Computational Study of Dipolar Noise in Molecular Spin Qubits

Trinity College Dublin
Coláiste na Tríonóide, Baile Átha Cliath
The University of Dublin

Student: Conor Ryan
Supervisor: Dr Alessandro Lunghi
School of Physics, Trinity College Dublin

LAIDLAW SCHOLARS

Introduction and Background

Molecular spins are amongst the most promising candidates for qubits, which are the basic units of quantum information and the building blocks of quantum computers. In the process of being used as qubits molecular spins undergo decoherence effects. This means information about the state of the system is lost and can't be extracted from the quantum computer. One way in which decoherence occurs is through spin-spin interactions. To bring us closer to having quantum computers which can tackle more practical and realistic problems the number of qubits needs to be increased and interactions such as spin-spin interactions need to be analysed and better understood to allow for this. This project aimed to provide some insight into these interactions by studying systems with an increasing rate of realism.

Aims

During the course of this project I aimed to analyse the decoherence behaviour of systems such as a chain of electronic spins, a chain of nuclear spins with a paramagnetic impurity at the centre, and the [CpTi(cot)] molecule which has shown some promising behaviour in terms of coherence in some new studies. My objective to accomplish this was to study the rate of decoherence in these systems with respect to different parameters and also determine the position of the spin diffusion barrier.

Methodology

To achieve the aims of this project I ran numerous computer simulations using the MolForge software designed by my supervisor. The main technique used was the spin-echo process, which flips the magnetisation in the *z*-direction, M_z, into the *xy*-plane and tracks M_x, giving an echo signal which can be plotted which allows for an analysis of the decoherence behaviour. I then converged the results with respect to the number of spins and the size of the Hilbert Space to see the rate of decoherence in each system.

Results

Chain of Electronic Spins

This system consisted of a chain of electronic spins along the *x*-axis and was analysed using the "fully polarized" initial condition where all spins were initialised along the +*z*-axis and the "thermal population" initial condition with an average temperature of 10K.

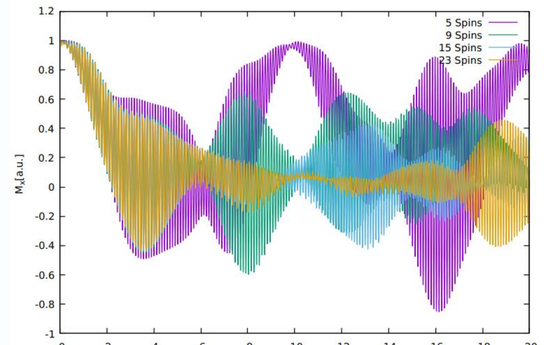


Fig 2: Convergence of polarized electron chain with respect to the number of spins

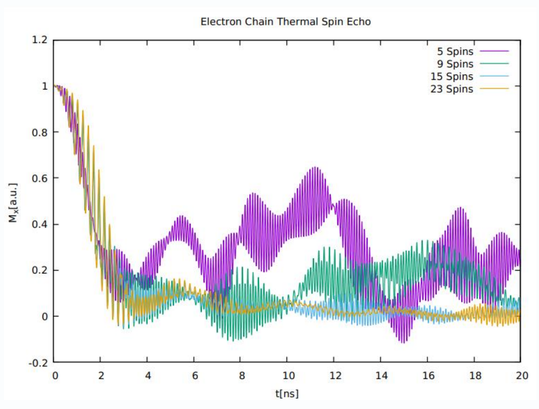
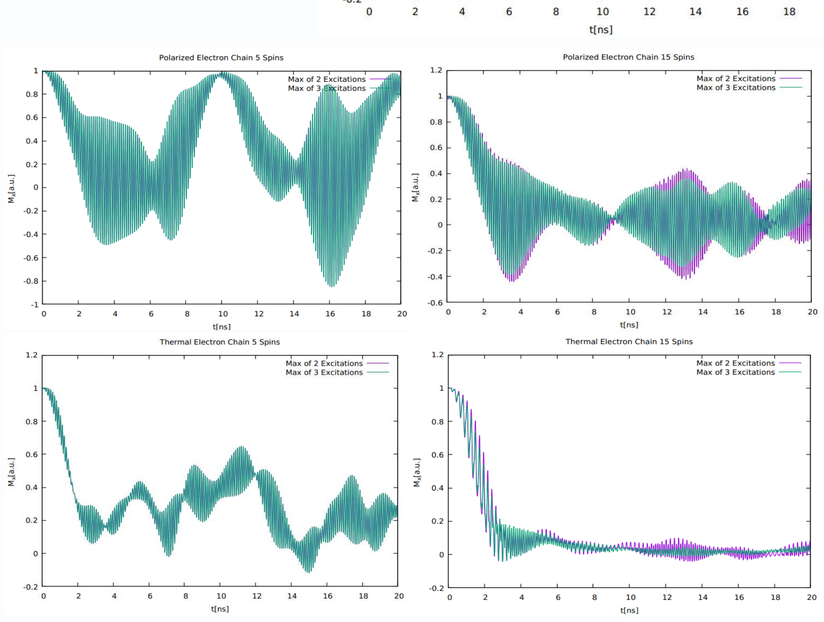


