Write up on Simulating coupled oscillator on Quantum computer

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1 Introduction

Quantum computing has emerged as a transformative domain with the potential to revolutionize various industries. Therefore, at the stage when we have made successful progress toward quantum technology development, the study of possibilities available and applications of quantum algorithms is significant. It has been shown that quantum computing can show strong complexity theoretic evidence for specific problems and achieve exponential speedup over the classical method[ref [2,3]]. Efficient simulation of quantum dynamics is one of the promising areas of quantum computing. In quantum dynamics, quantum computing offers exponential speed up over its classical counterpart[ref 1].

Hamiltonian simulation on a quantum computer is a method to model and analyze the time evolution of quantum dynamics. A strategy for harnessing the power of quantum computers is to find a range of problems that can be expressed in terms of, or reduced to, Hamiltonian dynamics, which are known to be suitable for quantum simulation. Efforts in the past have aimed to create Hamiltonian simulation techniques for a specific range of differential equations. However, the outcomes have been restricted to polynomial speedups, as in references [ref 4-6].

This article explores how Hamiltonian simulation can be applied to classical dynamics problems that strongly correlate with quantum systems. The methodology used in this article can simulate the dynamics of a multitude of coupled classical oscillators in polynomial time, harnessing the quantum mechanical for exponential speedup against its classical counterparts. The study of such systems using Hamiltonian simulation has the potential to offer some critical insights into the underlying mechanics of phenomena like mechanical oscillators to electrical circuits and even neuron activity models [ref 7-10]. The study of coupled classical oscillators can be done through Hamiltonian simulation, which is not surprising because solutions to the Schrödinger equation contain oscillatory terms and interference, and we are effectively using these properties to simulate the same phenomena in the classical system.

Mapping classical problems to quantum simulations involves encoding classical quantities, such as displacements and momenta, into quantum states with

technical subtleties. This encoding is essential for energy conservation and key to realizing exponential quantum speedup. This article's research demonstrates progress beyond current algorithms by presenting solutions that can scale polynomially in the Hilbert space for classical systems' full configuration. This advancement provides a new frontier in efficiently computing global properties like kinetic and potential energies.

The article further claims that the complexity of classical simulation presents an exponential lower bound, making problems intractable for classical computation but feasible for quantum processors and classified as BQP-complete if addressed using quantum circuits, indicating that quantum computing can transform the area of dynamical systems simulation.

2 Defining the Problem

Writing the Classical equation for N coupled oscillator,

$$m_j \ddot{x}_j(t) = \sum_{k \neq j} \kappa_{jk} \left(x_k(t) - x_j(t) \right) - \kappa_{jj} x_j(t). \tag{1}$$

We can also write it in a matrix form as:

$$\mathbf{M} \ddot{\vec{x}}(t) = -\mathbf{F} \vec{x}(t), \tag{2}$$

where $\mathbf{M}$ is a $N \times N$ diagonal matrix with entries $m_j > 0$ and $\mathbf{F}$ is the $N \times N$ matrix whose diagonal and off-diagonal entries are $f_{jj} = \sum_k \kappa_{jk}$ and $f_{jk} = -\kappa_{jk}$, respectively.

This is solvable classically with normal modes.

Now, we need the velocity and position at time t for the solution. Let us scale the problem with $\sqrt{M}$, so that the energy $\mathbf{E}$ becomes constant. Now we define the problem, by assigning a time evolved state variable.

Let $\mathbf{K}$ be the $N \times N$ symmetric matrix of spring constants $\kappa_{jk} \geq 0$ and assume it is d-sparse (i.e., there are at most d nonzero entries in each row). Let $\mathbf{M}$ be the $N \times N$ diagonal matrix of masses $m_j > 0$ and define the normalized state

$$|\psi(t)\rangle := \frac{1}{\sqrt{2E}} \begin{pmatrix} \sqrt{\mathbf{M}} \dot{\vec{x}}(t) \\ i \vec{\mu}(t) \end{pmatrix}, \tag{3}$$

where $E > 0$ is a constant, and $\vec{\mu}(t) \in R^M [M := N(N+1)/2]$ is a vector with N entries $\sqrt{\kappa_{jj}} x_j(t)$ and $N(N-1)/2$ entries $\sqrt{\kappa_{jk}} \left(x_j(t) - x_k(t) \right)$, with $k > j$.

Assume that we are given oracle access to $\mathbf{K}$ and $\mathbf{M}$, and oracle access to a unitary $\mathcal{W}$ that prepares the initial state, i.e., $\mathcal{W}|0\rangle \mapsto |\psi(0)\rangle$. Given $t \geq 0$ and $\epsilon > 0$, the goal is to output a state that is ϵ-close to $|\psi(t)\rangle$ in the Euclidean norm.

