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Understanding spin decoherence of molecular qubits.

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Understanding spin decoherence of molecular qubits

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Abstract

Quantum technologies rely on qubits, which encode and manipulate information in quantum states $|0\rangle$ and $|1\rangle$ simultaneously in a multidimensional manner. To fully harness the advantages of quantum computing, qubits must maintain their properties, such as entanglement, superposition, and constructive interference. However, qubits are highly susceptible to the environment, a problem that leads to decoherence, the loss of quantum information through the collapse of superposition. Due to the challenge represented by decoherence, the approach to simulate possible candidates for qubits has been generated. Nonetheless, simulating the complex nature of quantum phenomena requires substantial computational power to be carried out efficiently. Recently, new methods have been developed to simplify the simulation process of quantum dynamics. In the following report, the open-source Python library PyCCE is used to perform simulations on classical hardware of the compound $[CpTi(cot)]$ as a promising s = $\frac{1}{2}$ molecular qubit since the states of the spin-$\frac{1}{2}$ serve as a two-level system. The primary challenge relies on measuring the interaction of the central spin with the rest of the spin bath, which can be solved using the method Cluster Correlation Expansion (CCE). In this work, CCE is used to calculate the coherence of the central spin by varying the cluster order, the bath radius, the dipole interaction radius, the magnetic field, and the deuterium ^2H isotopic variation.

Keywords: Decoherence, Spin qubits, [CpTi(cot)], PyCCE, CCE

Introduction

Over the past few years, the scientific community has recognized the significance of the second quantum revolution. In the 1960s, physicist John Bell established a theory that laid one of the most crucial foundations for modern quantum systems—the correlation between entangled particles [1]. In the early 1980s, the potential of representing information within quantum systems for enhancing information processing mechanisms was acknowledged [2].

Currently, the primary objective is to attain control over individual quantum systems, leading to the realization of a universal quantum computer capable of executing arbitrary quantum algorithms. Such a development would have applications in various fields, including chemistry, biology, communication systems, as well as the creation of atomic clocks for GPS and cryptography, among numerous others [3]. To accomplish these goals, the quantum technology industry must collaborate in the areas of simulation, error correction, and the development of large-scale and efficient quantum hardware.

In a quantum computer, information is stored in quantum bits (qubits), which are the fundamental units of information. These qubits consist of two basis states represented as $|0\rangle$ and $|1\rangle$. Various physical systems have been engineered to serve as qubits, with trapped ions, photons, superconducting qubits, and spin qubits being the most extensively studied. The scope of this report centers around spin qubits.

Spin qubits

A spin-$\frac{1}{2}$ inside a magnetic field can act as a two-level system in which the spin up will act as a high energy state ($|\uparrow\rangle = |1\rangle$) and the spin down as a low energy state ($|\downarrow\rangle = |0\rangle$).

Electron spins have been widely studied for quantum information processing due to their reproducible nature and ability to engineer coupled systems [2]. Because of the negative charge of electrons, spin qubits can be manipulated using an external magnetic field in the z-direction to split the energies of the spin states [4]. This allows the creation of single-qubit gates represented as rotations of the Bloch sphere around an axis and at some angle. Rotations about the x-y plane can be performed with microwave pulses, and rotations about other axes can be performed by decomposition into a series of x and y rotations.

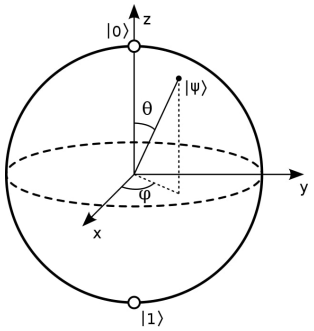


Figure 1: Bloch sphere representation. If the direction of the state ψ is pointing in the positive z-direction the qubit is in the $|1\rangle$ state (spin up) if pointing in the negative z-direction the qubit is in the $|0\rangle$ state (spin down) [5]. $|\psi\rangle$ point is represented by $|\psi\rangle = \alpha|0\rangle + \beta|1\rangle$

[22]

Decoherence

However, one of the main issues with physical quantum systems is the loss of information due to the system's interaction with the environment. This interaction causes an undesirable phase shift. In quantum information processing, information is expressed as a superposition of the basis states $|1\rangle$ and $|0\rangle$, when the system interacts with the environment, these states become mixed, resulting in the loss of the superposition state [6]. To measure and characterize the loss of coherence, two quantities are considered: the relaxation time T_1 which involves the evolution of an initial state towards a steady state, and the dephasing time T_2 (also named spin-spin relaxation time) which can be thought as the loss of quantum coherence over time, generally we would expect for $T_1 > T_2$ [8] . In this study, our focus is on T_2.

