

Building an NMR Quantum Computer

Pauli Matrices and Spin Precession

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I. THE PAULI MATRICES

Now that we've come up with a good way to represent the states in the Stern-Gerlach experiment, we need to come up with some way to mathematically describe the Stern-Gerlach devices (what we've been calling $SG(\hat{n})$). Before we can do this, however, we need to understand a little bit about how we measure quantum states.

Measurement is the assignment of a particular value to some attribute of the system under study. One of the postulates of quantum mechanics is that for every possible measurement you can do, there exists a Hermitian operator. Recall that a Hermitian operator, A , satisfies $A = A^\dagger$. The outcomes that are possible for the measurement are the eigenvalues of the operator. It might help to see an example:

Let's say we have some state: $|\hat{n}+\rangle = \cos(\theta/2)|0\rangle + \sin(\theta/2)e^{i\phi}|1\rangle$, and we want to measure its magnetic moment in the \hat{z} direction. We know from the discussion above that we should get one of two values, "aligned" or "antialigned." Because we're building a mathematical theory, let's call "aligned" = 1 and "antialigned" = -1. So now we have our eigenvalues. The eigenstates that correspond to these eigenvalues are the states $|\hat{z}+\rangle = |0\rangle$ and $|\hat{z}-\rangle = |1\rangle$. In order to represent our operators as matrices, we need to represent our states as vectors,

$$|\hat{z}+\rangle = |0\rangle \longrightarrow \begin{pmatrix} 1 \\ 0 \end{pmatrix} \quad |\hat{z}-\rangle = |1\rangle \longrightarrow \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

In this notation,

$$|\hat{n}+\rangle \longrightarrow \begin{pmatrix} \cos(\theta/2) \\ \sin(\theta/2)e^{i\phi} \end{pmatrix} \quad |\hat{n}-\rangle \longrightarrow \begin{pmatrix} \sin(\theta/2) \\ -\cos(\theta/2)e^{i\phi} \end{pmatrix}$$

So, our task now is to find a matrix $S(\hat{z})$, that has eigenvalues ± 1 and eigenvectors $(1, 0)^\top$ and $(0, 1)^\top$. This is easy:

$$\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

Now we need to find $S(\hat{n})$, the matrix corresponding to a measurement along \hat{n} . The eigenvalues are still (± 1) , but the eigenvectors have changed. We have already written down the eigenvectors, $|\hat{n}+\rangle$ and $|\hat{n}-\rangle$, so we can use the eigenvalue decomposition of a matrix,

$$S = P\Lambda P^{-1}$$

where Λ is the diagonal matrix of eigenvalues and P is the matrix of eigenvectors. Let's use this to explicitly construct $S(\hat{x})$. The eigenvectors are

$$|\hat{n}+\rangle \longrightarrow \begin{pmatrix} 1/\sqrt{2} \\ 1/\sqrt{2} \end{pmatrix} \quad |\hat{n}-\rangle \longrightarrow \begin{pmatrix} 1/\sqrt{2} \\ -1/\sqrt{2} \end{pmatrix}$$

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So,

$$P_x = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}$$

$$\Lambda_x = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

Which gives,

$$S(\hat{x}) = P_x \Lambda_x P_x^{-1} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

This case was a little special, because $P_x = P_x^{-1}$. Doing the same for $S(\hat{y})$,

$$P_y = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ i & -i \end{pmatrix} \Rightarrow \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$$

These three matrices we've just derived are very special. So special, in fact, that we are going to give them special names:

$$\begin{aligned} S(\hat{x}) &\rightarrow \sigma_x \equiv X \\ S(\hat{y}) &\rightarrow \sigma_y \equiv Y \\ S(\hat{z}) &\rightarrow \sigma_z \equiv Z \end{aligned}$$

Where $\sigma_{(x,y,z)}$ is the notation preferred by physicists and (X, Y, Z) is the notation preferred by computer scientists. These are the Pauli matrices, and you'll see them a lot this semester. A nice feature of them is that any matrix $S(\hat{n})$ can be written as

$$S(\hat{n}) = \hat{n} \cdot \vec{\sigma} = n_x \sigma_x + n_y \sigma_y + n_z \sigma_z$$

This is a nice exercise, and I recommend you try to show that you try to show that it's true. Something else to keep in mind is that these matrices are Hermitian, and *they don't commute*. In fact, their commutation relations may be summarized compactly as,

$$[\sigma_i, \sigma_j] = 2i\epsilon_{ijk}\sigma_k$$

Where ϵ_{ijk} is the Levi-Civita symbol and takes the value +1 for even permutations of x, y, z (such as y, z, x) and -1 for odd permutations (such as y, x, z). Once again, it is a worthwhile exercise to verify this relationship.

II. SPIN PRECESSION

Nearly every important concept in quantum computing can be illustrated with nuclear magnetic resonance (NMR). The first quantum factoring algorithm with implemented with NMR quantum computing, and it's the perfect platform to discuss decoherence and quantum control. Electron spin resonance (ESR), the topic we'll discuss, is almost exactly the same thing in principle.

