Building Mock Quantum Devices using Amazon Braket and CUDA-Q

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Abstract

Due to their long coherence times and exhibiting quantum coherence at room temperature, Nitrogen-Vacancy (NV) Centers in diamond are promising candidates for emerging quantum technologies [1]. Quantum registers, which are foundational in quantum computing, may be built from the electron and nuclear spins addressable in NV Centers.

To understand this approach in developing quantum computing better, researchers share a great interest in classically simulating the dynamics of a NV Center embedded in diamond with accuracy. However, conventional methods run into the challenge of complexity: simulating quantum systems with many particles ($N > 10$) requires demanding resources that are even challenging in high performance computing.

In our project, we approach this challenge using GPU acceleration through NVIDIA's CUDA-Q platform and AWS' Amazon Braket quantum computing service. By using GPU acceleration in hybrid quantum-classical algorithms, we explore the possibilities of scalability and the effects of noise in NV Centers as candidates for quantum computing hardware.

Dynamics in CUDA-Q

NVIDIA's open-source quantum computing development platform, CUDA-Q, includes their Dynamics API. The API provides tools for researchers to model and observe the dynamics of their systems; how the state of a quantum system evolves over time. In the context of quantum computing, these dynamics illustrate how the states of qubits (quantum bits) are shaped by control pulses over time. It is the quantum mechanical analog to observing the voltage or current changes over time across transistors.

The functionality of CUDA-Q Dynamics is centered around finding computational solutions to the Lindbladian, shown in the equation below. In this form of a quantum master equation, noise may be modeled in the form of jump operators, which describe dissipative dynamics in the system:

$$\dot{\rho} = -\frac{i}{\hbar}[H, \rho] + \sum \gamma_i \left(L_i \rho L_i^\dagger - \frac{1}{2}\{L_i^\dagger L_i, \rho\} \right)$$

for a system initiated in ρ that evolves under $H . L_i$ are jump operators that act with damping rates γ_i. Additionally, CUDA-Q leverages NVIDIA graphics hardware to speed up dynamics computations, showing significant improvement over non-GPU accelerated approaches with 10 or more qubits.

The Nitrogen-Vacancy Center

Nitrogen-Vacancy (NV) Centers are point defects in diamond lattices. A single carbon is substituted with nitrogen and an adjacent carbon is replaced by a lattice vacancy. When placed in an external magnetic field aligned with the NV-axis, the electron of a negatively charged NV centers (NV⁻) experiences Zeeman splitting providing the magnetic sublevels $m_S = 0$ and $m_S = \pm 1$. The NV nitrogen has nuclear spin $I = 1$, and the diamond carbons have nuclear spin $I = {}^1/_2$. We model their interaction with the electron using

$$H_1 = \omega_L I_z + A_\parallel S_z I_z + A_\perp S_z I_x,$$

which describes their interaction in the rotating frame of the electron for the corresponding nuclear hyperfine interaction tensor A. Here, ω_L is the Larmar frequency of the respective nuclear spin.

