Simulation and Analysis of Singlet–Triplet Interconversion in a Radical Pair Model

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Abstract

This project simulates the time evolution of a radical pair initially in a singlet spin state under the influence of external magnetic fields and hyperfine interactions. The model is motivated by biological magnetoreception mechanisms, such as those hypothesized in migratory birds. By evolving the quantum state and projecting onto the singlet state, the singlet fraction $P_S(t)$ is computed and analyzed under various magnetic field orientations. Noise, singlet–triplet dephasing, and detector uncertainty are incorporated to produce realistic outputs. Nonlinear curve fitting, error propagation, and χ^2 analysis are performed to extract physical parameters from the simulated data.

1 Introduction

Migratory birds exhibit remarkable sensitivity to the Earth's magnetic field, a phenomenon hypothesized to be mediated by magnetically sensitive radical pair reactions in proteins such as cryptochrome. These reactions involve quantum spin dynamics between two unpaired electron spins, coupled by hyperfine interactions to surrounding nuclei and perturbed by external magnetic fields. A key feature of the radical pair mechanism is the oscillation between singlet and triplet spin states, which affects chemical reaction pathways.

The probability of remaining in the singlet state at time t, denoted $P_S(t)$, reflects the influence of magnetic field strength and orientation. The evolution of $P_S(t)$ is governed by the system Hamiltonian:

$$\hat{H} = \underbrace{\mu_B \mathbf{B} \cdot (\hat{S}_1 + \hat{S}_2)}_{\text{Zeeman interaction}} + \underbrace{A \hat{\mathbf{S}}_1 \cdot \hat{\mathbf{I}}}_{\text{Hyperfine interaction}}, \tag{1}$$

where μ_B is the Bohr magneton, $\mathbf{B}$ is the magnetic field, $\hat{S}_1$ and $\hat{S}_2$ are the electron spin operators, A is the hyperfine constant, and $\hat{\mathbf{I}}$ is the nuclear spin.

2 Methods

The simulated system models a radical pair consisting of two electrons and one spin-$\frac{1}{2}$ nucleus. Each particle is represented in a two-level quantum system, yielding a total Hilbert space dimension of $2 \times 2 \times 2 = 8$. The initial state is a singlet configuration of the electron spins combined with a nuclear spin-up state.

The time evolution of the density matrix $\rho(t)$ is governed by the Schrödinger equation in matrix form. Evolution is computed using a unitary time-stepping method:

$$\rho(t + \Delta t) = U\rho(t)U^\dagger, \quad \text{with } U = e^{-i\hat{H}\Delta t/\hbar},$$

where $\hat{H}$ is the total Hamiltonian of the system, including both Zeeman and hyperfine interaction terms.

The Zeeman interaction accounts for the influence of an external magnetic field on the two electron spins:

$$\hat{H}_Z = \mu_B \mathbf{B} \cdot (\hat{\mathbf{S}}_1 + \hat{\mathbf{S}}_2),$$

while the hyperfine interaction couples one of the electron spins to the nuclear spin:

$$\hat{H}_{\text{HF}} = A\hat{\mathbf{S}}_1 \cdot \hat{\mathbf{I}},$$

where μ_B is the Bohr magneton, A is the hyperfine coupling constant, and $\hat{\mathbf{S}}_1$, $\hat{\mathbf{S}}_2$, and $\hat{\mathbf{I}}$ are vector spin operators.

At each time step, the probability of the system remaining in the singlet state is calculated using the projection:

$$P_S(t) = \text{Tr}(P_S\rho(t)), \tag{2}$$

where P_S is the projection operator onto the initial singlet state.

To simulate realistic experimental conditions, thermal noise and environmental decoherence are added to the ideal quantum result. This is implemented by adding Gaussian noise and applying exponential damping to each time step:

$$P_S^{\text{noisy}}(t) = (P_S(t) + \mathcal{N}(0, \sigma))\, e^{-t/\tau},$$

where σ is the standard deviation of the simulated measurement noise and τ is the singlet–triplet dephasing time.

