Building an NMR Quantum Computer

Spin, the Stern-Gerlach Experiment, and the Bloch Sphere

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I. INTRODUCTION

For the past few weeks you have been learning about the mathematical and algorithmic background of quantum computation. Over the course of the next couple of lectures, we'll discuss the physics of making measurements and performing qubit operations in an actual system. In particular we consider nuclear magnetic resonance (NMR). Before we get there, though, we'll discuss a very famous experiment by Stern and Gerlach.

II. SPINS AS QUANTIZED MAGNETIC MOMENTS

The quantum two level system is, in many ways, the simplest quantum system that displays interesting behavior (this is a very subjective statement!). Before diving into the physics of two-level systems, a little on the history of the canonical example: electron spin.

In 1921, Stern proposed an experiment to distinguish between Larmor's classical theory of the atom and Sommerfeld's quantum theory. Each theory predicted that the atom should have a magnetic moment (i.e., it should act like a small bar magnet). However, Larmor predicted that this magnetic moment could be oriented along any direction in space, while Sommerfeld (with help from Bohr) predicted that the orientation could only be in one of two directions (in this case, aligned or anti-aligned with a magnetic field). Stern's idea was to use the fact that magnetic moments experience a linear force when placed in a magnetic field gradient. To see this, not that the potential energy of a magnetic dipole in a magnetic field is given by:

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

Here, $\vec{\mu}$ is the vector indicating the magnitude and direction of the magnetic moment. The direction of the moment is analogous to the orientation of a bar magnet. This expression for the potential energy can also be used to derive a force that acts on the dipole (dipole is just another name for something that posesses a magnetic moment). Recall that the force is defined as the negative gradient of the potential:

$$F = -\nabla U = \nabla \left(\vec{\mu} \cdot \vec{B} \right)$$

Let's suppose that the magnetic field looks like $\vec{B} = B_0 z \hat{z}$; this field doesn't satisfy Maxwell's equations, but it makes the analysis easier. We get a force,

$$F = \nabla \left(\vec{\mu} \cdot B \right) = \nabla \left(\mu_z B z \right) = \mu B \cos(\theta)\, \hat{z}$$

The $\cos\theta$ term comes from the dot product, and θ is the angle between the magnetic field and the magnetic moment of the atom. If, for example, the dipole is initially aligned with the field, it will experience an 'upward' force, and if it is antialigned, it will experience a 'downward' force.

Now consider a beam of dipoles passing through this field gradient. Larmor's classical theory predicts that the dipole moment could point in *any* direction, so the beam would spread out homogenously. The Bohr-Sommerfeld

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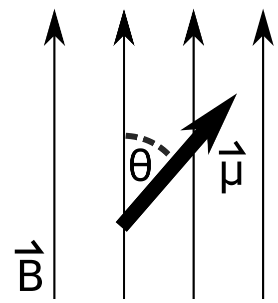

Figure 1: A magnetic moment in a magnetic field. The magnetic field is indicated by the vector $\vec{B}$, the magnetic moment of the atom is given by $\vec{\mu}$, and the angle between the two vectors is θ.

theory, though, predicts that the dipole moment can take only two values, aligned or anti-aligned with the field, so the beam would be *split* into two beams.

In 1922 Gerlach performed this experiment using silver atoms. (It turns out that electrons are a bad choice for this experiment because they are also affected by the Lorentz force, which is proportional to their velocity. Any spread in the initial velocity causes a spread in the output that overwhelms the spin-gradient force.) Gerlach saw his beam split into two distinct beams, thereby demonstrating the spatial quantization of the magnetic moment and falsifying the Lorentz theory. In an interesting twist, the Sommerfeld theory was *also* incorrect, even though it predicted the correct result of this experiment. In 1925/1926, Uhlenbeck and Goudspit postulated that the electron carried its own spin magnetic moment independent of its orbital angular momentum.

In any case, the Stern-Gerlach experiment provides a toy model that we can use to learn about quantum two level systems. Let's make the language a but more precise by labeling some things:

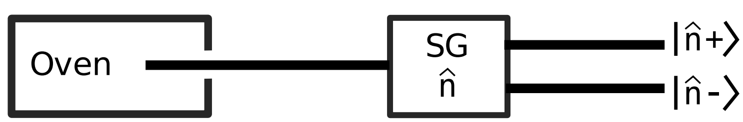

Figure 2: Schematic of Stern-Gerlach device.

In this diagram we have a cartoon picture of the Stern-Gerlach device. An oven produces a beam of particles which enters a region with an inhomogenous magnetic field, that gradient of which points in the $\hat{n}$ direction. The two beams that emerge we label $|\hat{n}+\rangle$ and $|\hat{n}-\rangle$. These symbols are what we use to label a quantum state, and what is written inside gives some information about this particular state. However, we should stress that what we write inside the ket is simply a label that we give to help us remember how the state behaves. We could have just as easily called the two states $|\text{Bob}\rangle$ and $|\text{Alice}\rangle$. Here, though, $|\hat{n}+\rangle$ denotes the state that is directed upwards when the field gradient is along the vector $\hat{n}$, and $|\hat{n}-\rangle$ is the state directed downwards.