Noise Modeling

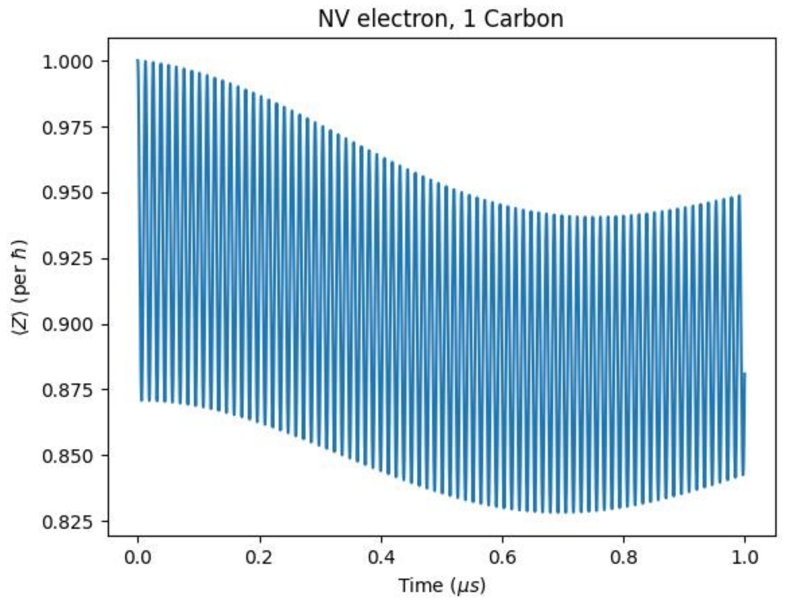
Dipolar interactions between the electron and neighboring carbon nuclear spins produces energy fluctuations of δE in the electron $|1\rangle$ state. These energy fluctuations manifest in the density matrix of the electron as decays in the off-diagonal terms. This aspect of noise may be modeled as pure dephasing at a damping rate $\gamma = \frac{\langle \delta E^2 \rangle - \langle \delta E \rangle^2}{2}$.

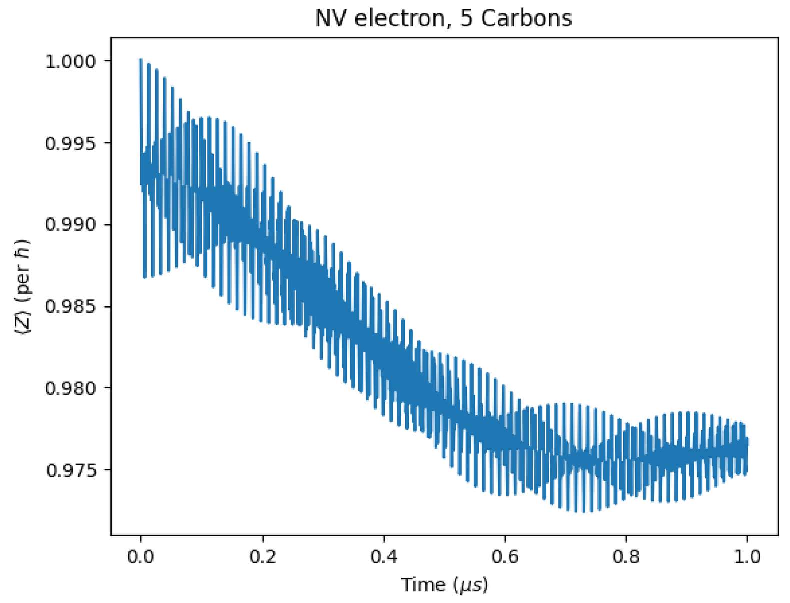
The damping rate depends on the strength of the dipolar interaction between the electron and nuclear spin. Nuclei closer to the electron will have a stronger damping rate, and the spatial distribution of the carbon nuclei is non-Markhovian. However, we approximate these dipolar interaction damping rates as 100kHz per carbon nucleus based on experimental measurements.

To model this, we simulated the following Hamiltonian for an NV Center with 1 and 5 system carbons prepared in the ground state:

$$H = 2\pi\Omega_e S_x + H_1$$

Where $\Omega_e = 10MHz$ is the driving rabi frequency of the electron, and H_1 is the interaction Hamiltonian from before.