2.1 Quantum Problem

Let us use the change of variables where $\vec{y}(t) := \sqrt{\mathbf{M}}\vec{x}(t)$ allows us to write the equation. (1) as

$$\ddot{\vec{y}}(t) = -\mathbf{A}\vec{y}(t), \tag{4}$$

where $\mathbf{A} := \sqrt{\mathbf{M}}^{-1}\mathbf{F}\sqrt{\mathbf{M}}^{-1} \succeq 0$ is positive semi-definite and real symmetric, and $\mathbf{M} \succ 0$ is the diagonal matrix with entries m_j.

Any solution to Eq. (4) satisfies

$$\ddot{\vec{y}}(t) + i\sqrt{\mathbf{A}}\dot{\vec{y}}(t) = i\sqrt{\mathbf{A}}[\dot{\vec{y}}(t) + i\sqrt{\mathbf{A}}\vec{y}(t)]. \tag{5}$$

This is simply Schrödinger's equation induced by the Hamiltonian $-\sqrt{\mathbf{A}}$. The solution therefore is,

$$\dot{\vec{y}}(t) + i\sqrt{\mathbf{A}}\vec{y}(t) = e^{it\sqrt{\mathbf{A}}}[\overrightarrow{\dot{y}}(0) + i\sqrt{\mathbf{A}}\vec{y}(0)]. \tag{6}$$

For a simplified version, we define, $\mathbf{B}$ as a NxM matrix which satisfies, $\mathbf{B}\mathbf{B}^\dagger = \mathbf{A}$ and define the block diagonal Hamiltonian as:

$$\mathbf{H} := -\begin{pmatrix} \mathbf{0} & \mathbf{B} \\ \mathbf{B}^\dagger & \mathbf{0} \end{pmatrix}, \tag{7}$$

where $\mathbf{0}$ are the matrices of all zeros.

Schrödinger's equation induced by $\mathbf{H}$ is

$$|\dot{\psi}(t)\rangle = -i\mathbf{H}|\psi(t)\rangle, \tag{8}$$

where $|\psi(t)\rangle \in C^{N+M}$ is the state of a quantum system at time t. It can be verified by direct substitution that

$$|\psi(t)\rangle \propto \begin{pmatrix} \dot{\vec{y}}(t) \\ i\mathbf{B}^\dagger\vec{y}(t) \end{pmatrix}$$

Hence, we have

$$\begin{pmatrix} \dot{\vec{y}}(t) \\ i\mathbf{B}^\dagger\vec{y}(t) \end{pmatrix} = e^{-it\mathbf{H}} \begin{pmatrix} \dot{\vec{y}}(0) \\ i\mathbf{B}^\dagger\vec{y}(0) \end{pmatrix}, \tag{9}$$

Now we have a specified Hamiltonian to simulate, for which we can use any algorithm for exponential time evolution. The problem is to define an oracle, which gives us the initial state to evolve and the matrices constituting the hamiltonian.

3 Results and Discussion

In this report, we have discussed a method of mapping a classical physics problem onto a quantum system, which then utilizes specific quantum algorithms to run a Hamiltonian simulation. The main process consists of mapping physical

quantities (like potential energies of the springs and kinetic energies of the oscillaitng bodies) onto the amplitude of quantum states of "n" qubits. Therefore, since the entire classical system scales exponentially with 2^n balls, it can be mapped onto a quantum system consisting of qubits that scale only in polynomial 'n.' As a result, the quantum algorithm allows the system of 2^n balls to be modeled only in poly(n) time. Furthermore, it has been proven that such simulations cannot be executed efficiently on a classical algorithm, since in the worst case the oracle will need 2^n queries to compute the system classically. Nevertheless, one must remember that the presented quantum algorithm relies on assumptions that make the preparation of quantum state of n qubits efficient, since the qubits must represent the full configuration of the classical system. Like for instance, the matrix that represents the potential and kinetic energies of the balls in the classical system must be sparce, meaning that only certain configuration of ball-spring systems can provide exponential speed-up, or that the energy is conserved, meaning that the algorithm - when applied to real-life oscillating systems - can provide at best very good approximations. Also, one must not forget that such quantum algorithms, like most quantum algorithms, provide an exponential-speed up for larger amount of qubits. Therefore, the speed-up justifies the operation costs of a quantum ocmputer only for systems where a large amount of qubits is utilized (larger than the maximum amount that a classical computer can simulate efficiently).

However, this is still an important development, since the algorithm can become a basis for future algorithm development and can provide a speed-up towards analyzing the energies for individual elements within systems that can be modeled using the coupled ball-spring model. For example, electrical circuits with capacitors and inductors, vibrations of molecules, and other systems that oscillate in a harmonic motion due to a slight perturbation.