Novel Control of Quantum Harmonic Oscillator System

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***Abstract*— This study proved that a permutated matrix *u*(t) can effectively control a quantum harmonic oscillator, unlike a scalar function that previous studies claim. Schrodinger's equation was solved using optimal control theory to determine a control matrix *u*(t), which was modeled in MATLAB with Simulink to confirm its controllability based on deBroglie's relationship.**

I. INTRODUCTION

The foundation of quantum mechanics and a wide variety of physical situations rests on the unique properties of the quantum harmonic oscillator. Unlike the classical oscillator, the quantum oscillator is capable of infinite energy levels. The multitude of eigenstates allows the controllability of the quantum oscillator, which is important because different energy levels affect the behavior of the oscillator. Through controlling the oscillator, it increases the flexibility and usefulness of modeling other quantum situations. For instance, the quantum harmonic oscillator is used to model the modes of vibrations in large molecules, the motions of atoms in a solid lattice, the theory of heat capacity, and the behavior of diatomic molecules. Any quantum system near an equilibrium state can often be expressed in terms of one or more harmonic oscillators.

Previous studies, [7], used modern laser technology to control molecular systems based on physical intuition. The limitations of such techniques prompted investigations on optimal control theory, where optimal control is a calculus-based method that uses state equations to determine the control law needed to attain a desired outcome from a given initial state.

To mathematically calculate the control function, previous studies examined Schrödinger's equation. The equation describes the behavior and the outcome of a dynamic system such as the quantum harmonic oscillator. The quantum system uses Schrödinger's equation solution in the form of a wave function. The state that is the wave function ψ measures position of a particle at a specific time such that $\psi^*\psi$= the probability of finding that particle at that given position and time.

The Schrödinger's equation is modified with a control input u(t):

$$i\frac{\partial \psi}{\partial t} = \left(H_0 + u(t)H_1\right)\cdot \psi \qquad (1)$$

where H_0 refers to the unperturbed Hamiltonian, H_1 represents the interaction Hamiltonian, and i is the imaginary number (square root of -1). (1) describes the effect the control function u(t) has on the quantum harmonic oscillator wave function. Mathematically, given any integer n>0, H_0 and H_1 are the following $(n+1)\times(n+1)$ Hermitian matrices (i.e., $\mathbf{A}^{T*} = \mathbf{A}$):

$$H_0 = \begin{bmatrix} \frac{1}{2} & & & \cdots & 0 \\ & \frac{3}{2} & & & \\ & & \frac{5}{2} & & \vdots \\ \vdots & & & \ddots & \\ 0 & & \cdots & & \frac{2n+1}{2} \end{bmatrix} \qquad (2a)$$

and

$$H_1 = \begin{bmatrix} 0 & 1 & 0 & \cdots & & 0 \\ 1 & 0 & \sqrt{2} & \ddots & & \vdots \\ 0 & \sqrt{2} & 0 & \sqrt{3} & & \vdots \\ \vdots & & \sqrt{3} & & \ddots & 0 \\ \vdots & & \ddots & & & \sqrt{n+1} \\ 0 & \cdots & & 0 & \sqrt{n+1} & 0 \end{bmatrix}. \qquad (2b)$$

Suppose the system is initially in state $\psi(0)=\psi_0$. The intention to control the oscillator is to use an external control function u(t) to force the system to a derived state ψ_d [1].

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This state, calculated with Schrödinger's equation, is a sinusoidal wave at a different frequency. According to the deBroglie relationship given that $n = 1, 2, 3 \ldots$,

$$E_n = \left(n + \frac{1}{2}\right)\lambda * \text{Planck's constant} \qquad (3)$$

the energy level E_n depends on the frequency, λ,of the oscillator. Therefore, a change in frequency suggests a change in the eigenstate of the oscillator. Unfortunately, the Hamiltonians (2) are unable to control the system with a scalar u(t) as implied by the literature.

II. Controllability

Some of the first few investigations of controllability assessed quantum systems with finite energy levels. For example, Mirrahimi et al.., used Lie groups to determine that finite quantum systems are controllable [1]. They focused on the situation where the external Hamiltonian, H_1 of the Schrödinger equation is time varying.

