Dipolar Couplings Simulation

Maria Paula Jimenez Moreno, Raghav Juyal, Mankrit Singh, Bhoomika Tanikonda

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Abstract

This project takes a look into the spin dynamics caused by the dipolar coupling between spins. We have identified different scenarios for our central spin surrounded by two other spins and found their effects on the central spin, which are then generalized to N bath spin systems for some scenarios. The insights and generalizations in this project can serve as a check and help in reducing the amount of computation or calculation required for similar systems.

1 Introduction

The ability to control a single electron or nuclear spin holds a lot of importance for potential applications, especially in quantum computing[1]–[3]. When looking into spin dynamics, it is important to consider the effect of surrounding spins[4]. One particular interaction between spins that is of interest to us is the dipolar coupling given by,

$$H = \sum_i \frac{\hbar\omega_{0i}}{2}\sigma_i^z + \sum_{i<j} \frac{\gamma_i\gamma_j\hbar}{4r_{ij}^3}\left[3(\vec{\sigma}_i \cdot \vec{n}_{ij})(\vec{\sigma}_j \cdot \vec{n}_{ij}) - \vec{\sigma}_i \cdot \vec{\sigma}_j\right]$$

We consider magnetic field along Z, giving us the following secular Hamiltonians for like and unlike spins respectively

$$H_{like} = \frac{\gamma^2\hbar}{4r_{ij}^3}\left(1 - 3\cos^2(\theta_{ij})\right)\left(3\sigma_i^z\sigma_j^z - \vec{\sigma}_i \cdot \vec{\sigma}_j\right) \tag{1}$$

$$H_{unlike} = \frac{\gamma_i\gamma_j\hbar}{2r_{ij}^3}\left(1 - 3\cos^2(\theta_{ij})\right)\sigma_i^z\sigma_j^z \tag{2}$$

In this project, we look into the effect of dipolar coupling between neighbouring spins and how it affects the dynamics of the central spin. In particular, we consider 3 spin systems and vary the inter-spin distances r_{ij}, initial polarizations and gyromagnetic ratios γ(see Appendix). We analyze the graphs generated by simulating the dynamics in QuTiP, compare analytical solutions derived using SymPy, and generalize some particular results to N spins.

2 Results

2.1 Effect of distance

One of the first noticeable behaviours when performing the simulations for the evolution of a 3 spin system relates to the effect of the distance between the spins. Considering the case where the distance between all spins is 100Å; and, taking as an example, the initial polarization of all spins is along the x-axis, it can be seen that there is no effect in the evolution of the spins as seen in Figure 1.

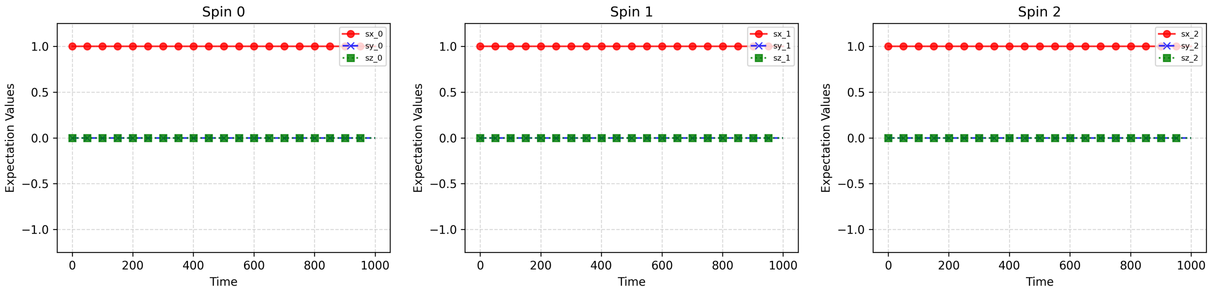

Figure 1: Spin expectation values of S_x at distances 100Å

Taking this into account, it is evident that spins that are far away($r = 100$Å) have negligible effects in the spin of interest. The effect of the distance in the spin dynamics can also be seen from the interaction Hamiltonian term which is inversely proportional to the cube of the distance.

Since a bath spin that is at a considerable distance from the central spin does not have influence in its spin dynamics, the cases in which the distances between all spins is 100Å(Figure 2(e)) and when one of the spins is at 100Å from the other two spins(Figure 2(b),(c),(d)) corresponds to the situations of having effectively a one spin system and a two spin system, accordingly. With this in mind, the analysis of the spin dynamics can be narrowed to only taking into account the nearest neighbours of the spin of interest, that is, the ones located at 1Å.

2.2 Effect of gyromagnetic ratio

Another relevant finding from the simulations is evidenced when we have two nearby spins with gyromagnetic ratio 0.02 as seen in Figure 2(d). This case is effectively the same as having two spins with gyromagnetic ratio 0.1 next to each other (Figure 2(b)). The only difference lays in having an slower evolution in the system that has $\gamma = 0.02$. This effect is also evident from the interaction Hamiltonian of like spins which is proportional to γ^2.

