3 Simulation Lab

23. Spinny Spin Spin

It is well known that the spin of an electron is related to its magnetic moment by $\boldsymbol{m} = -g\mu_B \boldsymbol{S}$, where μ_B is the Bohr magneton, g is a dimensionless factor that depends on the electron's environment, and $\boldsymbol{S}$ is a vector of magnitude $\frac{1}{2}$. The angular momentum of the electron is given by $\hbar \boldsymbol{S}$.

Now, an ensemble of $N = 100000$ electron spins are distributed roughly evenly along a rod of length 2. The rod points in the x direction. The left end of the rod is given the coordinate $\boldsymbol{\xi} = -1$ and the right end of the rod is given the coordinate $\boldsymbol{\xi} = 1$. The magnetic field along the rod points in the z direction and is given by $B_z = B_0 + B_1\xi$. It is known that B_0 is on the order of $0.01T$ and $B_1 \ll B_0$. You can also add a bias magnetic field $\boldsymbol{B} = b\hat{z}$ which is uniform, but due to budget constraints this magnetic field must be limited to a magnitude of $0.01T$.

The spins are placed in a thermal bath and allowed to thermalise. In this initial stage, the spin will either align with the magnetic field or antiparallel to it according to the Boltzmann distribution. At time $t = 0$, a strong magnetic field pulse is applied to the system to rotate all spins 90° anticlockwise about the y axis. You can then set a sensor to detect the total magnetisation around the x and y axes at certain times (for convenience it will be given in units of μ_B), but remember these measurements are subject to noise! Also, a protection circuit is in place to prevent the initial magnetic field pulse from destroying the measurement circuit, so nothing will be recorded before $t = 100$ns. After $t = 10000$ns the measurement circuit runs out of memory and nothing will be recorded either.

Your goal is to find g, B_0 to 5% accuracy, as well as B_1 to 15% accuracy. Give the magnetic fields in units of Tesla. You may assume the spins do not interact with the environment or with each other after $t = 0$.

Solution 23: Writing out the equation of motion for each individual spin:

$$\frac{d(\hbar \boldsymbol{S})}{dt} = (-g\mu_B \boldsymbol{S}) \times \boldsymbol{B} = g\mu_B \boldsymbol{B} \times \boldsymbol{S}$$

Therefore the spins rotate at what is known as the Larmor frequency $\omega_L = \frac{g\mu_B B}{\hbar}$. Since $B_0 \gg B_1$ the precession will be chiefly at the central frequency B_0+b (unless B_0+b is close to 0). To determine the frequency with good accuracy, we can take measurements at 1-ns intervals and extrapolate the phase using $\arctan \frac{M_y}{M_x}$ (using the atan2 function common in many programming languages will do the trick without fuss). We need to 'unwrap' the phase by adding a multiple of 2π where the phase suddenly jumps from π to $-\pi$. Fitting this phase to a straight line we can then obtain the Larmor frequency for a certain b. If we repeat this experiment for a few values of b, we can plot a graph of the Larmor frequency with b. The slope will be $\frac{g\mu_B}{\hbar}$ while the y-intercept will be $\frac{g\mu_B}{\hbar}B_0$. Alternatively to find B_0 one can choose a value of b which minimises the signal (as we would expect from a low Boltzmann factor) but this is slightly less accurate. In the end we should find $g = 1.83$ and $B_0 = 5.27$mT.
The effect of B_1 is to modulate the envelope of oscillations. Because of the parameters of the problem, B_1 does not significantly affect the Boltzmann distribution of spins (unless we choose b such that $B_0 + b$ becomes very close to 0) and therefore we can ignore that effect, but just to be safe it is wiser to choose $b = 0.01$T just to take advantage of a larger Boltzmann factor (which will lead to a larger signal anyway). Define $\Delta\omega \equiv \frac{g\mu_B}{\hbar}$ Taking the magnetisation to be constant throughout the material, we can find the way the envelope evolves in time:

$$M_x \propto \int_{-1}^{1} \cos(\omega + \Delta\omega\xi)t \, d\xi = \frac{1}{\Delta\omega t}\left(\sin(\omega + \Delta\omega)t - \sin(\omega - \Delta\omega)t\right) \propto \frac{\sin \Delta\omega t}{\Delta\omega t}\cos \omega t$$

and similar for M_y confirms that the envelope will be of the form $\frac{\sin \Delta\omega t}{\Delta\omega t}$. The first root of the envelope will be at $\frac{\pi}{\Delta\omega}$ from which we can extract $\Delta\omega$ and hence B_1. We can initialise the ensemble many times and find the time at which the first minimum occurs, and average over several runs to obtain an estimate of B_1 and also its standard error. We should find $B_1 = 73\mu$T. (It is not quite so good to take more roots as the noise in the system along with approximations made mean that further roots are prone to systematic errors.) Of course, many people also fit the magnitude of M directly to a sinc curve using curve fitting tools which is a perfectly valid way to do things as well.