Additionally, they proved that the controllable part of the quantum harmonic oscillator corresponds to the classical dynamics of the average position q. They analyzed this derivation of Schrödinger's equation:

$$i\frac{\partial \psi}{\partial t} = -\frac{1}{2}\frac{\partial^2 \psi}{\partial q^2} + \left(\frac{1}{2}q^2 - u(t)q\right)\psi . \qquad (4)$$

Through Lie Algebra and the Schrödinger's equation, they also confirmed that the original infinite-dimensional system is not controllable.

Recently, Mirrahimi and Rouchon applied a Lyapunov-based approach that also verified the controllability of a finite dimensional oscillator [2]. The Lyapunov tracking design employs convergence analysis on a dynamic system. The researchers added a fictitious control ω to increase the degrees of freedom in their calculations. Furthermore, those studies proved that the tracking design method is valuable in clarifying state space problems and helping to simulate more realistic designs of molecular systems.

The objective of this research is to confirm controllability through a new law in controlling quantum harmonic oscillators. The study is conducted in three phases. First, the control function u(t) is generalized for an $(n+1) \times (n+1)$ matrix and calculated for controlling Schrödinger's differential equations. Then, the u(t) is applied to a MATLAB with a Simulink model of Schrödinger's equation to confirm the effectiveness of u(t) and the controllability of the system.

In order to determine the control function u, the Schrödinger differential equation had to be solved. We chose to solve a finite 3 x 3 quantum harmonic oscillator based on equation (1). Instead of using a scalar, which is equivalent to a diagonal matrix u(t), we used a permutation of the diagonal matrix:

$$\frac{\partial}{\partial t}\begin{bmatrix}\psi_1\\ \psi_2\\ \psi_3\end{bmatrix} = \begin{bmatrix}\frac{1}{2} & 0 & 0\\ 0 & \frac{3}{2} & 0\\ 0 & 0 & \frac{5}{2}\end{bmatrix} * \begin{bmatrix}\psi_1\\ \psi_2\\ \psi_3\end{bmatrix} + \begin{bmatrix}0 & u_1 & 0\\ 0 & 0 & u_2\\ u_3 & 0 & 0\end{bmatrix} * \begin{bmatrix}0 & 1 & 0\\ 1 & 0 & \sqrt{2}\\ 0 & \sqrt{2} & 0\end{bmatrix} * \begin{bmatrix}\psi_1\\ \psi_2\\ \psi_3\end{bmatrix} \quad (5)$$

Let

$$\mathbf{A} = \begin{bmatrix}\frac{1}{2} + u_1 & 0 & \sqrt{2}u_1\\ 0 & \frac{3}{2} + \sqrt{2}u_2 & 0\\ 0 & u_3 & \frac{5}{2}\end{bmatrix},$$

such that

$$i\frac{\partial \psi}{\partial t} = \mathbf{A}\psi .$$

This differential equation is solved by setting

$$\psi = \psi_0 e^{\mathbf{A}t} .$$

Laplace transforms were used to solve for a matrix set of solutions and obtained a solution in matrices:

$$\psi = \psi_0 \cdot \begin{bmatrix} e^{-i\left(\frac{1}{2}+u_1\right)t} & 0 & 0\\ 0 & e^{-i\frac{3}{2}t} & 0\\ 0 & 0 & e^{-i\frac{5}{2}t}\end{bmatrix} \qquad (6)$$

Where u_2, u_3 and initial conditions ψ_{02} and ψ_{03} are set to 0 to eliminate wave interference. Additionally, equation (6) was expressed as three separate equations through the relationship:

$$e^{it} = \cos t + i \sin t$$

$$\psi_1 = \psi_{01}\left(\cos\left(\left(-u_1 - \frac{1}{2}\right)t\right) + i\sin\left(\left(-u_1 - \frac{1}{2}\right)t\right)\right), \qquad (7a)$$

$$\psi_2 = 0 , \qquad (7b)$$

and

$$\psi_3 = 0 , \qquad (7c)$$

where (7b) and (7c) equal 0 because of the set initial conditions. It is evident that by varying u_1, that ψ_1 can change frequency. An integer u_1 would effect a change in discrete eigenstates through frequencies of $\frac{1}{2}$, $\frac{3}{2}$, $\frac{5}{2}$, and so on.

