Simulation of Spin-Spin Coupling Dynamics in EPR

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ABSTRACT:

Simulations of the dynamics of spin-spin coupling were made in MATLAB. A system of two coupled spins 1/2 was defined, then the MATLAB libraries of Easyspin were used to evaluate the system's Hamiltonian eigenvalues as well as the magnetization over time.

INTRODUCTION:

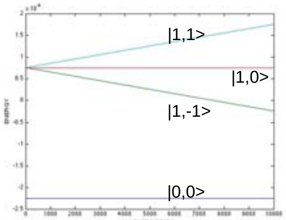
Spin-1/2 systems such as electrons are the physical representation of a qubit. The ability of a qubit to store information relies on the precession of these particles in a static magnetic field. When an electron is placed in a magnetic field, there is a torque on the electron due to its intrinsic spin, causing the spin to precess around the magnetic field similar to a gyroscope at the Larmor frequency. When a magnetic field in the plane perpendicular to the static field (such as a microwave) is applied, the electron will begin to precess around it as well. If the microwave's frequency equals the Larmor frequency, resonance occurs and the electron's spin flips from up to down. This corresponds to a transition from the ground state to the excited state. These two energy levels are represented in the Hamiltonian. The periodic flipping of the electron's magnetization is called Rabi oscillation.

HAMILTONIAN:

The spin Hamiltonian for this system is:

$$H = \gamma \vec{B}\cdot\left(\vec{S}_{1z}+\vec{S}_{2z}\right) + J\left(\vec{S}_1\cdot\vec{S}_2\right) + \vec{b}\cdot\left(\vec{S}_{1y}+\vec{S}_{2y}\right)\cos\omega t$$

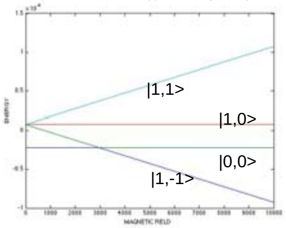
where γ is the gyromagnetic ratio, $\vec{B}$ is the static magnetic field, $\vec{b}$ is the microwave field, $\vec{S}_1$ and $\vec{S}_2$ are the spin operators for particles 1 and 2, and J is the electron-electron coupling. It includes the electron Zeeman interaction, the electron-electron coupling interaction, and the dynamic RF coupling.



Zeeman Energy Levels (J/B=3)

ZEEMAN LEVELS:

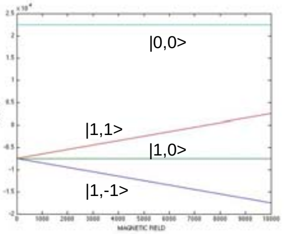
The 4 eigenvalues of the spin Hamiltonian give the energy states of the system. They are described by $|S, S_z\rangle$. S Is the total spin and S_z is the projection of the spin on the z-axis. 3 levels form a triplet (S=1), and 1 forms a singlet (S=0).



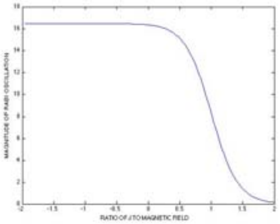
Zeeman Energy Levels (J/B=.3)

TWO OSCILLATIONS:

Conservation of angular momentum prohibits transitions from the singlet to the triplet. At low temperature, two transitions occur in the triplet: between the ground state |1,-1> and the intermediate state |1, 0> (1-photon transition) and between |1,-1> and the excited state |1,1> (2-photon transition).



Zeeman Energy Levels (J/B=-3)



Change in magnitude of Rabi oscillations with increasing J (0.1K)

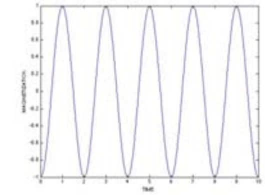
EFFECT OF COUPLING:

Varying the coupling constant compared to the magnetic field changes the energy of the singlet state. Selection rules prohibit transitions from the singlet to the triplet (angular momentum must be conserved), so Rabi oscillations only occur for low J.

RABI OSCILLATIONS:

At low temperature all electrons start out in |1,-1> and 2 Rabi oscillations occur:

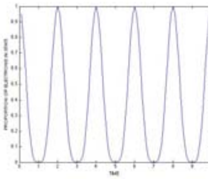
|1,-1> ↔ |1,0> and |1,-1> ↔ |1,1>. In an isotropic system, the energy levels are equally spaced and all these oscillations have the same frequency.

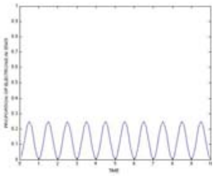


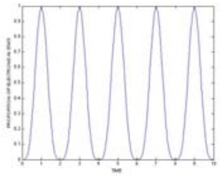
Rabi oscillations for isotropic coupled spin-1/2 system

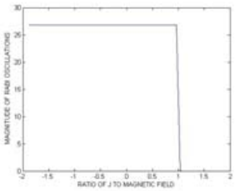
STATE POPULATION:

Our simulation gives the proportion of electrons in each state. Initially, each state has zero population except for the ground state |1,-1>, but they vary with time as the proportion of spins in each state oscillates.