All simulations and data analysis were performed using `Python` in Jupyter notebooks. The simulation used `NumPy` for linear algebra and matrix operations, `SciPy` for computing the matrix exponential, and `Matplotlib` for plotting. Nonlinear curve fitting was carried out using `scipy.optimize.curve_fit`. Each dataset was evolved over a 2 µs time window with 400 time steps of $\Delta t = 5$ ns.

3 Results

To understand the fundamental behavior of the radical pair system, the singlet fraction $P_S(t)$ was simulated under ideal conditions — with no noise or environmental dephasing. The ideal model includes only the unitary quantum dynamics governed by the Zeeman and

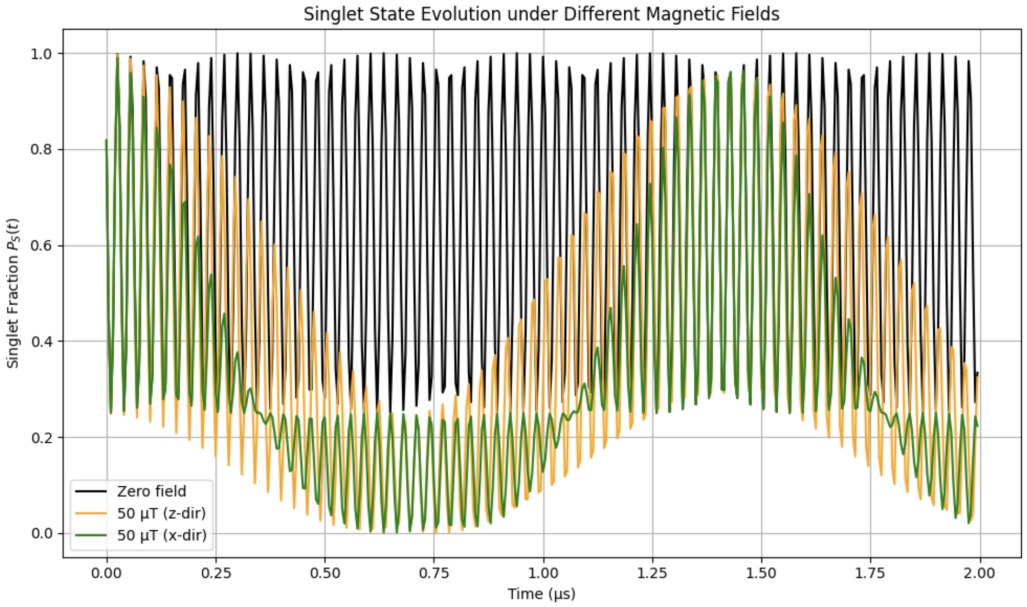

Figure 1: Simulated $P_S(t)$ under ideal (noise-free) conditions for 0, 50 μT (z), and 50 μT (x) magnetic fields.

hyperfine interactions. Figure 1 shows the resulting time evolution for three magnetic field configurations: no external field, a 50 μT field in the z-direction, and a 50 μT field in the x-direction.

Each trace exhibits oscillatory behavior due to coherent singlet–triplet interconversion. The oscillation frequency and envelope differ depending on the orientation and strength of the magnetic field, reflecting how external fields modify spin dynamics through the Zeeman effect.

To make the simulation more physically realistic, Gaussian noise was added to model detector uncertainty and an exponential decay was applied to simulate singlet–triplet dephasing. These effects represent the influence of thermal fluctuations and environmental decoherence that occur in real systems.

Figure 2 shows both the noisy simulated data and the fitted damped cosine curves for all three magnetic field configurations. Visibly, the noise obscures high-frequency components of the signal and suppresses long-term oscillations, especially in the zero-field case.

To quantify these results, the noisy data for each magnetic field was fit to the function

$$f(t) = A\cos(\omega t + \phi)e^{-t/\tau} + \text{offset},$$

and the best-fit parameters were extracted. Table 1 summarizes the fitted dephasing times, oscillation frequencies, and reduced chi-squared values.

The fitting procedure allowed extraction of physical parameters such as oscillation frequency, phase, and dephasing time. The reduced chi-squared statistic was lowest for the 50 μT fields and significantly higher for the 0 μT case, reflecting a mismatch between the fitting model and the hyperfine-driven dynamics in the absence of an external field.