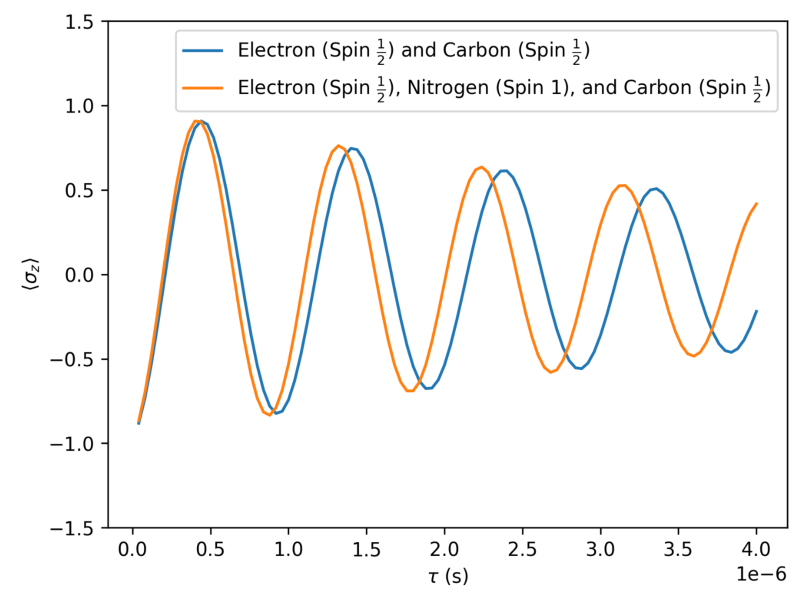


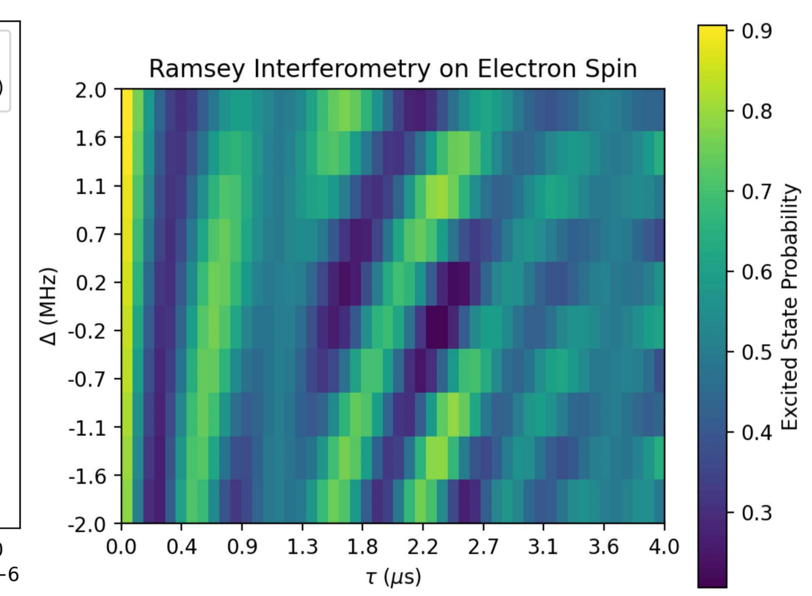


Simulating Coherence

We simulated Ramsey interferometry to model the coherent dynamics of the system. The electron spin was driven with ${}^\pi/_2$ pulses along the Y-axis of the Bloch sphere, with varying free evolution times in between these pulses. The system was modeled with a single coherently coupled carbon spin, as well as a nitrogen nuclear spin. Noise modeling of an incoherently interacting bath of carbon nuclear spins was incorporated as pure dephasing of the electron spin with a characteristic decay rate of 100 kHz.

When the hyperfine coupling strength between the electron and nuclear spins was simulated in the kHz frequency range, a clear decay of the Ramsey fringes was observed. When hyperfine coupling was increased to the MHz range to simulate stronger coupling, we observed collapse and revival behavior in the measured electron spin population due to entanglement and disentanglement over time between the electron and strongly-coupled nuclear spins.





Future Work and References

Our future work will be centered on applying numerous carbon nuclear spins in Ramsay interferometry and exploring dynamical decoupling.

The primary benefit of using CUDA-Q Dynamics instead of other quantum dynamic simulation tools is the speed up from GPU acceleration in complex systems. Expanding beyond 10 spin ${}^1/_2$ particles will help demonstrate the advantages of this platform.

Our work isn't only aimed at simulating realistic dynamics but also at exploring solutions to physical challenges faced by NV Centers if they are to be used in quantum hardware. Dynamical decoupling may be a feasible method at noise reduction and could further advocate for this approach to quantum computing.

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