Multiparticle Quantum Tunneling Simulation

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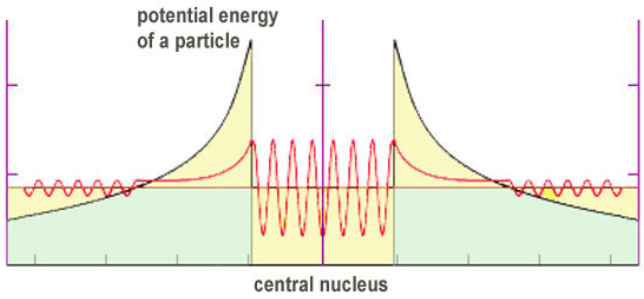
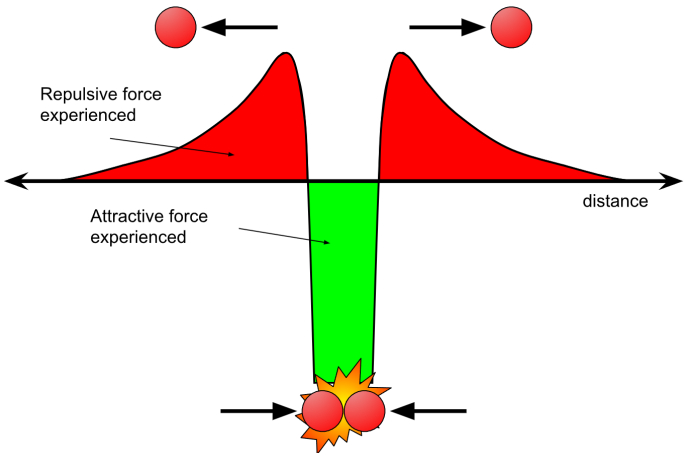
1 Abstract

In this study, we address the challenge of simulating multi-particle quantum tunneling, a phenomenon crucial to understanding various quantum mechanical systems but limited by the computational complexity of existing simulation methods. By developing an extension to the Benenti-Strini Method (2018), which originally facilitated quantum simulation of the single-particle Schrödinger equation through trotterization of the complex Hamiltonian, we introduce an approach capable of simulating multi-particle systems.
We **simulated Nuclear Fusion** between two particles, governed by Quantum Tunneling, as illustrated in the Figure.





The probabilities of occurrence of tunneling and positions of particles match the theoretically predicted results.
This method of simulation could be easily used to provide accurate insights into other **multi-particle** systems governed by **Quantum Tunneling**.

2 Introduction

Quantum tunneling is a fundamental phenomenon in quantum mechanics where particles pass through a barrier that they classically should not be able to surmount due to insufficient energy. Unlike classical particles, which require enough energy to overcome a barrier, quantum particles have a non-zero probability of "tunneling" through barriers without the requisite energy level. The Figure illustrates the Existence of the Wave Function of a Particle in the Classically Forbidden Region (Created where Kinetic Energy is Insufficient to cross the Potential Barrier). This phenomenon is crucial to many processes in physics, chemistry, and technology, including nuclear fusion in stars, radioactive decay, and the operation of quantum devices like tunnel diodes.
Historically, the simulation of quantum tunneling on quantum computers has been limited to single-particle systems. This limitation stems from the complexities associated with simulating the behavior of multiple interacting particles in a quantum system. The **Hamiltonian** that governs the time evolution of the system **becomes too complex**, and a suitable **method to break it down** to implement it on a Quantum Circuit is crucial.
Trotterization is a powerful method in quantum computing used to simulate the time evolution of quantum systems, particularly when dealing with complex Hamiltonians that describe the energy and dynamics of these systems. The core idea behind trotterization is to break down the exponential of a sum of non-commuting operators, which typically describe the Hamiltonian of a quantum system, into a product of exponentials of individual operators.
Trotterization, followed by **implementation of the exponentials of individual operators** as Quantum Gates can finally produce a simulation that would depict the time evolution of the system.