In an experimental setup, T_2 can be measured following a sequence of operations, first a qubit is prepared in a superposition state $|\psi\rangle = \alpha|0\rangle + \beta|1\rangle$ (where α and β are probability amplitudes) by applying a $\frac{\pi}{2}$-pulse to the qubit, wait some time τ and apply another pulse of the same magnitude to bring the qubit back to the ground state. After this process, the state of the qubit is measured [5].

In the context of spin qubits, the central spin and the spin bath form an isolated subsystem within the environment. Consequently, the decoherence of the qubit arises from its entanglement with the bath during the coherent evolution of the system [7].

Certain molecular systems with a low natural abundance of nuclear spins, such as carbon and silicon, have exhibited coherence times (T_2) in the range of several hundreds of microseconds [2]. The qubit is prepared in the state: $|\psi\rangle = \frac{1}{\sqrt{2}}(|0\rangle + e^{i\phi}|1\rangle)$. The loss of coherence is determined by the loss of the relative phase between the $|0\rangle$ and $|1\rangle$. This is characterized by:

$$L(t) = \frac{\langle 1|\hat{\rho}(t)|0\rangle}{\langle 1|\hat{\rho}(0)|0\rangle} = -e^{\frac{t^2}{T_2}}\,[8] \tag{1}$$

Where $\hat{\rho}(t)$ is the density matrix of the central spin [8].

The interaction between the central spin and the spin bath can be described by the Hamiltonian of the interaction:

$$\hat{H} = \hat{H}_S + \hat{H}_{SB} + \hat{H}_B \tag{2}$$

Where:

$$\hat{H}_S = \sum_i ((S_i D_i S_i + B_{\gamma S_i} S_i + \sum_{i<j} S_i K_{ij} S_j) \quad (3)$$

Is the Hamiltonian of the central spin, which typically includes terms accounting for the Zeeman energy due to an external magnetic field and local energy contributions.

$$\hat{H}_{SB} = \sum_{i,k} S_i A_{ik} I_k \quad (4)$$

Is the Hamiltonian of the interaction which captures the coupling between the central spin and the bath spins. It is typically modeled using the dipolar interaction between the central spin and bath spins.

$$\hat{H}_B = \sum_k I_k P_k I_k + B_{\gamma_k} I_k + \sum_{k<l} I_k J_{kl} I_l \quad (5)$$

Is the Hamiltonian of the spin bath

- $\hat{H}_S$: Hamiltonian of the free central spin
- $\hat{H}_{SB}$: Interaction hamiltonian between the spin and the bath spin.
- $\hat{H}_B$: Intrinsic spin bath interactions
- $D(P)$: Interaction tensor of the central spin bath.
- γ_i :Gyromagnetic ratio of the i-spin describing the interaction with the external magnetic field.
- A : Interaction tensor between central and bath spins.
- $J(K)$: Interaction tensor between center spins.
- B: External magnetic field.
- S_z: Z-component of the central spin operator.
- D_i: Dipolar coupling strength between the central spin and the i-th bath spin

The parameters of the Hamiltonian will depend on the details of the system like the nature of the central spin, the size of the cluster and the length limit for the interaction [8].

The decoherence of a central spin qubit poses a challenge for spin-based technologies, and to understand it, it is required to investigate the dynamics of the bath. The primary approach to studying bath dynamics is through quantum many-body theory. Realistically, it is challenging to achieve complete isolation of quantum systems since external perturbations can interfere with information processing. When a central spin interacts with coupled spins in the environment, information loss occurs in the central qubit, resulting in a decay of phase coherence [21].

It is possible to solve the Schrodinger equation of the total system, although the complexity of that calculation grows exponentially as the bath grows. Thence, a most suitable approach is to reduce the contributions from the bath with spin clusters in terms of the coherence function, which is the core idea of the Cluster Correlation Expansion (CCE) method, the goal is to mitigate the complexity by decomposing the bath into a series of spin clusters.

The coherence function in this context can be expressed as:

$$L(t) = \prod_p Lc = \prod_i \tilde{L}_i \prod_i j\tilde{L}_{ij} \quad (6)$$

Where L_i is the contribution of the single bath spin i and L_{ij} is the contribution of a spin pair ij.