Evolution of state population: |1,-1>


Evolution of state population: |1,0>

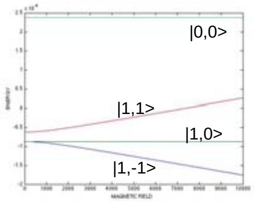

Evolution of state population:|1,1>



Transitional Coupling Region (.001K)

TEMPERATURE:

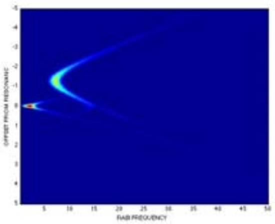
When the temperature is not 0K, particles will be excited to the singlet state according to the Boltzmann distribution. These electrons do not participate in Rabi oscillations, so the magnitude of the total oscillation decreases. At very low temperature the curve is very sharp because electrons only begin in |0,0> state when it is the lowest energy state.



Zeeman Energy Splitting with Coupling Anisotropy in X

ANISOTROPY:

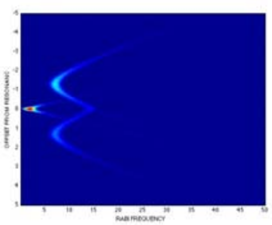
A system that has a directional dependence in its magnetic properties is anisotropic. Introducing anisotropic coupling changes the energy levels, breaking the degeneracy in the triplet.



Effect of offset from resonance on Rabi frequencies (.01K)

OFF-RESONANCE EFFECTS:

When the microwave frequency is slightly off-resonance, the Rabi oscillations have a higher frequency and lower magnitude. The Fourier transform makes a hyperbolic shape around the resonance frequency. There are two curves: the 2-photon resonance transition at 0 offset and the one-photon transition above it.



Effect of offset from resonance on Rabi frequencies (1K)

THIRD TRANSITION:

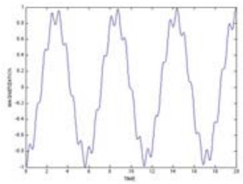
At 1 K, some of the electrons start out at |1,0> and the third transition is observed:

|1,0> ↔ |1,1>.

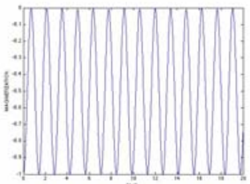
ANISOTROPIC RABI OSCILLATIONS:

The resonant frequency for the isotropic system is no longer resonant for both transitions. Because the |1,0> level was shifted, the one-photon transition is off resonance. The summed magnetization shows two frequencies: the faster off-resonance one-photon transition and the slower resonance two-photon frequency.

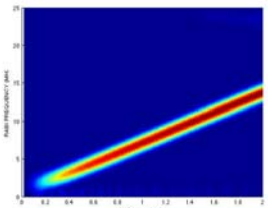
At the one-photon resonance frequency, only the one-photon transition takes place so the magnetization only shows one frequency.



Total magnetization with coupling anisotropy (2-photon resonance)



Total magnetization with anisotropy (1-photon resonance)

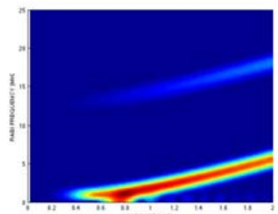


Rabi frequencies versus power (1-photon resonance)

POWER:

Increasing the power of the electromagnetic wave increases the Rabi frequency, but the magnitude of the magnetization is not altered because the pulse is still resonant and the magnetization still flips between its two maximum values.

At the two-photon resonance frequency, there are two lines, one for each of the Rabi frequencies. The line for the one-photon transition has a smaller magnitude and it is at a higher frequency; this is due to off-resonance effects .



Rabi frequencies versus power (2-photon resonance)

CONCLUSIONS:

Spin-1/2 systems contain the basic quantum unit of information, the qubit. A simple simulation of the effects of temperature, anisotropy, power, and coupling on a system of coupled spin-1/2 particles using MATLAB and Easyspin gives insight into the dynamics of multi-qubit systems.

Acknowledgements:

Irinel Chiorescu, Sylvain Bertaina, Nickolas Groll, and Lei Chen

Research funded by the NSF, the Alfred P. Sloan Foundation, NSF-CAREER, NHMFL, FSU, and DARPA and supported by the Center for Integrating Research and Learning

References:

Cohen-Tannoudji, Claude; Diu, Bernard; and Laloe, Franck. Quantum Mechanics: Volume 1. John Wiley & Sons: Singapore, 2005.

Stefan Stoll, Arthur Schweiger. "EasySpin, a comprehensive software package for spectral simulation and analysis in EPR". J. Magn. Reson. 178(1), 42-55 (2006).