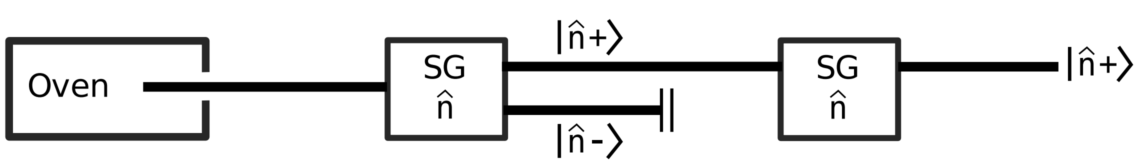

Figure 3: Cascaded Stern-Gerlach devices.

This all becomes much more interesting if we consider multiple, cascaded Stern-Gerlach devices. Let's add another identical SG device, which we'll denote as SG($\hat{n}$), after the first, but we'll discard the $|\hat{n}-\rangle$ state.

Notice that if we measure the output of the first SG($\hat{n}$) with a second SG($\hat{n}$) then we only get one beam out, the

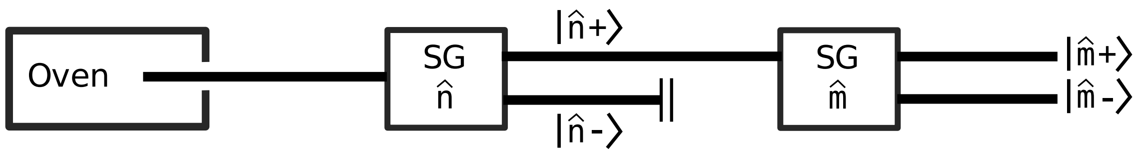

Figure 4: Cascaded Stern-Gerlach devices.

$|\hat{n}+\rangle$ state again. This shouldn't be surprising, as we have established with the first SG device that the dipole moment points along $\hat{n}$. But what would happen if we rotated the device?

Now we get two beams! The probability that $|\hat{n}+\rangle \to |\hat{m}\pm\rangle$ is found experimentally to be

$$P(|\hat{n}+\rangle \to |\hat{m}+\rangle) = \frac{1}{2}\left(1 + \hat{n}\cdot\hat{m}\right),$$

and also

$$P(|\hat{n}+\rangle \to |\hat{m}-\rangle) = \frac{1}{2}\left(1 - \hat{n}\cdot\hat{m}\right).$$

These probabilities can also be considered as the relative intestates of the two outgoing beams, $|\hat{m}\pm\rangle$, given an incoming beam $|\hat{n}+\rangle$.

Our task now is to seek a quantum mechanical description of this experiment. One way to do this is to search for the simplest description we can come up with, adding complexity only as we need to. Because the result of any measurement we can do is either "aligned" or "antialigned," the simplest model we can try is that the Hilbert space is two-dimensional. Since we can make a measurement for which the states $|\hat{n}\pm\rangle$ are eigenstates (measurement with a SG device in the $\hat{n}$ direction) with different eigenvalues (aligned or antialigned), they must be orthogonal states. Because we have two orthogonal states in a two-level space, these states can form a basis. The states $|\hat{m}\pm\rangle$ then form a different basis. Let's pick a special basis, $|\hat{z}\pm\rangle$ and express all other states as linear combinations of these vectors. To indicate that this basis is special, we relabel the vectors:

$$|\hat{z}+\rangle \to |0\rangle$$

$$|\hat{z}-\rangle \to |1\rangle$$

We can now represent any other state as a linear combination of the $\{|0\rangle, |1\rangle\}$ states:

$$|\hat{n}+\rangle = \alpha\,|0\rangle + \beta\,|1\rangle\,,$$

where α and β are complex numbers. Now that we know, roughly, how to express our states, we need to figure out what the α and β are. We can start by considering the following double Stern-Gerlach experiment.

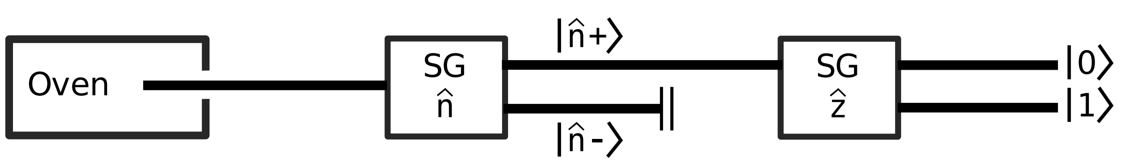

Figure 5: Cascaded Stern-Gerlach devices.