The maximum size of the cluster included into the expansion determines the order of the CCE approximation, each cluster contribution is defined as:

$$\tilde{L}(t) = \frac{L_C}{\prod'_C \tilde{L}_{C' \subset C}} \quad (7)$$

For a pair of spins, the coherence function can be written as:

$$\tilde{L}_{ij} = \frac{L_{ij}}{\tilde{L}_0 \tilde{L}_i \tilde{L}_j} \quad (8)$$

PyCCE

In the field of quantum technologies, simulating quantum operations serve as valuable tools for researching physical applications and algorithms. However, a major limitation arises from the high degree of complexity exhibited by quantum systems, which demands significant computational power [9].

PyCCE is an open-source Python library that provides a solution to this challenge. It enables the simulation of spin decoherence in a realistic spin bath using the cluster correlation expansion method (CCE). The library facilitates the necessary calculations of the central spin and allows for the modification of interaction parameters [8]. With PyCCE, researchers can acquire insights about the behavior of the central qubit and visualize the impact of the bath on decoherence. Simulators offer a practical approach to studying the properties of a quantum system, avoiding the need of experimental trial and error which can be resource and time-consuming [10].

[CpTi(cot)] Complex

Organometallic sandwich complexes represent a versatile class of compounds characterized by two planar, cyclic, and π-bonded ligands [11]. They have gained significance in organometallic chemistry and have recently been utilized in experiments involving single-molecule manipulation and spin sensing. CpTi[cot] is an organometallic complex with the formula $[(\eta 8 - C_8H_8)M(\eta 5 - C_5H_5)]$, where Cp represents $\eta 8 - C_8H_8$, cot represents $\eta 5 - C_5H_5$, and M represents a metallic element. These compounds have found applications as single molecule magnets for spintronics and in the implementation of quantum gates due to the presence of an unpaired electron in the nonbonding d_z^2 orbital [12].

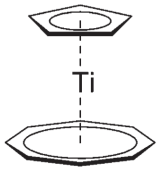


Figure 2: Visualization of a $[(\eta 8 - C_8H_8)Ti(\eta 5 - C_5H_5)]$

[14]

In a recent experimental study conducted at the University of Florence, pulsed electron paramagnetic resonance (EPR) was employed to investigate the coherence properties of the s=$\frac{1}{2}$ organometallic sandwich [CpTi(cot)] in frozen deuterated toluene solution at a temperature of 4.5 K ($-258.65°C$). The study utilized Hahn-echo decay experiments and found a coherence time in the range of tens of microseconds. To mitigate the contribution of solvent-induced decoherence, a deuterated solution was utilized, as deuterons lead to longer time scales of the echo decays [13]. It is worth noting that this experiment considered weak spin-phonon coupling.

The presence of decoherence in paramagnetic molecules limits their viability as qubits. In the case of organic molecules like [CpTi(cot)] diluted in frozen solutions at cryogenic temperatures, the main source of decoherence arises from neighboring nuclear spins, this can be predicted by studying the molecular structure of the organic complex [13].

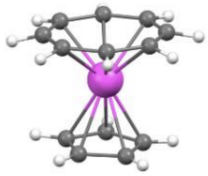


Figure 3: Visualization of the chemical structure of the [CpTi(cot)]complex

[12]

Methods

PyCCE was developed by Mykyta Onizhuk and Giulia Galli from the University of Chicago in 2021. The software aims to provide a reliable implemen-

tation of the Cluster Correlation Expansion (CCE) method for predicting the dynamics of a spin qubit within a bath and estimating the coherence times for different materials. This makes it a valuable tool for experimental research in the field of spin qubit engineering.. To run simulations using PyCCE, users need to follow the workflow outlined in the documentation [15]. Here, I provide a general overview of the steps involved in creating the spin bath and localizing the central spin qubit.

The first step is to initialize the structure of the supercell of the material and populate it with spins using the BathCell class. This class allows users to specify the properties of the spin bath, parameters for the unit cell, and properties of the nuclear spins using the EasySpin database. PyCCE utilizes concentrations of the most common stable isotopes with non-zero spin based on the database. However, users can explicitly define the abundance of each isotope if desired [8].