3 Theory

3.1 Deriving the Time Evolution

Let x_1, x_2 be the positions of particle 1 and 2 in a system at time t.
To simulate a pair of particles on a quantum computer, we must discretize the continuous variables x_1, x_2, and t. If the motion takes place inside a finite region, $-d \leq x_1, x_2 \leq d$, we decompose this region into n intervals of length l =

2d/n. Let the equivalent circuit have 2log(n)-qubits. Let the Hilbert space formed by the first log(n) qubits represent the be corresponding to the discretized positions of x_1. And similarly, the Hilbert space formed by the other log(n) qubits correspond to the discretized positions of x_2. **The state of the qubit register can be written as** $|x_1\rangle |x_2\rangle$
Hence, the wave function $\psi(x_1, x_2, t)$ is approximated by:

$$\sum_{k,l=0}^{2^n-1} c_{kl}(t) |k\rangle |l\rangle = \frac{1}{\sqrt{N}} \sum_{k,l=0}^{2^n-1} \psi(x_k, x_l, t) |k\rangle |l\rangle$$

So now solving the TDSE (Time Dependent Schrodinger Equation):

$$i\hbar \frac{d}{dt}\psi(x_1, x_2, t) = H\psi(x_1, x_2, t)$$

Where the Hamiltonian, H, will be:

$$H = KE_1 + KE_2 + V(x_1, x_2)$$

For a n-particle system with Coulombic potential between particles,

$$\hat{H} = -\frac{\hbar^2}{2}\sum_{j=1}^{N}\frac{1}{m_j}\nabla_j^2 + \frac{1}{8\pi\epsilon_0}\sum_{j=1}^{N}\sum_{\substack{i=1\\ i\neq j}}^{N}\frac{q_i q_j}{|\vec{r_i} - \vec{r_j}|}$$

When modeling our system for Nuclear Fusion between two particles, the potential term in the Hamiltonian will be $V(x_1, x_2) = \frac{1}{4\pi\epsilon_0|x_1 - x_2|}$

$$H = -\frac{\hbar^2}{2m_1}\frac{\partial^2}{\partial x_1^2} - \frac{\hbar^2}{2m_2}\frac{\partial^2}{\partial x_2^2} + \frac{1}{4\pi\epsilon_0|x_1 - x_2|}$$

On Integrating the TDSE with respect to time, from t to $t + \epsilon$ we obtain:

$$\psi(x_1, x_2, t + \epsilon) = e^{-\frac{i}{\hbar}(KE_1 + KE_2 + V(x_1, x_2))\epsilon}\psi(x_1, x_2, t)$$

The Hamiltonian is too complicated to have a direct implementation, so we will need to perform various transformations to implement the time evolution operator using Quantum Gates.

3.2 Trotterization

The first step in the simplification of the time evolution operator is Trotterization.

The Trotterization method is generally used to approximate the exponential of a sum of non-commuting operators. The core idea is to decompose the evolution of a quantum system into a sequence of simpler steps.

Consider a quantum system's Hamiltonian expressed as $H = H_1 + H_2 + \cdots + H_n$, where the components H_i do not necessarily commute (*i.e.*, $[H_i, H_j] \neq 0$ for $i \neq j$). The system's evolution over time t is given by the exponential of the Hamiltonian, e^{-iHt}. Trotterization approximates this evolution by dividing it into a series of shorter time steps, applying the exponential of each Hamiltonian part separately, and then repeating this sequence multiple times. The simplest form of this approximation is provided by the Trotter formula:

$$e^{-iHt} \approx \left(e^{-iH_1 t/n} e^{-iH_2 t/n} \cdots e^{-iH_n t/n}\right)^n,$$

for a sufficiently large n. This approximation approaches exactness as $n \to \infty$. Similarly,

$$e^{-\frac{i}{\hbar}(KE_1 + KE_2 + V(x_1, x_2))\epsilon} \approx e^{-\frac{i}{\hbar}KE_1\epsilon} e^{-\frac{i}{\hbar}KE_2\epsilon} e^{-\frac{i}{\hbar}V(x_1, x_2)\epsilon}$$

is a good approximation for small ϵ

3.3 Encoding KE into Quantum Gates

Now, to simplify $e^{-\frac{i}{\hbar}KE_1\epsilon} e^{-\frac{i}{\hbar}KE_2\epsilon} e^{-\frac{i}{\hbar}V(x_1, x_2)\epsilon}$ further, we look at the individual terms.
From the implementation of the Quantum Fourier Transform circuit, we know that Controlled Unitaries can be used to implement:

$$|x\rangle \to e^{if(x)} |x\rangle$$

In order to simplify the implementation of this phase shift, controlled unitary gates will be used to apply a phase shift to only the least significant bit. Consider the state $|k\rangle$ where k represents the integer representation of the binary string of log(n) - 1 qubits. Hence, if the last qubit is in state $|0\rangle$, $x = 2k$ otherwise $x = 2k + 1$. Thus, a phase shift controlled unitary of the form $|0\rangle \to e^{if(2k)} |0\rangle$ and $|1\rangle \to e^{if(2k+1)} |1\rangle$ must be applied.

$$U_k = \begin{bmatrix} e^{if(2k)} & 0 \\ 0 & e^{if(2k+1)} \end{bmatrix}$$

Since $\frac{\partial^2}{\partial x_1^2}$ isn't easy to convert into a Quantum Circuit gate, we use the Fourier Transform F to convert from the x-basis to the p(momentum operator)-basis, where a Quadratic Function of p is formed (hence the operator is diagonal in this basis and can easily be implemented). This can be implemented using Quantum Circuit Gates and then, be converted back to the x-basis by using the inverse Fourier Transform F^{-1}

$$e^{-\frac{i}{\hbar}KE_1\epsilon} = F^{-1} e^{-\frac{i}{\hbar}\left(\frac{p_1^2}{2m_1}\right)\epsilon} F$$

$$e^{-\frac{i}{\hbar}KE_2\epsilon} = F^{-1} e^{-\frac{i}{\hbar}\left(\frac{p_2^2}{2m_2}\right)\epsilon} F$$

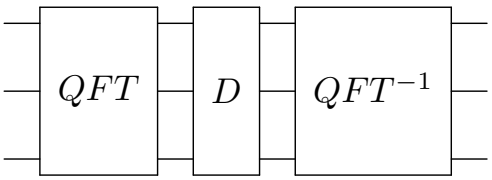
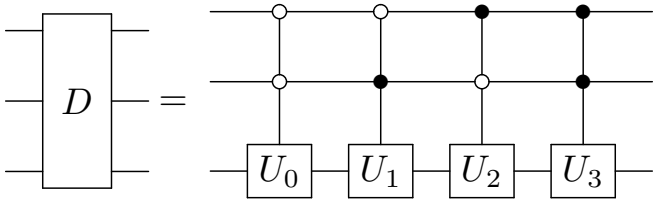


Figure: Quantum circuit gates representing the kinetic energy operator where D implementing $e^{-\frac{i}{\hbar}\left(\frac{p^2}{2m}\right)\epsilon}$ operation



3.4 Encoding Potential into Quantum Gates

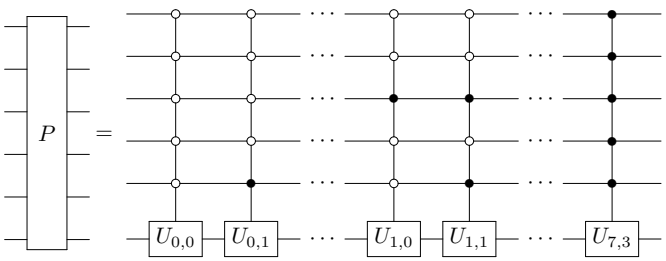
We can use Controlled Unitary Operations to implement the Potential as:

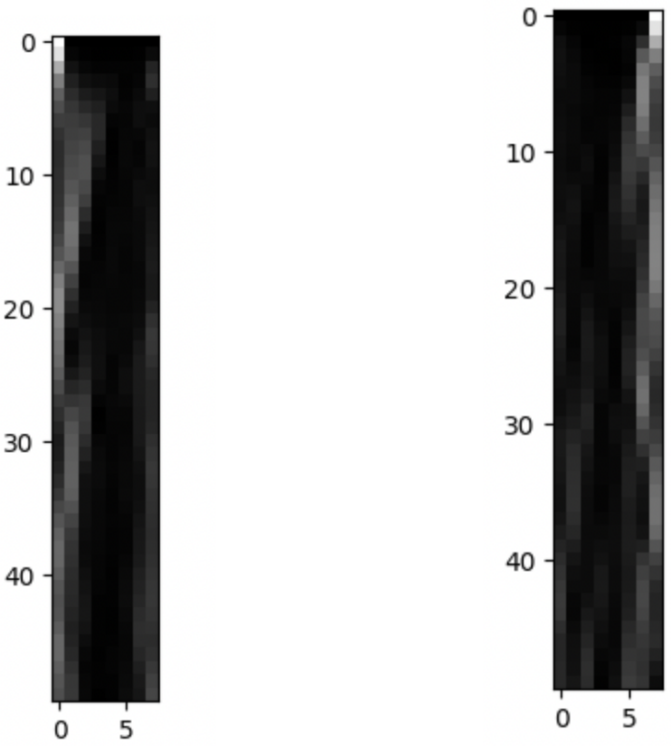
$$|x_1\rangle |x_2\rangle \rightarrow e^{if(x_1,x_2)} |x_1\rangle |x_2\rangle$$

Let x_1 be fixed and the phase shift must then applied with respect to x_2. Following a process similar to the one outlined above, the following unitary is obtained with a control on the state $|x_1\rangle |k\rangle$,

$$U_{x_1,k} = \begin{bmatrix} e^{if(x_1,2k)} & 0 \\ 0 & e^{if(x_1,2k+1)} \end{bmatrix}$$

Iterating through values of x_1, all combinations of x_1 and x_2 are covered and desired multi-particle transformation is applied.



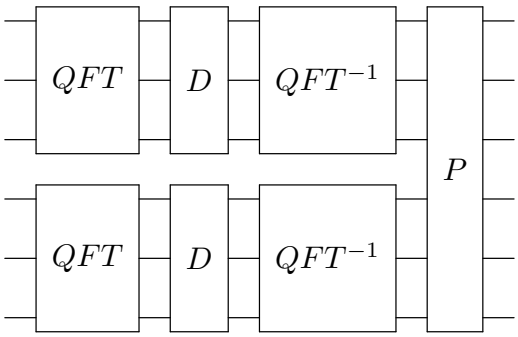


(a) Particle 1

(b) Particle 2

4 Final Circuit Diagram

The final circuit diagram to Encode the Hamiltonian into a Quantum Circuit is:



5 Results

This method was used to simulate the **Nuclear fusion of two Particles**. 3 Qubits were used for each Particle, to store the region(denoted by x) in which the particle is present out of the 8 distinct regions formed by the Hilbert space formed by the 3 Qubits(an approximation for the position of the particle).
Initially, Particle 1 is at x = 0 and Particle 2 is at x = 7. **The size of the region is such that whenever both the particles are in the same region, Nuclear fusion occurs** due to the dominance of the Strong Force.
By implementing this circuit in **Pennylane** for Encoding the Hamiltonian into a Quantum Circuit, We obtain the following **time evolution** :

Plot describes the position probabilities of each particle as a grayscale plot where white corresponds to certain probability of particle in that distance interval whereas black indicates 0 probabilty of the particle being within that distance interval. The distance intervals are plotted over the x-axis while the time is plotted on the y-axis. It can be clearly seen that there are slight probabilities of either particle tunnelling into the other towards the bottom of the plot. We have also created an animation of this concept using our quantum circuits within the attached zip file.

6 References:

- Wiesner, S. (1996). Simulations of Many-Body Quantum Systems by a Quantum Computer. https://doi.org/10.48550/arxiv.quant-ph/9603028
- Benenti, G., and Strini, G. (2008). Quantum simulation of the single-particle Schrödinger equation. American Journal of Physics, 76(7), 657–662. https://doi.org/10.1119/1.2894532
- Hegade, N. N., Kortikar, N. L., Das, B., Behera, B. K., and Panigrahi, P. K. (2017). Experimental Demonstration of Quantum Tunneling in IBM Quantum Computer. arXiv (Cornell University). https://doi.org/10.48550/arxiv.1712.07326