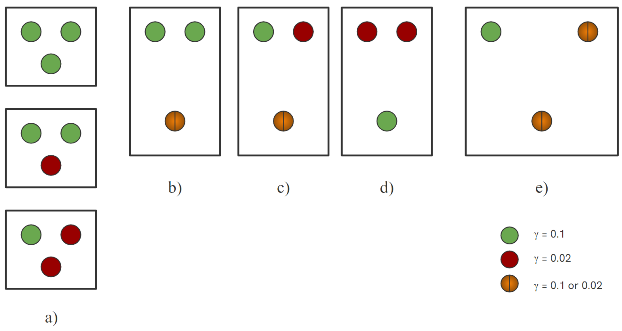

Figure 2: Different configurations for simulations. The spin at the top left corner on each of the combinations corresponds to the central spin. a) The distances between all spins is 1Å; spin pairings w.r.t spin 1 and spin 2 are like-like, like-unlike, unlike-unlike. In (b), (c) and (d) only one of the spins is at 100Å and the spin close by is like, unlike, or like to the central spin, respectively. e) All spins are at 100Å.

2.3 Effect of initial polarizations

For our simulations and analytical solutions, we took into account all 4 different kinds of initial polarizations - Unpolarized (U), polarized along X, Y and Z. Our findings are as follows:

- X and Y initial polarizations have the same behavior for "simple" cases: This means that for cases involving just X, Y and U polarizations (eg. XUU), we can replace X with Y to get results for a different configuration (eg. YUU), obtaining the same solutions for the $\langle S_y \rangle$ component that we get for $\langle S_x \rangle$ in the original polarization and vice versa.

- For such simple cases, we can usually "add up" different graphs to obtain results for other configurations. An example is illustrated in Figure 3. This behaviour is not observed in cases like $\gamma_0 = \gamma_1 = \gamma_2$ with all spins seperated by a distance of 1Å, as we see additional oscillations in $\langle S_z \rangle$.

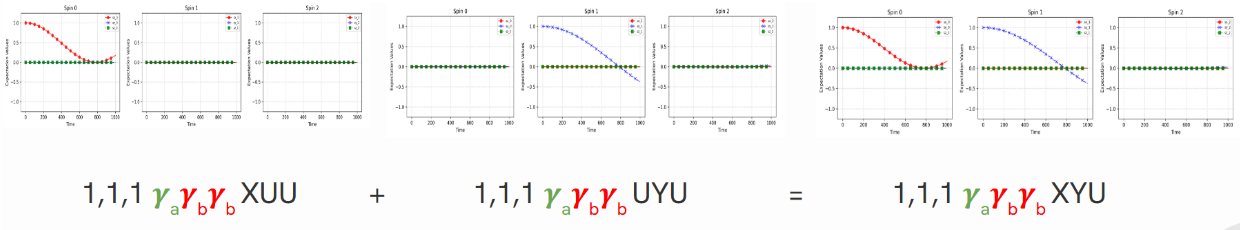

Figure 3: Spins are polarized as $\gamma_a = 0.1, \gamma_b = 0.02$. This demonstrates the additivity of "simple" graphs like XYU.

- Polarizations along Z create interesting effects when mixed with other polarizations like X and Y, as we see additional oscillations in the remaining components as demonstrated in Figure 4. This implies that Z polarizations cannot be added trivially as mentioned above for X and Y. Also, this demonstrates that X and Y polarizations behave anti-symmetrically in presence of a Z polarization.

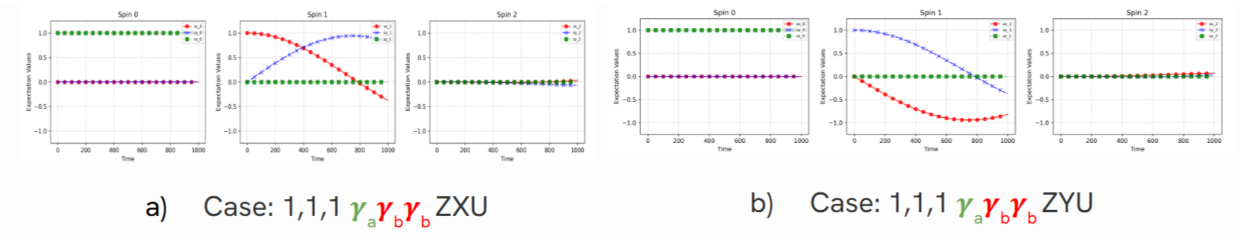

Figure 4: Spins are polarized as $\gamma_a = 0.1, \gamma_b = 0.02$. Here, we see that for ZXU there are additional oscillations in the $\langle S_y \rangle$ component, and for ZYU there are inverted oscillations in the $\langle S_x \rangle$ component

- Finally, a universal observation was that the total sum of $\langle S_z \rangle$ components of all the spins always add up to the total number of initial qubits polarized along Z at all times.

$$\sum_{n=1}^{N} \langle S_z \rangle = N_z$$

  Here, N_z is the total number of spins initially polarized in Z.

