Simulation and optimization of CPMG sequences for a nitrogen-vacancy center in a diamond

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1 Introduction

A single nitrogen-vacancy center in a diamond has been an emerging topic of research with applications in quantum-sensing [5] and quantum-computing [2] possible at ambient conditions. Read-out and initialization of the electron spin can be done optically. Extending the electron spin's coherence time we can increase the system's quantum volume for potential applications. One the methods to extend the T_2 time of an NV center is the usage of Carr-Purcell-Meiboom-Gill (CPMG) sequences with results showing a factor of 6 improvement [3]. The goal of this project is to simulate these sequences on a single NV center and investigate how can the pulse sequences be further optimized with the usage of machine learning, even apply these new pulses in quantum sensing protocols to showcase their effectiveness.

2 Motivation

As part of my student research I work on compiling and designing quantum algorithms on NV-centers for both quantum sensing and computational applications. Implementing the simulation of CPMG sequences will help me gain a deeper knowledge of NV centers and how I can gain computational advantage beyond the gate level.

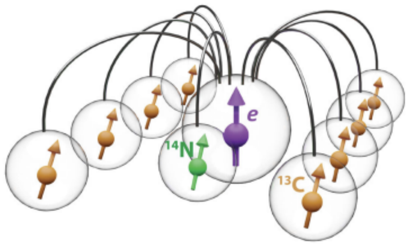

Figure 1: **Example of a central spin NV-center with several ^{13}C nuclear spins.** figure taken from [1]

3 Basic ideas

The spin system hamiltonian can be described by the following equation for an NV center with multiple nuclear spins:

$$H = \sum_i \gamma_i S_i [B_{static} + B_{drive}(t)] + \sum_i \Delta S_{z,i}^2 + \sum_{i,j} S_i A_{ij} S_j$$

where

- $S_i = (S_{x,i}, S_{y,i}, S_{z,i})$ are the spin operators
- γ_i are the gyromagnetic rations
- B_{static} and B_{drive} are magnetic fields
- Δ_i are the zero-field splitting or nuclear quadrupole parameters
- A_{ij} describes the interaction (e.g., hyperfine or dipolar) between the i-th and j-th spin

The first term represents the Zeeman interaction with static and driving fields. The second term accounts for zero-field splitting (for spin-1) and nuclear quadrupole effects. The last term describes interactions between spins, such as hyperfine coupling between an electron spin and nearby nuclear spins. CPMG pulses can be defined by first applying a $\frac{\pi}{2}$ pulse, after which n number of π pulses are applied with a final $\frac{\pi}{2}$ pulse applied at the end.

4 Proposed solution

The main goal of my project is to implement the simulation using Simphony, and open-source python based package with JAX and autodiff support. Simphony includes not only the basic Hamiltonian, but a quasistatic noise model as well, applying random local magnetic noise, providing us a framework to test effectiveness of the optimized sequences.
Thanks to the research of [4] we can use a hyperfine tensor calculated via a first-principles method giving the results a ground in reality as well.

5 Expected results

We expect to see an increase T_2 coherence time, but a difference between factors seen in literature is not unexpected as most ignore the hyperfine interaction between spins.

References

[1] C.E. Bradley, J. Randall, M.H. Abobeih, R.C. Berrevoets, M.J. Degen, M.A. Bakker, M. Markham, D.J. Twitchen, and T.H. Taminiau. A Ten-Qubit Solid-State Spin Register with Quantum Memory up to One Minute. *Physical Review X*, 9(3):031045, September 2019.

[2] F. Jelezko. Observation of Coherent Oscillation of a Single Nuclear Spin and Realization of a Two-Qubit Conditional Quantum Gate. *Physical Review Letters*, 93(13), 2004.

[3] Boris Naydenov. Dynamical decoupling of a single-electron spin at room temperature. *Physical Review B*, 83(8), 2011.

[4] István Takács and Viktor Ivády. Accurate Hyperfine Tensors for Solid State Quantum Applications: Case of the NV Center in Diamond, May 2024. arXiv:2309.03983 [quant-ph].

[5] J. M. Taylor, P. Cappellaro, L. Childress, L. Jiang, D. Budker, P. R. Hemmer, A. Yacoby, R. Walsworth, and M. D. Lukin. High-sensitivity diamond magnetometer with nanoscale resolution. *Nature Physics*, 4(10):810–816, October 2008. Publisher: Nature Publishing Group.