Computational Study of Dipolar Noise in Molecular Spin Qubits

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Introduction:

Quantum computing is a field that is making rapid progress today, both academically and financially. One of the biggest areas of research within it is looking at obtaining better quantum coherence times, that is, how long a qubit(quantum computing equivalent of a bit) can remain intact. This will be of great benefit as it will make quantum computers better equipped to solve practical problems. Atomic/molecular spins are one of the most promising candidates to be successful as a qubit and they are the focus of this project.

The goal of this project is to study how interactions between the electrons and nuclei in atoms/molecules affect quantum coherence. This goal will be achieved using computer simulations and by comparing the results of these simulations to existing results from recent studies. These studies are very promising in terms of telling us how accurate these simulation methods are and what the criteria are for providing better quantum coherence times.

This research topic interests me because quantum computing is a very modern field of research with plenty of problems to tackle and make further progress in. I feel once more progress is made in establishing quantum coherence there will be plenty of benefits, such as advances in computer simulation in physics and medicine, and positive impacts to other industries. I feel that during the course of this project I will be able to produce my own original work to compare with some of the studies from researchers actively working on these problems.

My objective upon completion of this project is that I will have produced an accurate set of results that can provide further clarity on answering the question of how to establish better quantum coherence times in atomic/molecular spin systems.

Methodology:

The methods I will use throughout this project will be strongly based around the theory of molecular spin dynamics and how to utilise the theory to put together an accurate computer simulation using several numerical strategies[1]. The completion of this project will be split into two main parts.

(1)Using a model system to observe spin decoherence. I will look at model systems that may not be considered completely realistic which will allow me to test computational efficiency and will make the results easier to interpret. I will simulate a single electronic spin surrounded by an increasing number of nuclear spins that are arranged linearly and equidistant from each other. In this section I hope to better understand the interactions between electric and nuclear spins and familiarise myself with the simulation software developed by Dr Lunghi.

(To be completed-weeks 1-3)

(2)Reproduction of existing experiments. I will move on from looking at model systems to looking at realistic systems that have been investigated in other studies. The first of these systems is a series of molecular qubits where the distance between the spin of the electron and the spin of the nucleus is progressively increased using a synthetic strategy[2]. The second system to be looked at is a Titanium ion as a qubit[3]. This system is of particular interest because no concluding interpretation of the decoherence mechanism observed could be provided on a sole experimental basis, so in looking at this system I hope to be able to produce results that will allow definite conclusions to be drawn.

(To be completed-weeks 4-6)

As the methods mentioned are theory and computer simulation based, this project is equipped to be completed remotely as that could be a possibility in the current climate, although in person work would help for making the completion of some sections easier if restrictions were reduced.

During this project I will simulate the various systems and interpret the results obtained from the computer simulations. In interpreting these results I will look for what factors allow for longer quantum coherence times and also where there is decoherence. At the end of this project I will bring all this together to see where the results can be built upon and lead to with further research. I will organise meetings with Dr Lunghi at regular intervals to discuss the progress of the project and how to proceed in the event of a problem arising. In doing this work I aim to develop my computer simulation and work presentation skills to effectively produce and explain the results obtained from this project so the main questions can be answered. The work being undertaken in this project is strongly linked to the work being researched by Dr Lunghi and his research group but it is still self-contained and can stand on its own with original results that will be produced during the course of my work on this project.

Collaboration and Interdisciplinary/International Focus:

This project has the possibility to look at the current international work being undertaken by researchers from various backgrounds and could even look at certain pieces of work here at Trinity College from schools such as the School of Physics, the School of Chemistry and the School of

Computer Science as concepts from each of these areas will be necessary to complete this project. I will also have the opportunity to work with other members of Dr Lunghi's research group in the case that any questions/problems arise and Dr Lunghi may be unavailable at the time.

Outcomes:

The main outcomes of this project will be to gain first-hand experience in working on a central topic in quantum science and familiarise myself with the fundamental theory of spin dynamics and decoherence. I will also tackle a real problem in developing quantum technologies and have tackled this problem using high level numerical computer simulation methods. Another outcome is the production of original results from a computer simulation of real molecular spin systems which would be of interest to the molecular magnetism community and can be used as a starting point for further, more-detailed research. All of this will then hopefully become a part of the success of the academically fascinating and financially promising field of quantum computing.

References:

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[2]*Graham, M. J., Yu, C. J., Krzyaniak, M. D., Wasielewski, M. R. & Freedman, D. E. Synthetic Approach To Determine the Effect of Nuclear Spin Distance on Electronic Spin Decoherence. J. Am. Chem. Soc. 139,3196–3201 (2017).*

[3] *Camargo, L. C. D. et al. Exploring the Organometallic Route to Molecular Spin Qubits: The [CpTi(cot)] Case. Angew. Chem. Int. Ed. 132, 1–7 (2020).*