Abstract—The project investigates theoretical approaches of optimal control to study the issues of quantum computer. The main research is focused on the Carbon monoxide (CO) molecules model which have vibrational and rotational and many body entanglement coupling model of Nitrogen-vacancy center. Besides, we also study the optimal solutions for chloroform (CHCl$_3$) molecule under NMR system. This project integrates two methods, i.e. optimal control and genetic algorithm, to overcome a series of quantum control problems.

Introduction

In recent years, quantum computing and quantum information science have become one of the most important and attractive research areas in a variety of disciplines, e.g., mathematics, information science, physics, chemistry, etc. These new kinds of technologies are predicted to be much more advantageous compared with the classical computers and classical information science and the benefit obtained by these technologies is assumed to be beyond measure in our every-day life. For instance, quantum computers are predicted to be able to solve mathematical problems that today’s fastest computers could not solve in years. In particular, entanglement or entangled state plays a key role for quantum computing and quantum information processing. Based on above important events, this project integrates optimal control and genetic algorithm to overcome a series of quantum control problems.

Methodologies

Since the chloroform system is a liquid substance, the interatomic effect is considered to be a coupling effect, and its Hamiltonian can be expressed as,

$$H^J_{ij} = \sum_{ij} \hbar \pi J_{ij} I^{(i)} \cdot I^{(j)}$$

$$I^{(i)} = I^{(i)}_x \hat{x} + I^{(i)}_y \hat{y} + I^{(i)}_z \hat{z}$$

where $J_{ij}$ is called J coupling tensor.

The three spin operators are defined as:

$$I_x = \frac{1}{2} \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}, \quad I_y = \frac{1}{2} \begin{bmatrix} 0 & i \\ -i & 0 \end{bmatrix}, \quad I_z = \frac{1}{2} \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$$

Results and Discussion

The results integrated optimization and genetic algorithms in the NMR environment are presented in the following figures. The energy step of the transition field is used to simulate the entangled logic gates of two qubits.

Conclusion

In this study, the entangled logic gates of two qubits are successfully simulated the chloroform system under the nuclear magnetic resonance (NMR) environment, and the state fidelity and process fidelity were 0.9922 and 0.9839 respectively.

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