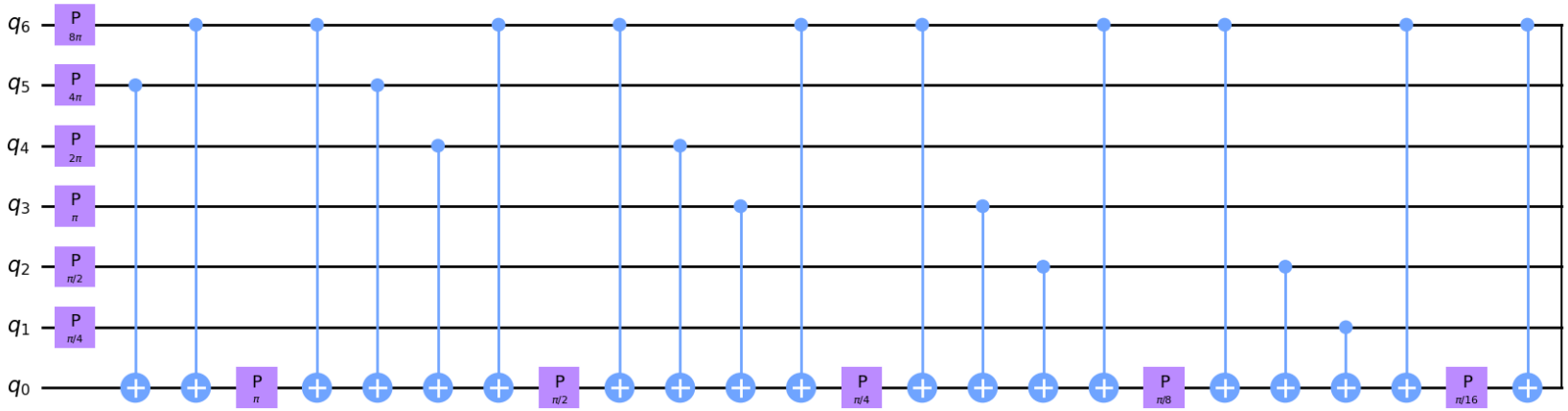
Appendix

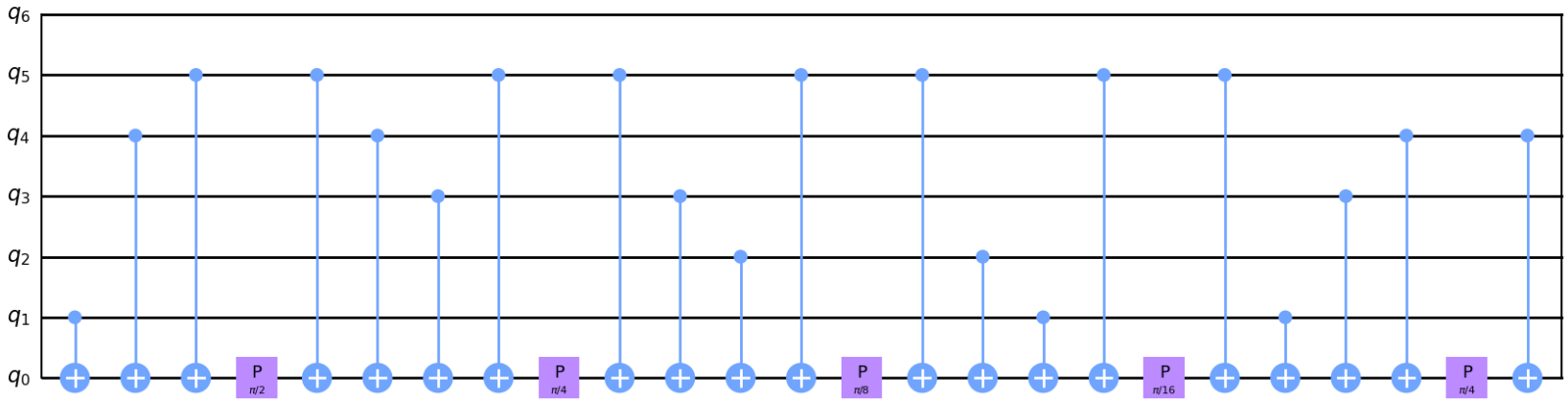
2. Quantum circuit for Inverse Quantum Fourier Transform for 6-qubit system



