ELEC4605 ASSIGNMENT 2 – TERM 3, 2020

Quantum Simulation

For your second assignment, you are to perform a quantum simulation of a particle in a 1D parabolic potential (i.e. a 1D quantum harmonic oscillator). To do this, you will build a circuit that simulates the time evolution of a particle with dynamics governed by the Schrodinger equation

$$\mathcal{H} = \frac{P^2}{2m} + V(X)$$

where $V(X) = \frac{1}{2}m\omega^2 X^2$ is a parabolic potential, P is the momentum operator and X is the position operator. The wavefunction of the particle in the continuous x basis is written as

$$|\psi(t)\rangle = \int_{-\infty}^{\infty} |x\rangle\langle x|\psi(t)\rangle dx = \int_{-\infty}^{\infty} \psi(x,t)|x\rangle dx$$

which exists in an infinite-dimensional Hilbert space. It is usually sufficient to consider the wavefunction over a finite region $-d \leq x \leq d$, which is certainly the case when the particle is confined in a parabolic potential (provided you choose d to be much greater than the extent of the wavefunction). In addition, we can sample the wavefunction at discrete points, so long as we choose the step size Δx to be shorter than the relevant length scale of our problem, providing us a way to simulate such a system on a digital quantum computer. With n qubits, we have 2^n computational basis states $|0\rangle, \ldots, |2^n - 1\rangle$. You will use these computational basis states to represent discrete samples of the position basis, with points separated by $\Delta x = 2d/2^n$

$$x_j = -d + \left(j + \frac{1}{2}\right)\Delta x$$

The discretised wavefunction becomes

$$|\psi(t)\rangle = \sum_{j=0}^{2^n-1} \psi(x_j, t)|j\rangle$$

where $|j\rangle = |j_{n-1}\rangle|j_{n-2}\rangle \ldots |j_0\rangle$ is the computational basis state of the n-qubit register. We wish to compute the time evolution of the wavefunction from a time t to a later time $t + \varepsilon$

$$|\psi(t+\varepsilon)\rangle = e^{-i\mathcal{H}\varepsilon/\hbar}|\psi(t)\rangle$$

The aim is to produce a quantum circuit that implements the unitary time evolution operator above.

(a) Use the Trotter approximation (that is correct up to the second-order terms) to express the time evolution operator as a product of the kinetic and potential components. You can assume ε to be a very small incremental time. [*5 marks*]

(b) The system will be initialised in some state

$$|\psi(0)\rangle = \sum_{k=0}^{2^n-1} \psi(x_j, 0)|j\rangle$$

Expressed in the position basis. The unitary operator for the potential energy $e^{-iV(X)\varepsilon/\hbar} = e^{-i\beta X^2}$(where $\beta = m\omega^2\varepsilon/2\hbar$) is diagonal in this basis, which as we will see, amounts to a conditional phase operation.

Explain why the transformation $U_{QFT}^{\dagger} e^{-i\alpha P^2} U_{QFT}$ (where $\alpha = \varepsilon/2\hbar m$ and U_{QFT} is the unitary for a Quantum Fourier Transform) makes it easier to evaluate the time evolution for the kinetic energy component of the Schrodinger equation. [*5 marks*]

(c) The combined unitary describing the time evolution of the particle for a single Trotter iteration is given by

$$e^{-i\mathcal{H}\varepsilon/\hbar} = U_{QFT}^{\dagger} e^{-i\alpha P^2} U_{QFT} e^{-i\beta X^2}$$

Repeating this operator l times evolves the state to a time $t = l\varepsilon$. The diagonal operator $e^{-i\beta X^2}$ performs the following transformation on the computational basis states

$$e^{-i\beta X^2}|j\rangle = e^{-i\beta x_j^2}|j\rangle$$

with x_j the discrete position previously defined. Write down a circuit that implements a unitary of the form $e^{-i\beta X^2}$ for a computer with three qubits ($n = 3$).

