# Simulating Spin-Field Interactions in Simple Molecules for Quantum Circuits

*Oxford Physics Summer School, Quantum Experience, University of Oxford*

*By Mackenzie Ward,*
*William Martin*
*Supervisor Niccolo Fontana*

## Introduction

By using a Hamiltonian equation for our designed system, we can observe how the different eigenvalues for the system change as the magnetic field changes. These systems can be used to model how certain types of qubits will react to certain magnetic fields, using this information to determine gates for that quantum computer.

## Terms

$\gamma_e$: •Describes how an electron's spin reacts to the applied magnetic field.
$\gamma_n$: •Describes how the nucleus' spin reacts to the applied magnetic field.
$A$: •Describes the interaction between the nucleus and the electrons.
$D$: •Explains the effect electrons have on each other.
$\boldsymbol{B}$: •The magnetic field, we have ignored the y-component as it is typical to fix the direction.
$\boldsymbol{S}$: •The collection of rotation matrices defining the electrons.
$\boldsymbol{I}$: •The collection of rotation matrices defining the nucleus.

## General Hamiltonian Used

$$\hat{H} = \frac{\mu_B g_e}{\hbar}(B \cdot S) + \frac{\mu_N g_n}{\hbar}(B \cdot I) + A(S \cdot I) + D(S_z^2 \otimes \mathbb{I})$$

### Electron Zeeman Used

$$\gamma_e(B \cdot S) \quad where\, \gamma_e = \frac{\mu_B g_e}{\hbar}$$

This takes into account the effect the external magnetic field has on the electron.

### Nuclear Zeeman Used

$$\gamma_n(B \cdot S) \quad where\, \gamma_n = \frac{\mu_n g_n}{\hbar}$$

Alike the Electron Zeeman but with respect to the nucleus.

### Hyperfine Interaction

$$A(S \cdot I)$$

This is the effect the electron spin has on the nuclear spin and vice versa.

### Magnetic Anisotropy Interaction

$$D(\hat{S}_z^2 \otimes \mathbb{I})$$

This is the effect that electrons induce into each other.

## Calculating Energy Differences

$$\hat{O}\mathbf{v} = \lambda\mathbf{v} \qquad \hat{H}\,|\psi> = E\,|\psi>$$

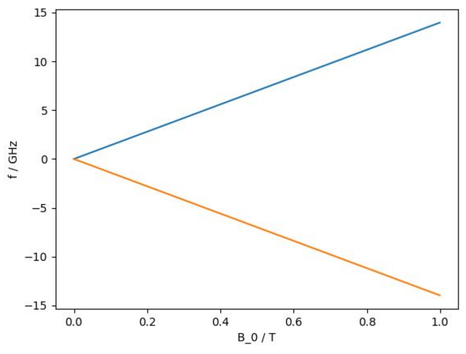
As each eigenvalue for the Hamiltonian is the energy for a given state, the change in the eigenvalues for a given Hamiltonian is the change in energy. This change in energy identifies different states for the molecule; the goal is to maximize the energy difference while ensuring each gap is identifiable to ensure the correct gate is applied to the correct qubit.

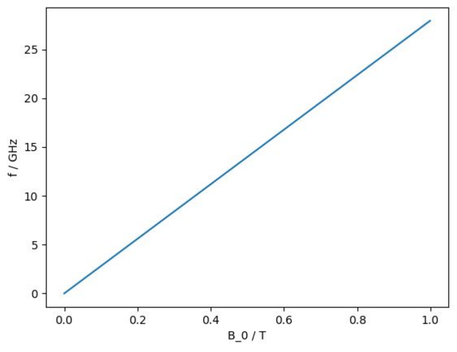
Overall, we have created a system to compute and plot Spin-Field interactions in simple molecules, this simulation demonstrate the difficulty of using the nucleus as a qubit due to the small energy differences between energy states. The model also promotes high values of the Hyperfine and Magnetic Anisotropy components.
The model's code can be accessed at https://github.com/Me-Mac-Ward/Oxford_physics_summer_school

# Program Implementation

## Single Electron

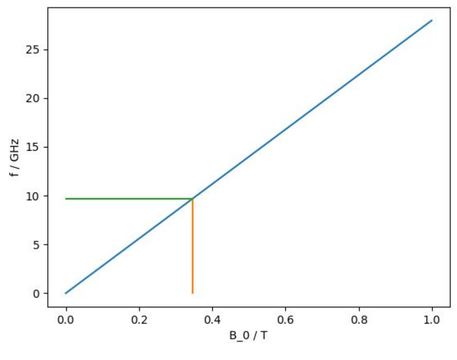
$$\hat{H} = \gamma_e B_0(S_x \sin\theta + S_z \cos\theta)$$