Fig 3: Convergence of thermal electron chain with respect to the number of spins

Fig 4-7: Convergence with respect to "max_ex" for polarized chain (top), thermal chain (bottom) for 5 spins (left) and 15 spins (right)



Chain of Nuclear Spins with a Paramagnetic Impurity

This system was made up of a chain of nuclear (^{1}H) spins with a paramagnetic impurity (electronic spin) at the centre. It was analysed with just the "thermal population" initial condition with an average temperature of 10K.

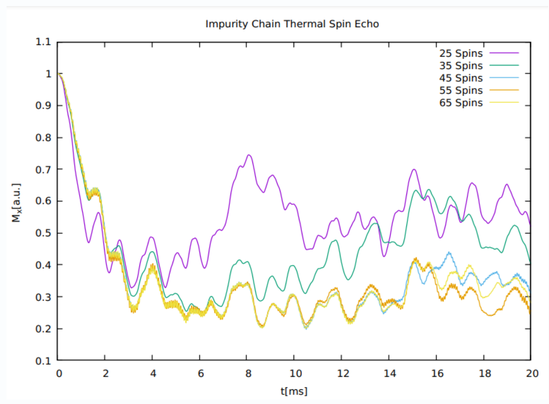


Fig 8: Convergence of thermal nuclear chain with respect to the number of spins

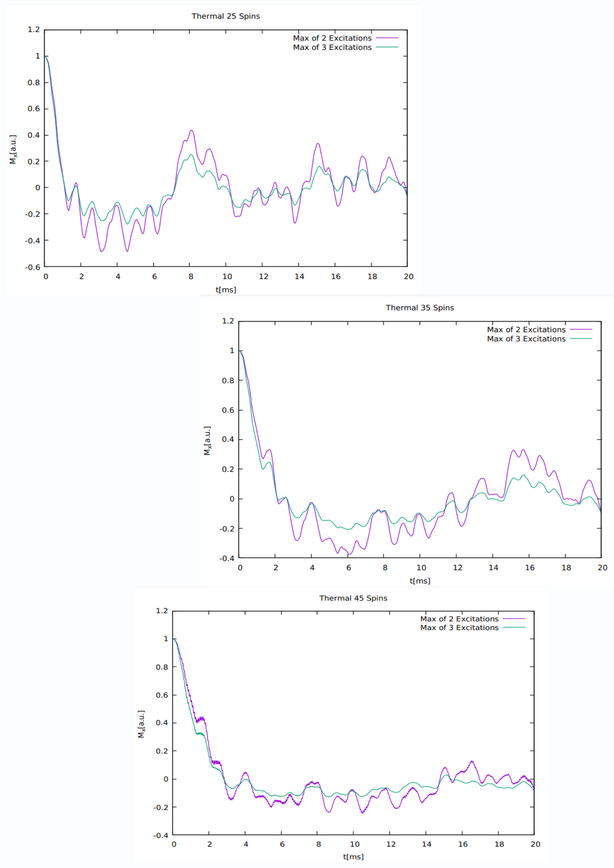


Fig 9-11: Convergence of nuclear chain with respect to "max_ex" for 25 spins (top), 35 spins (centre) and 45 spins (bottom)

[CpTi(cot)] Molecule

This system consists of a ^{48}Ti atom(purple), ^{12}C atoms (black) and ^{1}H atoms (white). The spin-spin interaction between the Ti atom and H atoms were studied by cutting spheres of increasing radius around the Ti atom.