Hint: one method is to use the first two qubits as controls for a phase gate applied to the third qubit. See the attached research paper for inspiration. [*15 marks*]

(d) To realise a single Trotter step, we also need to implement the Quantum Fourier Transform (QFT) and the kinetic energy operator $e^{-i\alpha P^2}$. We have already seen the circuit that performs the QFT in class, so all that remains is to build a circuit for the unitary $e^{-i\alpha P^2}$.

The QFT transforms the basis from position space to reciprocal space (k-space). The separation between each point in k-space is given by $\Delta k = 2\pi/(2^n \Delta x) = \pi/d$, since the smallest momentum corresponds to the largest possible wavelength in position space ($\lambda = 2^n \Delta x = 2d$). Furthermore, the discrete set of wavenumbers span a range of $2\pi/\Delta x = \pi 2^n/d$ (as the minimum wavelength in position space is $\lambda = \Delta x = 2d/2^n$). We define a discrete set of wavenumbers for our simulation, ranging from $-\pi 2^n/2d$ to $\pi 2^n/2d$:

$$k_m = -\frac{\pi 2^n}{2d} + m\Delta k$$

Here m represents the computational basis state in the new Fourier basis ($|m\rangle = |0\rangle, \dots, |2^n - 1\rangle$). To obtain momentum we simply use the relation $p = \hbar k$, so the kinetic energy operator $e^{-i\alpha P^2}$ acting on the basis states $|m\rangle$ is then given by

$$e^{-i\alpha P^2}|m\rangle = e^{-i\alpha \hbar^2 k_m^2}|m\rangle$$

Write down a circuit that implements the operator $e^{-i\alpha P^2}$ for $n = 3$ qubits. You may assume the QFT has been applied so that you are already in the $|m\rangle$ basis. [*10 marks*]

(e) For technical reasons that we won't go into, we need to perform a "cyclic shift" on the $|m\rangle$ basis states directly after the QFT, translating each state by 2^{n-1}. For the case of $n = 3$ qubits, the cyclic shift implements the following mapping of the basis states: $|0\rangle \leftrightarrow |4\rangle, |1\rangle \leftrightarrow |5\rangle, |2\rangle \leftrightarrow |6\rangle$ and $|3\rangle \leftrightarrow |7\rangle$.

Write down a circuit that performs the cyclic shift operation U_{CS} for $n = 3$ qubits. [*10 marks*]

(f) The full Trotter increment now reads as:

$$e^{-i\mathcal{H}\varepsilon/\hbar} = U_{QFT}^{\dagger} U_{CS}^{\dagger} e^{-i\alpha P^2} U_{CS} U_{QFT} e^{-i\beta X^2}$$

Code a complete circuit that can perform the 1D quantum simulation *with an arbitrary number of qubits* in a suitable simulation software package (such as Matlab). [*20 marks*]

(g) In practice, you are limited in the number of qubits you can utilise for your simulation on a classical computer, though your results should be obtained with at least 6 qubits (64 position points). Use your circuit to compute the evolution of the particle in the 1D harmonic potential. Specifically, you should:

i. Try different initial states of the system, attempt to initialise in both stationary and superposition states. [*10 marks*]

ii. Apply several iterations of the infinitesimal time evolution operator listed in part (f), measuring the state of the qubits in the computational basis after each iteration. [*10 marks*]

iii. Play with the Trotter step size ε to ensure your results converge (e.g. start from a course time increment ε where the error is large and decrease the step size until the error reduces no further). [*10 marks*]

iv. Discuss your results. [*5 marks*]

Note: you need to select some reasonable values for m and ω. These will set the relevant length and timescales of your simulation. [*total: 35 marks*]

Submission: You are expected to complete this assignment and write a report summarising your results by yourself. The assignment is due Friday of Week 10 (20/11/2020) at 11:55pm. Submission will be via the Moodle course page. This is worth 12.5% of your total grade for the course and will be marked out of 100.