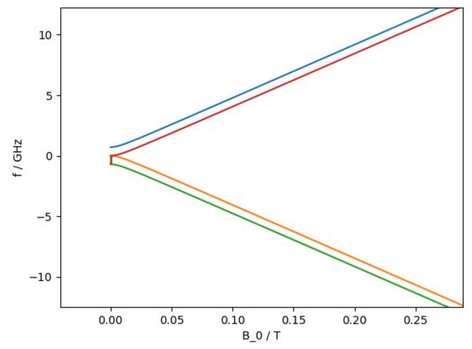

Above: graph of the eigenvalues against magnetic field strength

Right: graph of the differences of the eigenvalues, and the magnetic field strength identified when the change in frequency is 9.7 GHz, a common frequency used



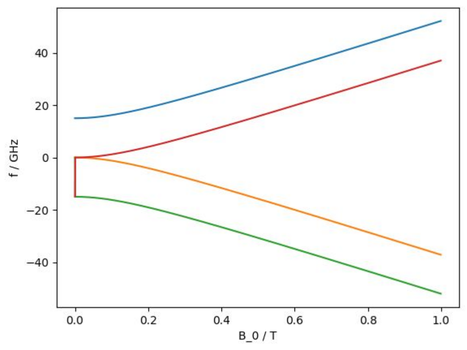

## One Electron One Hydrogen Nucleus

$$\hat{H} = \gamma_e B_0(\sigma_x \otimes \mathbb{I}\sin\theta + \sigma_z \otimes \mathbb{I}\cos\theta) + \gamma_n B_0(\mathbb{I} \otimes \sigma_x \sin\theta + \mathbb{I} \otimes \sigma_z \cos\theta) + A(\sigma_x \otimes \sigma_x + \sigma_z \otimes \sigma_z)$$



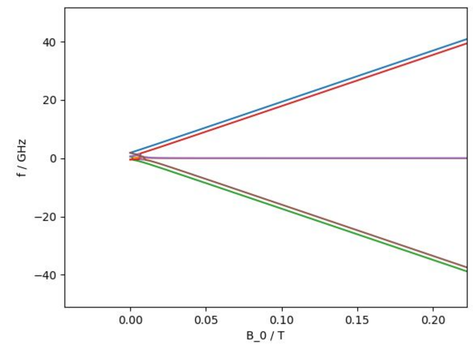

Left: graph of eigenvalues against magnetic field strength with the Hyperfine Term = 1.42e9 Hz/T, the value for an electron and a Hydrogen Nucleus

Right: graph of eigenvalues against magnetic field strength with the Hyperfine Term = 3e9 Hz/T



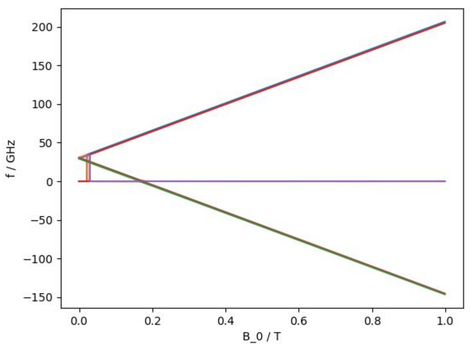

## Two Electrons One Hydrogen Nucleus

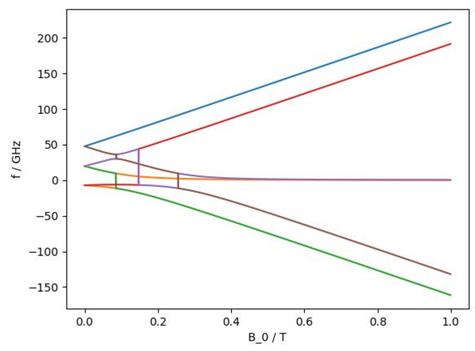
$$\hat{H} = \gamma_e B_0(S_x \otimes \mathbb{I}_2 \sin\theta + S_z \otimes \mathbb{I}_2 \cos\theta) + \gamma_n B_0(\mathbb{I}_3 \otimes I_x \sin\theta + \mathbb{I}_3 \otimes I_z \cos\theta) + A(S_x \otimes I_x + S_z \otimes I_z) + D(S_z^2 \otimes \mathbb{I}_2)$$




Left: graph of eigenvalues against magnetic field strength with the Hyperfine Term = 1.42e9 Hz/T and Magnetic Anisotropy = 1e9 , the values for an electron and a Hydrogen Nucleus

Right: graph of eigenvalues against magnetic field strength with the Hyperfine Term = 1.42e9 Hz/T and Magnetic Anisotropy = 3e9




Right: graph of eigenvalues against magnetic field strength with the Hyperfine Term = 3e9 Hz/T and Magnetic Anisotropy = 3e9, ideal qualities as the change in frequencies are large and different