Recall from the previous section that the Hamiltonian for a magnetic moment in a magnetic field is:

$$H = -\vec{\mu} \cdot \vec{B}$$

in that section we were concerned with the action of this Hamiltonian on the spatial part of the electron wavefunction. However, in this section we are going to neglect the spatial part and consider only the time evolution of the electron's spin. Hand wavingly, the spin angular momentum of an electron gives rise to a magnetic moment. We can make a (surprisingly) reasonable estimate of this magnetic moment by considering the electron to be a classical particle whirling around in a circle. The movement of the electron, a charged particle, is equivalent to a current loop. The magnetic moment of a current loop is given by the current times the area of the loop. Applying this to the whirling

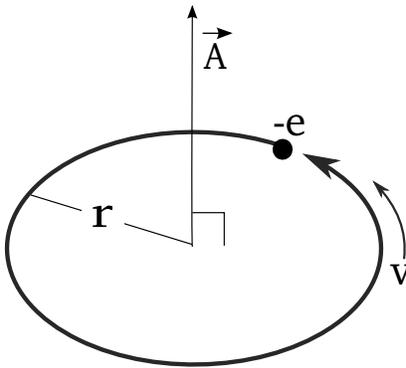


Figure 1: The magnetic moment associated with a whirling electron.

electron, we have

$$\vec{\mu} = I\vec{A} = \frac{-e}{2\pi r/v} \pi r^2 \hat{A} = \frac{-e m v r \hat{A}}{2m} = \frac{-e\vec{L}}{2m}$$

We will replace the angular momentum vector, \vec{L} , with the spin angular momentum operator, $\vec{S} = \hbar\vec{\sigma}/2$. This gives a magnetic moment, $\vec{\mu} = \frac{1}{2} \left(\frac{-e\hbar}{2m} \right) \vec{\sigma} \equiv -\mu_B \vec{\sigma}/2$. This expression also defines the Bohr magneton, μ_B . Our classical derivation is surprisingly close to the actual answer. We're just off by a relativistic factor (if you're interested, look up the Dirac and Pauli equations), which we'll call g , and is roughly equal to 2,

$$\vec{\mu} = -\frac{1}{2} g \mu_B \vec{\sigma}$$

Now let's rewrite the Hamiltonian for a spin in a magnetic field using this expression we've just derived for the magnetic moment operator,

$$H = -\vec{\mu} \cdot \vec{B} = \frac{1}{2} g \mu_B \vec{\sigma} \cdot B \equiv \frac{1}{2} \hbar \gamma \vec{\sigma} \cdot \vec{B}$$

This expression defines $\gamma = g\mu_B/\hbar$, the gyromagnetic ratio. To be consistent with what we did in class, we'll define $\mu_0 = \gamma/2$ as the magnetic moment, so that we don't have strange factors of 2 floating around.

So let's consider the time evolution of a state $|\psi(t)\rangle$ with the initial condition $|\psi(t)\rangle = |\hat{x}+\rangle = (|0\rangle + |1\rangle)/\sqrt{2}$ when placed in a constant magnetic field, $\vec{B} = B_0 \hat{z}$. The time evolution is given by solving the Schrödinger equation:

$$i\hbar \frac{d}{dt} |\psi(t)\rangle = H |\psi(t)\rangle$$

Recall that for a constant Hamiltonian, the evolution can be solved for exactly:

$$|\psi(t)\rangle = U(t) |\psi(0)\rangle = e^{-iHt/\hbar} |\psi(0)\rangle$$

Using the Hamiltonian and initial state above,

$$\begin{aligned} |\psi(t)\rangle &= e^{-i\mu_0 B_0 \sigma_z t} \left(\frac{1}{\sqrt{2}} (|0\rangle + |1\rangle) \right) \\ &= \frac{1}{\sqrt{2}} (e^{-i\mu_0 B_0 t} |0\rangle + e^{i\mu_0 B_0 t} |1\rangle) \\ &= \frac{1}{\sqrt{2}} (|0\rangle + e^{2i\mu_0 B_0 t} |1\rangle) \end{aligned}$$

In the last equality we noted that we exploited our freedom to multiply the wavefunction by an arbitrary phase, in

this case, $\exp(i\gamma Bt)$. Furthermore, we played some tricks with operators and their eigenfunctions. Let's say that we have some function $f(A)$, where A is some Hermitian operator. As a Hermitian operator, it possesses an orthogonal basis of eigenstates $\{|\alpha\rangle\}$ and their associated eigenvalues, $\{\alpha\}$. If we take that function and operate on one of the eigenstates, we can replace the operator A with its eigenvalue,

$$A|\alpha\rangle = \alpha|\alpha\rangle \implies f(A)|\alpha\rangle = f(\alpha)|\alpha\rangle$$

This allowed us to deal with the exponentiated operator $\exp(-i\mu_0 B_0 \sigma_z t)$ in a nice way.

So what does this evolution look like on the Bloch sphere? Recall that an arbitrary qubit state can be written as $|\hat{n}+\rangle = \cos(\theta/2)|0\rangle + \sin(\theta/2)\exp(i\phi)|1\rangle$. The phase, ϕ , is evolving in time as $\phi(t) = 2\mu_0 B_0 t$. So the Bloch vector is precessing around the applied magnetic field with a frequency $\omega_L = 2\mu_0 B_0$, known as the Larmor frequency.

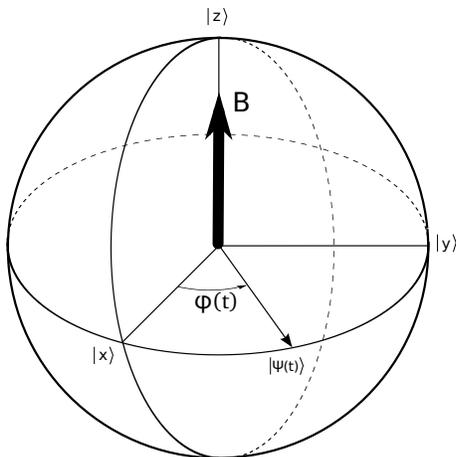


Figure 2: Bloch sphere representation of spin precession in constant field.