Since ψ is a complex vector, it can be decomposed into a real and an imaginary part. By solving each ψ separately in equation (5), we obtain:

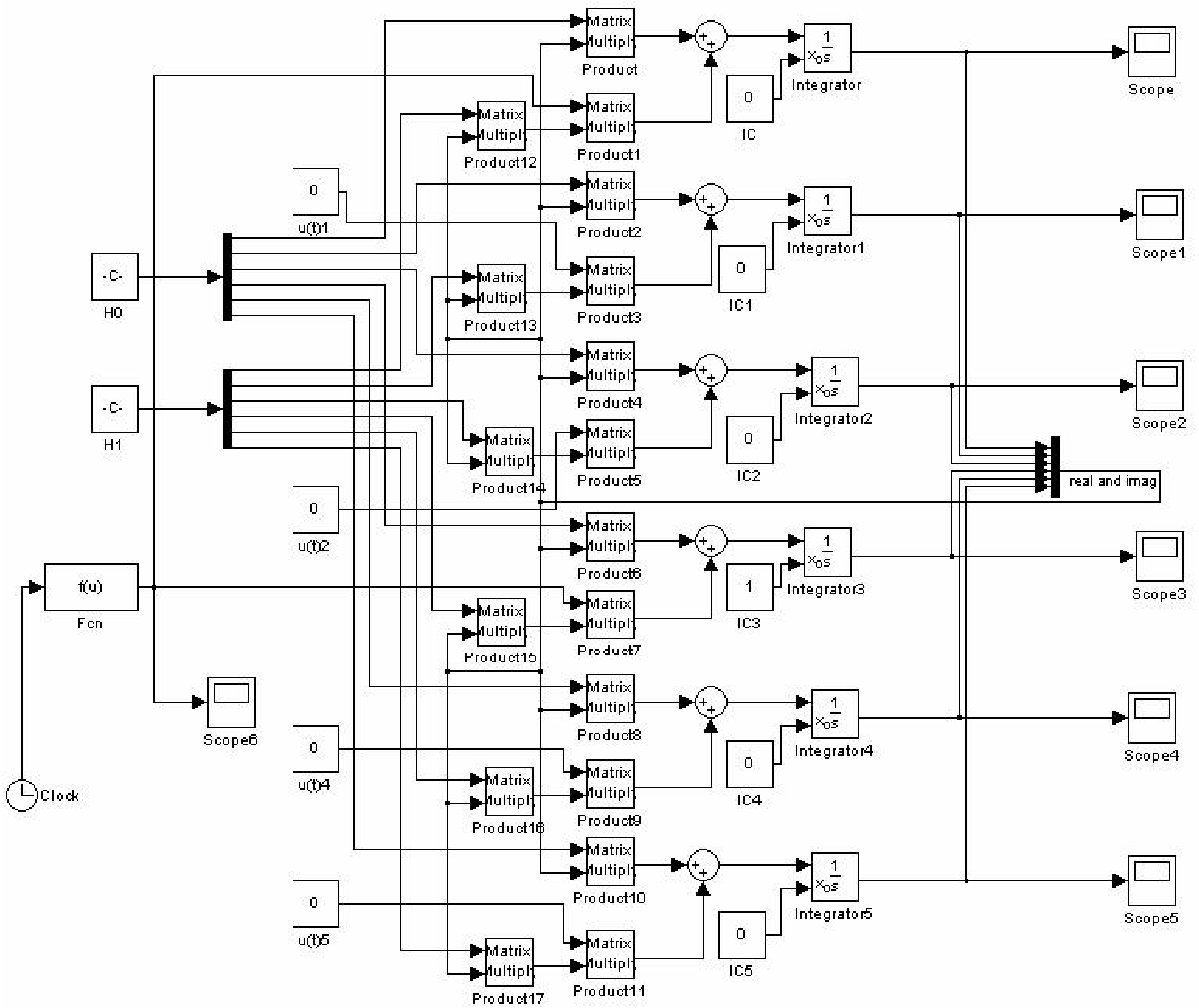

Figure 1. MATLAB with Simulink Model of a Controlled Quantum Harmonic Oscillator

$$\frac{\partial}{\partial t}\begin{bmatrix}\psi_{real}\\ \psi_{real}\\ \psi_{real}\\ \psi_{imag}\\ \psi_{imag}\\ \psi_{imag}\end{bmatrix}=\begin{bmatrix}0&0&0&\frac{1}{2}&0&0\\ 0&0&0&0&\frac{3}{2}&0\\ 0&0&0&0&0&\frac{5}{2}\\ -\frac{1}{2}&0&0&0&0&0\\ 0&-\frac{3}{2}&0&0&0&0\\ 0&0&-\frac{5}{2}&0&0&0\end{bmatrix}*\begin{bmatrix}\psi_{real}\\ \psi_{real}\\ \psi_{real}\\ \psi_{imag}\\ \psi_{imag}\\ \psi_{imag}\end{bmatrix}+\begin{bmatrix}0&u_1&0&0&0&0\\ u_2&0&0&0&0&0\\ 0&0&u_3&0&0&0\\ 0&0&0&0&u_1&0\\ 0&0&0&u_2&0&0\\ 0&0&0&0&0&u_3\end{bmatrix}*\begin{bmatrix}0&0&0&0&1&0\\ 0&0&0&1&0&\sqrt{2}\\ 0&0&0&0&\sqrt{2}&0\\ 0&-1&0&0&0&0\\ -1&0&-\sqrt{2}&0&0&0\\ 0&-\sqrt{2}&0&0&0&0\end{bmatrix}*\begin{bmatrix}\psi_{real}\\ \psi_{real}\\ \psi_{real}\\ \psi_{imag}\\ \psi_{imag}\\ \psi_{imag}\end{bmatrix} \tag{8}$$

Using MATLAB-Simulink (Natuck, MA) to model (8), a derivation of the controlled Schrödinger's equation is shown in Fig. 2. The control matrix function $u(t)$ was applied to the simulation in order to assess the effectiveness of $u(t)$.

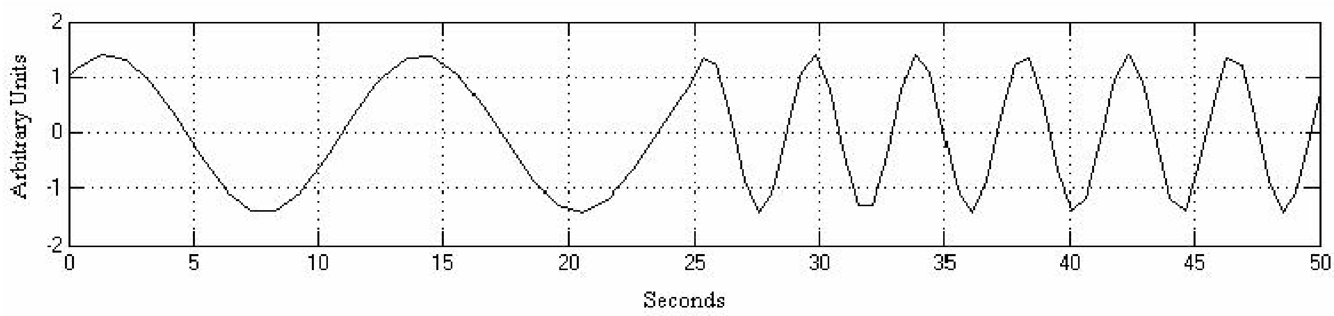

Figure 2. Quantum Harmonic Oscillator Curves with u_1 ramping from 0 to 1.

The determined matrix u(t) was then applied to Schrödinger's equation. The function was a step function for u_1 in (5) (u_2 and u_3 being zero due to initial conditions), ramping from 0 to 1 over 25 seconds. The oscillation curves produced by the controlled Schrödinger's equation are shown in Figure 2.

The frequency of the oscillator changes, which indicates a change in energy level.

The controllability of a finite Schrödinger's equation was confirmed with the calculation of u(t). Not only was the controllability confirmed, but a method was also determined that allows the change in energy of a molecular system. A matrix function, u(t), was shown to control quantum oscillators, and that a scalar function is not capable of such behavior. The generated sinusoidal waves, as shown in Figure 2, show the desired change in frequency and energy level. The successful change in state affirms the control function u(t) that was determined in equation (7).

III. CONCLUSIONS

A permutated matrix-based approach that systematically enables controllability is significant to the studies of quantum systems and quantum mechanics. However, this research only examined the controllability of finite systems. Future studies would reinvestigate the infinite level quantum harmonic oscillator and its possible applications in physics and quantum computing.

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