The research focused on obtaining a quantitative understanding of spin coherence in $CpTi[cot]$ to enable accurate predictions for future experiments. As part of this effort, a file containing the xyz coordinates for this chemical system was provided. Specifically, the coordinates in the x, y, and z directions were stored for each element. The file consists of 108 atoms, with 52 corresponding to hydrogen, 52 to carbon, and 4 to titanium. To better visualize the unit cell, which was constructed using these values and the BathCell parameters, a graphical representation was designed and can be seen in the figure 4 [8].

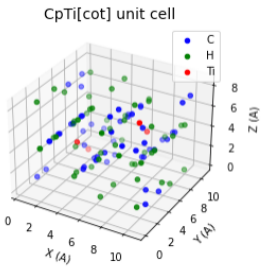


Figure 4: Visual representation of a unit cell for CpTi[cot]]

The BathCell class provides several functionalities for the user. It allows the user to define the direction of the Cartesian coordinates, add atoms at specific lattice sites, add isotopes with specific concentrations, and generate a supercell of a desired size. To populate the system with spins, the function gen-supercell is used, which specifies the position of the Ti atom to be removed. Removing the Ti atom from that position is necessary to place the spin-$\frac{1}{2}$ qubit in the chemical system [8].

Once the unit cell is constructed, the next step is to input the properties of the central spin into the Simulation object. PyCCE requires the user to provide the properties of the central spin using the CenterArray class. This class allows for the setup of an array of several central spins, with each central spin accessible as an element of the object [8]. For the simulation in this particular report, only one central spin was used.

The CenterArray class takes several inputs, including the number of central spins, the total spin-($\frac{1}{2}$), the position (which, in this case, corresponds to the coordinates of the previously removed Ti atom), and the states of the qubits (($|0\rangle$ and $|1\rangle$). The following lines of code show the transformation of the unit cell coordinates for the removed Ti atom to cartesian coordinates and the CenterArray class in which the spin-$\frac{1}{2}$ is specified, as well as the position for the qubit and its states:

```
position=titanium.to_cartesian
        ([xt[3], yt[3], zt[3] ])
spin = pc.CenterArray(spin=0.5,
                position=position,
                alpha=1, beta=0)
```

Once the properties of the central spin qubit are established, the next step is to set up the Simulator object to compute the coherence function. To do this, we need to define the size and parameters of the spin bath that PyCCE will use for calculating the Cluster Correlation Expansion (CCE). The parameters that need to be defined are as follows:

- Radius of the bath: This is the maximum distance from the central spin to a bath spin that will be considered in the calculation.

- Radius for the spin interaction: This parameter sets the maximum distance at which two bath spins (labeled i and j) are considered to have an "edge" or interaction between them.
- Order of the interaction (order): This parameter determines the maximum size of the total spin system that will be considered in the CCE method.
- The $|0\rangle$ and $|1\rangle$ states of the qubit: These states have already been specified in the CenterArray class.
- The external magnetic field: This field needs to be specified as it can influence the dynamics of the central spin qubit.

By setting up the Simulator object with these parameters, you can compute the coherence function and analyze the dynamics of the spin qubit within the spin bath using the CCE method.

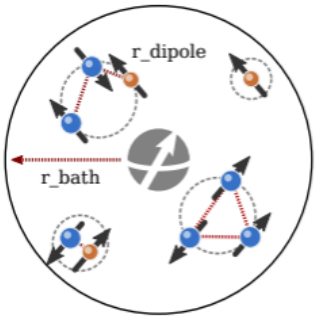


Figure 5: Visual representation for the properties of the central and cluster composition [8]

Once the parameters are determined, the Simulation object can compute the coherence function using either the conventional CCE or the generalized CCE. The main distinction between these two methods lies in the treatment of the interactions. In the conventional CCE, interactions are expressed as the sum of two effective Hamiltonians that are mapped onto two-level spins. On the other hand, the generalized CCE directly incorporates the degrees of freedom of the central spin, with the central spin included in each cluster [8].

Conventional CCE The sum of the two effective Hamiltonians are conditioned on the qubit levels:

$$\hat{H} = \langle 0|0\rangle \otimes \hat{H}^0 + \langle 1|1\rangle \otimes \hat{H}^1 \tag{9}$$

Where $\hat{H}^\alpha$: Effective Hamiltonian acting on the bath.

The initial state of the bath spin cluster C is characterized by the density matrix $\hat{\rho}_C$. And the coherence function is computed as:

$$L_C(t) = Tr[\hat{U}_C^0(t)\hat{\rho}_C\hat{U}_C^{1\dagger}(t)] \tag{10}$$

Where $\hat{U}_C^\alpha(t)$: Time propagator define in terms of the effective Hamiltonian.