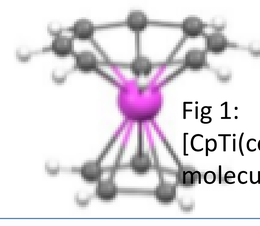
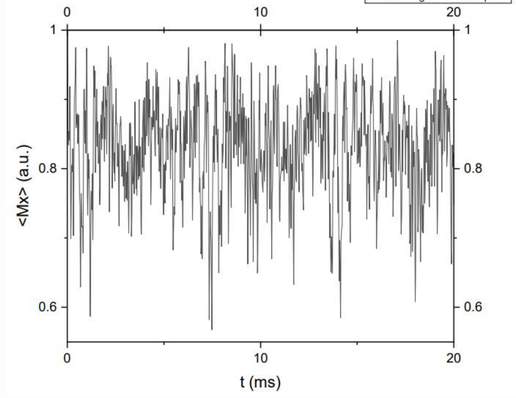


Fig 1: [CpTi(cot)] molecule



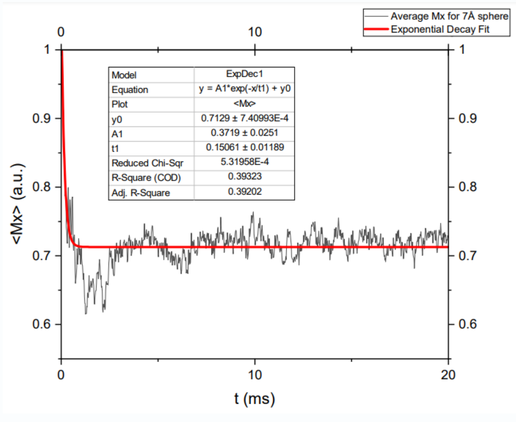


Fig 12-13: Average M_x over various rotations of the molecule for spheres of radius 5Å(top) and 7Å(bottom)

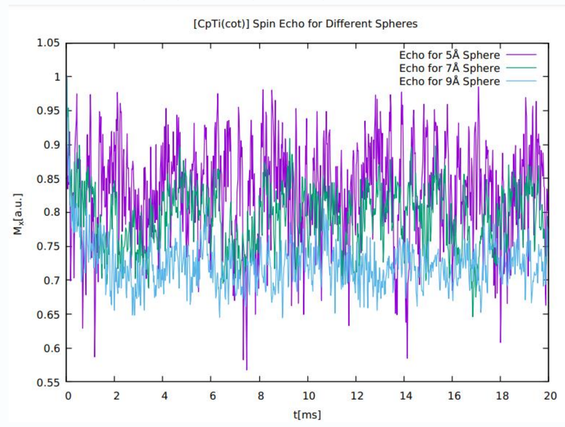


Fig 14: Overlapping plot comparing M_x from spheres of size 5Å(purple), 7Å(green) and 9Å(blue)

Conclusions

- The results for the electron spin chain converged well with respect to both the total number of spins and the maximum number of excited spins. The rate of decoherence in this system appears to be around 2ns and the effect of constraining the maximum number of excited spins gets stronger with an increasing number of spins.
- The nuclear chain has a rate of decoherence of 1-2ms because the interaction between the electron and nuclei takes longer since they do not have similar resonance energy levels.
- A boundary for the spin diffusion barrier of the [CpTi(cot)] system was found to be 4-6Å which agrees with [2].
- Coherence times, T_2, were found in the range of 150-470µs. This large range is because only the 7Å sphere could be averaged over different configurations.

References

[1] Lunghi, A. & Sanvito, S. Electronic spin-spin decoherence contribution in molecular qubits by quantum unitary spin dynamics. J. Magn. Magn. Mater. 487, 165325 (2019).
[2] 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).

Acknowledgements

I would like to acknowledge the Laidlaw Foundation for giving me the opportunity to do this project and also for funding it. I would also like to thank the Irish Centre for High End Computing for allowing me to use the supercomputer Kay to obtain several key results.