Problem Set 2

Due **Tuesday 4/8/2025 in class**

Problem 2-1 [45 points + 2 points for nice code and plotting style] Here you will simulate spin dynamics in QuTiP; please submit a Jupyter notebook via Canvas for this problem. In an experiment, you have a $B_0 = 1$ T magnetic field oriented along the $\hat{z}$ direction and an oscillating magnetic field with $\sin(\omega t)B_x\hat{x}$, with $B_x = 0.2$ mT and a frequency ω that is under your control.

(a) Express the Hamiltonian $H/\hbar$ in an appropriate rotating frame and insert it in QuTiP.

(b) Plot the energy spectrum (i.e. the eigenenergies) as a function of detuning $\Delta = \omega_0 - \omega$, where ω_0 is the spin precession frequency in B_0. Make sure that your axes are labeled and have units. Compare with the case where $B_x = 0$.

(c) What are the eigenvectors for positive and negative detuning, and for on-resonance driving. Compare these to the bare eigenstates without the driving field. This can be calculated done analytically or numerically. Please discuss the result.

(d) For resonant driving ($\omega = \omega_0$): Start with the spin in $|0\rangle$ and let it evolve with H. Plot the expectation values of $\sigma_{x,y,z}$. Don't forget labels and units on your axes.

(e) For resonant driving ($\omega = \omega_0$): What is the duration for a $\pi-$pulse and for a $\pi/2-$pulse?

(f) For resonant driving: Use the Hamiltonian to create the following Ramsey pulse sequence: $\pi/2 - \tau - \pi/2$ with the interval time $\tau = 25$ μs. Plot the evolution of the expectation values.

(g) Now consider a random magnetic field generated by a subway train at a distance of 100 m on the experiment. To model the random phase shifts that such a random magnetic field will cause, assume a Gaussian current distribution centered around 0 A with a width (sigma) of 1000 A, which produces a magnetic field in the $\hat{z}$ direction, effectively from an infinitely long straight wire perpendicular to $\hat{z}$, in the plane of the experiment at a distance of 100 m. For a single pulse sequence, this field will be have a fixed current, but will fluctuate from experiment to experiment. Perform 50 Ramsey experiments with 50 random values from the current distribution. Plot the average spin evolution.

(h) Now pick a few different evolution times τ_i and study the magnitude of the expectation values at the end of the Ramsey sequence (still with random B-fields from the subway and taking 50 measurements at each time step). Discuss the result.

(i) Perform a spin echo experiment $\pi/2 - \tau - \pi - \tau - \pi/2$ with the randomly fluctuating field from above (50 measurements). What is the behavior of the final expectation values as a function of τ? Discuss the result.

Problem 2-2 [10 points] Generating entanglement. Consider a chloroform molecule ($CHCl_3$) from Chuang et al., Nature **393**, 143 (1998). This problem may be done either by hand or implemented in QuTiP, as you prefer.

(a) Formulate the Hamiltonian in an appropriate rotating frame for ^1H and ^{13}C with values from the paper (including the exchange coupling).

(b) Assume that you can initialize both spins in the up-state. Specify a pulse sequence with which you can create the Bell state $|\psi^+\rangle = (|00\rangle + |11\rangle)/\sqrt{2}$. You may assume that you can switch the exchange coupling J on and off (in reality this would be done with refocusing pulses).