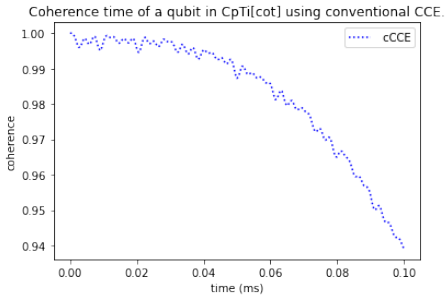
Generalized CCE The cluster Hamiltonian including the central spin degrees of freedom:

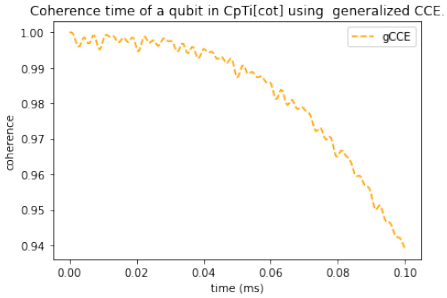
$$\begin{aligned}\hat{H}_C = \hat{H}_S + \\ \sum_{k,i\in C} S_k A_{ki} I_i + \sum_{i\in C} I_i P_i I_i + B\gamma_i I_i + \\ \sum_{i<j\in C} I_i J_{ij} I_j + \sum_{k,a\notin C} S_k A_{ka}[I_a] + \sum_{i,a\notin C} I_i J_{ia}[I_a]\end{aligned} \tag{11}$$

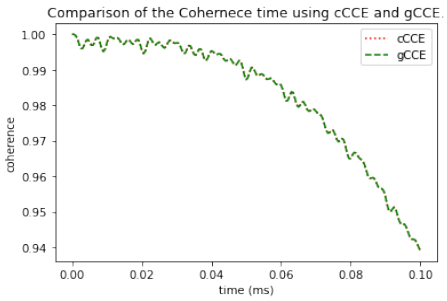
And the coherence function is computed as:

$$L_C(t) = \langle 0|\, \hat{U}_C(t)\hat{\rho}_C\hat{U}_C^{1\dagger}(t)\, |1\rangle \tag{12}$$

To explore any significant differences between the calculations performed by these two methods, I used both approaches. The graphs shown below were made with the conventional and generalized CCE, as well as a last graph showing that both behave in a similar way for the system that is being studied in this project.







Results

To compute the desired properties, we require to use the PyCCE method 'simulator.compute' which takes the following parameters:

- Timespace: These are the time points, expressed in milliseconds, at which the computation is performed.
- Quantity: You can choose to calculate either the coherence function or the noise autocorrelation function.
- Method: You can specify whether to use the conventional CCE or the generalized CCE method.
- Magnetic field External: The external magnetic field is already provided in the Simulator object.
- Pulses: This parameter corresponds to the magnetic pulses associated with the Hahn-Echo experiment.
- Delay: If the time points represent delayed time intervals, this parameter is set to True; otherwise, if the time points represent the total time, it is set to False.

By specifying these parameters and calling the simulator method, we can perform the desired calculations and obtain the results for the coherence function.

The following lines of code specify the time points in which the calculation will be carried out, starting from time 0 and ending in 0.5 milliseconds, 201 points will be computed using the previously specified parameters. Additionally, the line of code required to calculate consistency with the CCE method is shown.

```
time_space = np.linspace(0, 0.10, 201)
n = 1
b =25000

l_cCCE = calc.compute(time_space, pulses=n,
                      method='cce',
                      quantity='coherence',
                      as_delay=False)
```

The main goal for this project is to present the results obtained from simulating the spin decoherence of $CpTi[cot]$ using the cluster correlation expansion (CCE) method with the assistance of the Python package PyCCE. In the first simulation, an initial magnetic field of 1.2 T was applied, which corresponds to the magnetic field used in the experimental research conducted at the University of Florence [13]. This magnetic field strength is considered moderately high and has a significant impact in the compound since organometallic complexes containing transition metal ions exhibit significant magnetic properties [12]. Additionally, single-qubit gate operations can be achieved purely through magnetic field control, making the magnitude of the applied magnetic field a crucial factor of interest [16].