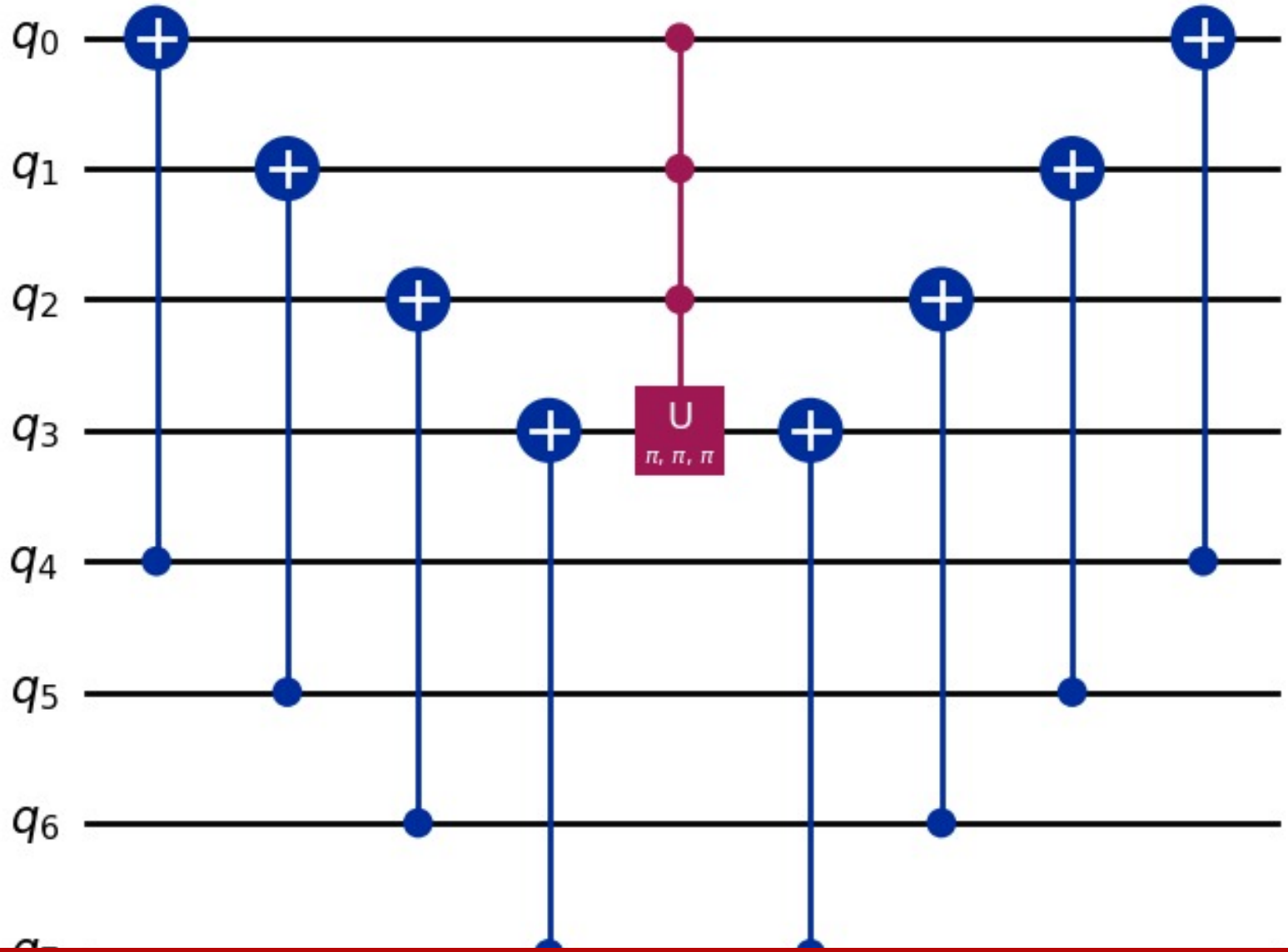
Appendix

2. Quantum circuit for Kinetic Energy Operator for 6-qubit system

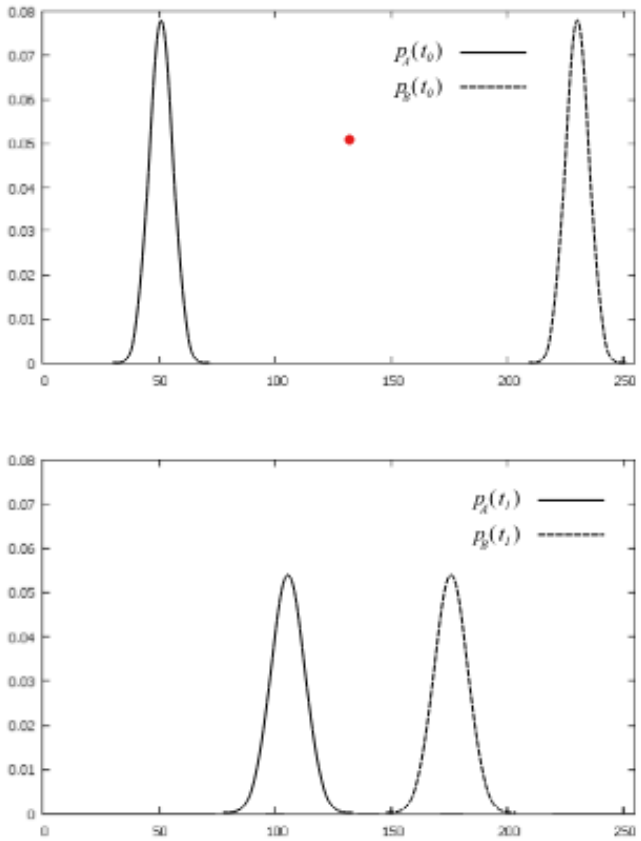


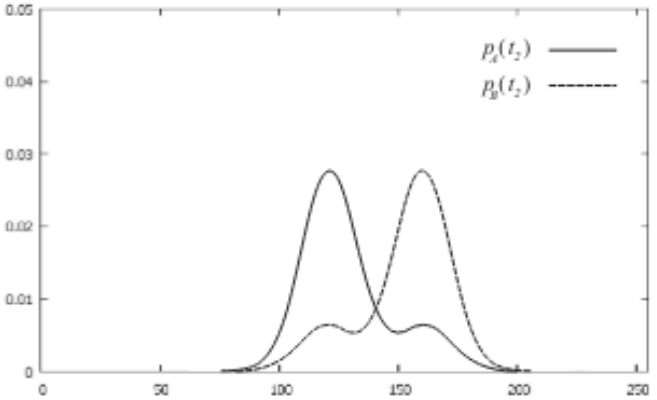


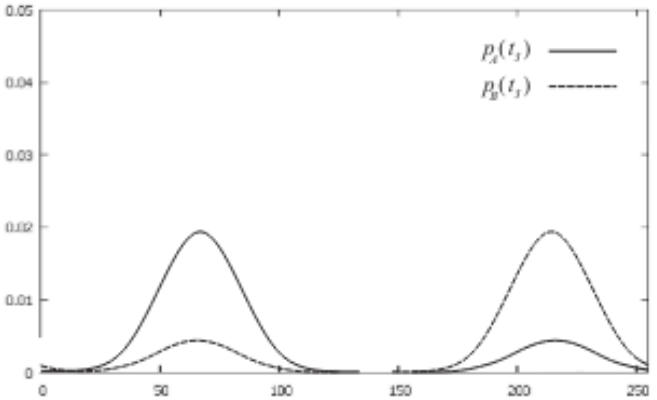
Two Particle interaction potential



Two Particle Refrence




$p_A(t_2)$
$p_B(t_2)$
0.05
0.04
0.03
0.02
0.01
0
0
50
100
150
200
250


$p_A(t_3)$
$p_B(t_3)$
0.05
0.04
0.03
0.02
0.01
0
0
50
100
150
200
250