2.4 Generalizations for N bath spins

With the central spin polarized in X, each additional like spin polarized in X in the bath impacts the $\langle S_x \rangle$ by a factor of $\cos\left(\frac{3\gamma_1\gamma_2 t}{2}\right)$ as can be seen in Figure 5, so if there are N bath spins, the central spin will have

$$\langle S_x \rangle = \cos^N \left(\frac{3\,\gamma_1\gamma_2\,t}{2} \right) \tag{3}$$

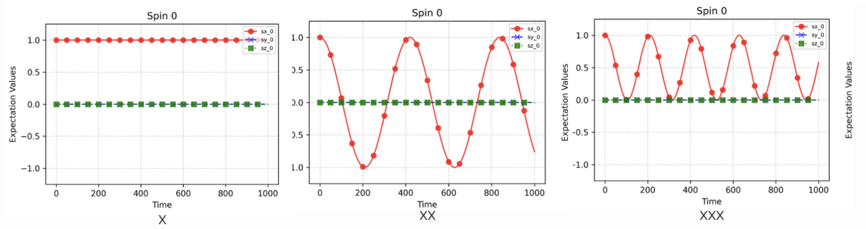

Figure 5: central spin: X, like bath spins: X

and for each additional unlike bath spin polarized in X, Y or U the $\langle S_x \rangle$ is multiplied by a factor of $\cos(\gamma_1\gamma_2\,t)$ as can be seen in Figure 6, so if there are N bath spins, for the central spin we have

$$\langle S_x \rangle = \cos^N(\gamma_1\gamma_2\,t) \tag{4}$$

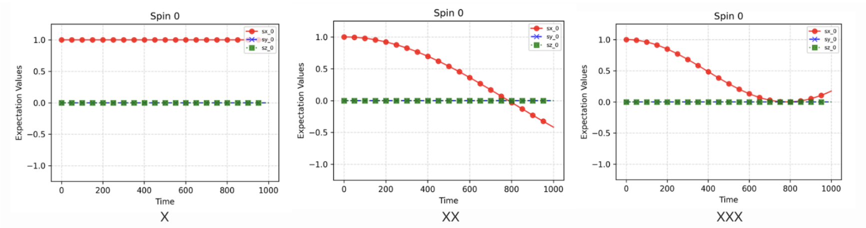

Figure 6: central spin: X, unlike bath spins: X

On the other hand, if the bath spins are unlike and are Z polarized then for N such spins the $\langle S_x \rangle$ and $\langle S_y \rangle$ are multiplied by factors $\cos(N\,\gamma_1\gamma_2\,t)$ and $\sin(N\,\gamma_1\gamma_2\,t)$ respectively, this can be seen in Figure 7. In this case the expectation values for the central spin correspond to

$$\langle S_x \rangle = \cos(N\,\gamma_1\gamma_2\,t) \text{ and } \langle S_y \rangle = \sin(N\,\gamma_1\gamma_2\,t) \tag{5}$$

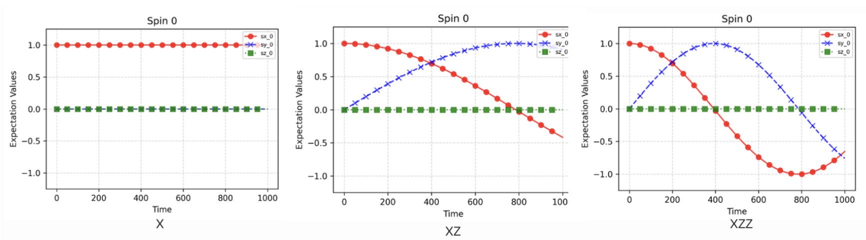

Figure 7: central spin: X, unlike bath spins: Z

3 Conclusion

This project aimed to analyze the effect of dipolar couplings in spin dynamics under varying configurations of distances, spin pairings, and initial polarizations. We have provided some insights based on the simulation results and our calculations. Using this we have been able to generalize some cases to N bath spins. All these observations could serve as either checkpoints or be used to speed up calculation or computation while solving for a system with many spins. Further research could include more studies on the generalization of like spins and including Rabi driving.

References

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Appendix

Code Availability

The code for this project is available at https://github.com/RaghavJuyal/Dipolar-Coupling-of-Spins.

Parameters Varied

Here we consider the following values for our parameters:

- Distance: The distance between spins, r_{ij} can be either 1Å or 100Å. We have the following combinations for (r_{01}, r_{02}, r_{12}): $\{(1,1,1),(1,100,100),(100,1,100),(100,100,1),(100,100,100)\}$
- Spin Polarization: All spins can be polarized along X, Y or Z or can be unpolarized.
- Gyromagnetic ratios: The central spin will have a constant gyromagnetic ratio $\gamma = 0.1$. The bath spins can have 2 possible values, $\gamma = 0.1$ or $\gamma = 0.02$ giving us combinations of like or unlike bath spins with respect to the central spin. Taking into account the symmetry, we have the following combinations of γ for the bath spins: $\{(0.1,0.1),(0.1,0.02),(0.02,0.02)\}$.

In total we generated $5 \times 4^3 \times 3 = 960$ graphs to analyze.