Using the parameters:

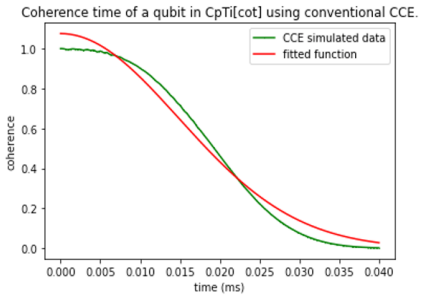
- Bath radius = 30 Å
- Dipole radius = 6 Å
- CCE order=2
- Magnetic Field = 12000 Gauss (1.2 T)

And uing the equation previously mention in the introduction:

$$L(t) = \frac{\langle 1|\,\hat{\rho}(t)\,|0\rangle}{\langle 1|\,\hat{\rho}(0)\,|0\rangle} = -e^{\frac{t^2}{T_2}}\,[8] \tag{13}$$

T_2 can be calculating using the curve fitting:

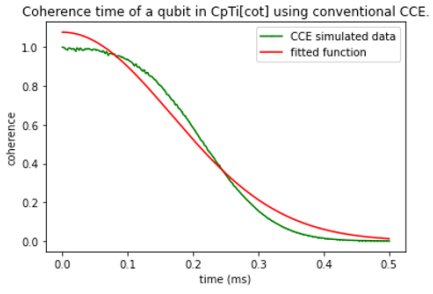
$$T_2 = \frac{t^2}{ln(t)} \tag{14}$$



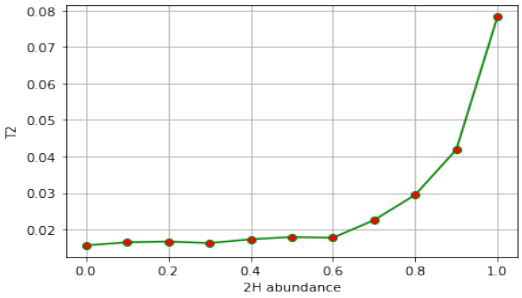
A T_2 of 14.52 μs was obtained.

As mentioned by the researchers in Florence, the coherence of the system improves when using a deuterated solution, this is because the gyromagnetic ratio of ^1H is 42.57608 MHz/T, while the one for ^2H is 6.53569 MHz/T [17]. This significant difference in gyromagnetic ratios makes ^2H an ideal candidate for improving coherence. The reason for this is that the spin-spin interaction between the central qubit and the surrounding spins becomes stronger as the gyromagnetic ratio increases [18].

When conducting the simulation with the same parameters as mentioned earlier, a T_2 value of 14.52 μs was obtained, however, in the presence of ^2H isotopes, the T_2 was 38.66 μs. This satisfies the theoretical conclusion that ^1H is the main source of decoherence.



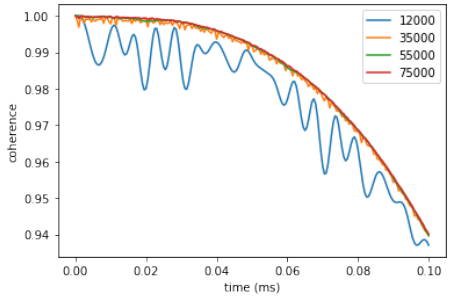
To visualize the effect of the presence of ^2H isotopes, multiple simulations were conducted varying isotope concentrations. The T_2 values were calculated for each simulation, and the following results were obtained:



$[^2H]$	T_2 (ms)
1.0	0.078246835
0.9	0.041864554
0.8	0.029467464
0.7	0.022541004
0.6	0.017709072
0.5	0.017918429
0.4	0.017290949
0.3	0.016264418
0.2	0.0166848
0.1	0.016472925
0.0	0.015624211

The results demonstrate that as the concentration of ^2H isotopes increases, the T_2 value also increases.

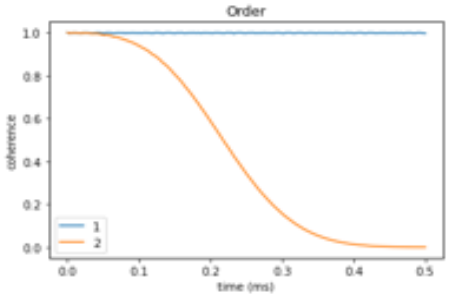
As mentioned earlier, the external magnetic field has a significant impact on the T_2 time. In order to gain a better understanding of the behavior of coherence, convergence tests were conducted by varying the magnitude of the external magnetic field from 1.2, 3.5, 5.5 and 7.5 T.