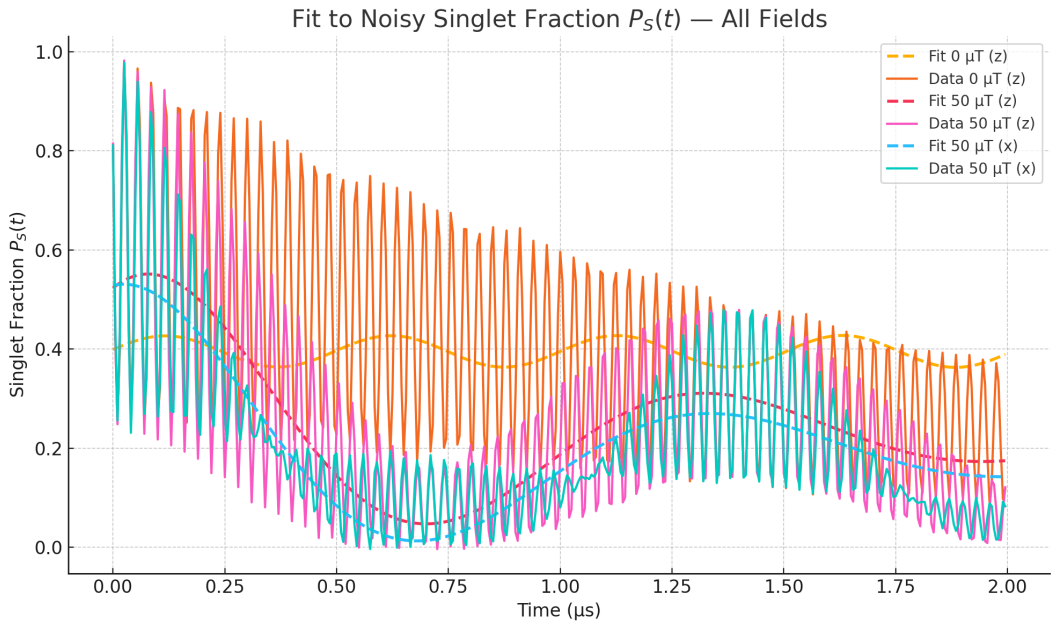

Figure 2: Noisy $P_S(t)$ data (solid) and best-fit damped cosine models (dashed) for each magnetic field case.

Field	**Fitted τ (μs)**	**Frequency (MHz)**	**Reduced χ^2**
0 μT (z)	Nonphysical	12.4	430.6
50 μT (z)	0.96	5.05	194.7
50 μT (x)	0.94	4.80	110.9

Table 1: Fit results: dephasing time τ, oscillation frequency $\omega/2\pi$, and reduced chi-squared.

4 Conclusion

The simulation of singlet–triplet interconversion dynamics in a radical pair system illustrates the fundamental role of quantum spin interactions in magnetically sensitive chemical processes. Under idealized conditions, coherent oscillations in the singlet fraction $P_S(t)$ arise from the combined effects of the Zeeman interaction and hyperfine coupling. These oscillations reflect transitions between spin states and reveal how external magnetic fields can alter the quantum evolution of electron-nuclear systems. Such behavior aligns with theoretical models proposed to explain magnetoreception in biological organisms, particularly migratory birds.

To approximate real-world conditions, the model was extended by incorporating Gaussian noise to simulate measurement uncertainty and exponential damping to mimic decoherence effects. These modifications resulted in attenuated and noisy signals that resemble the types of outputs expected from biological or solid-state spin systems exposed to environmental interactions. Curve fitting with a damped cosine model enabled the extraction of characteristic timescales and oscillation frequencies, and chi-squared analysis provided a measure of how well the fit captured the data. The model produced physically reasonable results

in the presence of external fields but failed to adequately fit the zero-field case, where spin evolution is driven purely by hyperfine interactions.

This study provides a computational framework for exploring the spin dynamics of radical pairs and the influence of magnetic fields on their evolution. The approach is adaptable and can be extended to more complex models, such as those involving multiple nuclear spins or anisotropic interactions. By combining quantum mechanics, numerical methods, and data analysis, the simulation offers insight into how weak magnetic fields can regulate spin-selective chemical pathways—supporting the broader hypothesis that spin chemistry may play a role in biological sensing.

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