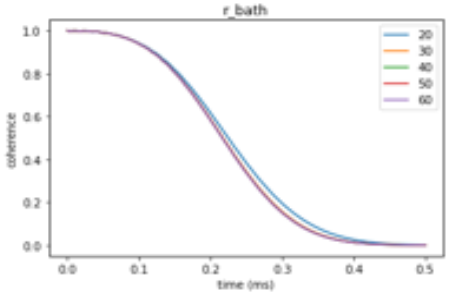


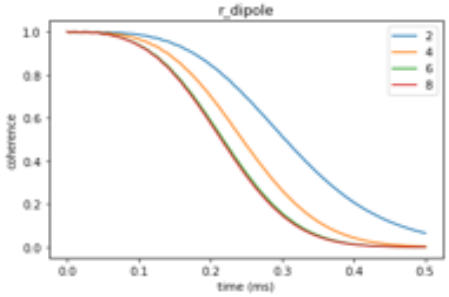
This graph indicates that a higher magnetic field

strength leads to enhanced coherence in the system. For the subsequent simulations, a magnetic field magnitude of 25000 Gauss (2.5 T) was employed. This magnitude is equivalent to the strength of a commercial magnetic resonance (MR) scanner used for routine clinical purposes [19].

The following are convergence tests were performed for variations of order, bath radius and dipole radius.







In the 'Order' graph, we can observe the visual representation for the decay in coherence which starts at CCE-2, implying that the nuclear spin-spin pair induces decoherence on the central spin, which agrees with the theory [2]. In CCE-1, there is only the contribution of the single bath spin i, which is the first element of the cluster expansion, and it is computed as:

$$L(i) = \frac{L_i}{L_0} \tag{15}$$

In the CCE-2 order, the spin i is paired with spin j which is computed as:

$$L(ij) = \frac{L_{ij}}{L_0 L_i L_j} \tag{16}$$

Observing the bath and dipole radius graphs, it is reasonable to conclude that lower amount of spins in the cluster will result in better coherence performance. If we perform the PyCCE calculation with a bath radius of 20 and a dipole radius of 2, which exhibited the best behavior in the convergence graphs, we will have a total of 491 spins and only 48 clusters of order 2. On the other hand, if we consider an bath radius of 60 and an dipole radius of 8, which represent the highest parameters, we will have a total of 11,221 spins and 188,251 clusters of order 2.

The nuclear spins are coupled to each other through magnetic dipolar coupling, and the nuclear spin bath interacts with the qubit via hyperfine interactions (which are neglected in this report). Therefore, as the size of the supercell increases and the bath and dipole radio becomes larger, the number of spins and the strength of the interactions also increase. Consequently, the decoherence effect become more significant. It is important to consider the balance between the number of spins and the coherence performance when selecting the parameters for the PyCCE calculation.

Conclusion

Spin qubits are one of the most promising platforms for quantum technologies because they meet the scalability criteria established for David DiVincenzo [25]. However, spin qubits require coherence times longer than logical quantum gate times, otherwise, the information is lost and the quantum algorithm cannot be completed [26]. To properly engineer spin qubits to achieve remarkably long coherence times, we must understand the system we are working with, computational methods that allow appropriate simulation of quantum many-body problems are

required.

In this report, I presented the results obtained from the open source library PyCCE [8] to approximate and predict the spin decoherence of [CpTi(cot)] organometallic complex. Through the simulations, it was determined that the presence of ^1H isotopes in the compound is the main source of decoherence. This finding suggests that implementing ^2H isotopes can effectively address this decoherence issue. It was also found that the external magnetic field has an important impact in the behavior of the central spin qubit.

Furthermore, through convergence graphs the parameters of bath and dipole radius as well as magnetic field and T_2 concentration were set to establish a precedent of the appropriate parameters to have better results. In addition, the influence of the variation in the magnetic field was shown to highlight the importance of carefully selecting and controlling its magnitude to optimize the coherence of the central spin.

Overall, PyCCE offers an efficient methodology to predict the qubit decoherence within a spin bath, it can be exploited in further simulations for other compounds, for example, to study the spin dynamics of the octacyanometallates $[Mo(CN)_8]^{3-}$ and $[W(CN)_8]^{3-}$ [23] or vanadium [24] since both have exhibited outstanding characteristics as qubit candidates.

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