So, given the initial state $|\hat{n}+\rangle$, the probability of measuring $|0\rangle$ is

$$P_0(\hat{n}+) = |\langle 0|\hat{n}+\rangle|^2 = |\alpha\,\langle 0|0\rangle + \beta\,\langle 0|1\rangle|^2 = |\alpha|^2 = \frac{1}{2}\left(1 + \hat{n}\cdot\hat{z}\right)$$

We have used that fact that $\langle 0|1\rangle = 0$ and $\langle 0|0\rangle = 1$. To make this a bit nicer, we are going to rewrite $\hat{n}\cdot\hat{z} = \cos\theta$, where θ is the angle between the two unit vectors $\hat{n}$ and $\hat{z}$. This angle is also equal to the spherical coordinate, θ, defined by the unit vector $\hat{n}$, which, in cartesian coordinates, becomes:

$$\hat{n} = (\sin\theta\cos\phi, \sin\theta\sin\phi, \cos\theta)$$

Applying the trig identity, $(1+\cos\theta)/2 = \cos^2(\theta/2)$, we can say that:

$$|\alpha| = \cos(\theta/2)$$

A similar analysis shows that $|\beta| = \sin(\theta/2)$. So this simple argument has given us the magnitudes of α and β, but what about their phases? Because they are complex, they can be written as:

$$\alpha = |\alpha|\, e^{i\psi} \qquad\qquad \beta = |\beta|\, e^{i\chi}$$

giving,

$$|\hat{n}+\rangle = |\alpha|\, e^{i\psi}\,|0\rangle + |\beta|\, e^{i\chi}\,|1\rangle = \cos(\theta/2)e^{i\psi}\,|0\rangle + \sin(\theta/2)e^{i\chi}\,|1\rangle$$

However, a quantum state is only defined up to an overall phase, so we can multiply this state by $e^{-i\psi}$ to get

$$|\hat{n}+\rangle = \cos(\theta/2)\,|0\rangle + \sin(\theta/2)e^{i(\chi-\psi)}\,|1\rangle \equiv \cos(\theta/2)\,|0\rangle + \sin(\theta/2)e^{i\phi}\,|1\rangle\,,$$

where $\phi = \chi - \psi$ is the relevant phase. So what is ϕ for a given $|\hat{n}+\rangle$? Let's look at $|\hat{x}+\rangle$ and $|\hat{y}+\rangle$:

$$|\hat{x}+\rangle = \frac{1}{\sqrt{2}}\,|0\rangle + \frac{1}{\sqrt{2}}e^{i\phi_x}\,|1\rangle$$

$$|\hat{y}+\rangle = \frac{1}{\sqrt{2}}\,|0\rangle + \frac{1}{\sqrt{2}}e^{i\phi_y}\,|1\rangle$$

If a double SG device is set up, with $\hat{x}$ first, then $\hat{y}$, the probability of seeing $|\hat{y}+\rangle$ given that the first beam emerged in $|\hat{x}+\rangle$, is $P(x \to y) = (1 + \hat{x}\cdot\hat{y})/2 = 1/2$. But this is also the overlap between the two states:

$$\begin{aligned}
P(\hat{x} \to \hat{y}) &= |\langle \hat{x} + |\hat{y}+\rangle|^2 \\
&= \left| \frac{1}{2}\,\langle 0|0\rangle + \frac{1}{2}e^{i(\phi_y-\phi_x)}\,\langle 1|1\rangle \right|^2 \\
&= \frac{1}{2} + \frac{1}{2}\cos(\phi_y - \phi_x) \\
&= \frac{1}{2}
\end{aligned}$$

So, $\cos(\phi_y - \phi_x) = 0 \to \phi_y - \phi_x = \pi/2$. This implies that we can associate the phase angle, ϕ_n, with the second spherical coordinate, ϕ, in:

$$\hat{n} = (\sin\theta\cos\phi, \sin\theta\sin\phi, \cos\theta)$$

So, for any vector $\hat{n}$, $|\hat{n}+\rangle = \cos(\theta/2)\,|0\rangle + \sin(\theta/2)e^{i\phi}\,|1\rangle$, where (θ, ϕ) are the polar coordinates of the vector $\hat{n}$. But what about $|\hat{n}-\rangle$? The states $|\hat{n}+\rangle$ and $|\hat{n}-\rangle$ must be orthogonal. This gives a unique solution, up to the standard quantum mechanical phase,

$$|\hat{n}-\rangle = \sin(\theta/2)\,|0\rangle + \cos(\theta/2)e^{-i\phi}\,|1\rangle$$

But this is the same as

$$|(-\hat{n})+\rangle = \cos((\pi-\theta)/2)\,|0\rangle + \sin((\pi-\theta)/2)e^{-i\phi}\,|1\rangle = |\hat{n}-\rangle$$

So, $|\hat{n}+\rangle$ is orthogonal to $|(-\hat{n})+\rangle$! This representation we have been using (θ, ϕ as parameters for a qubit state) is known as the Bloch Sphere representation. Every point on the Bloch Sphere (a unit sphere in $\mathbb{R}^3$) corresponds to a unique state, with the orthogonal state being represented by the antipodal point on the sphere.

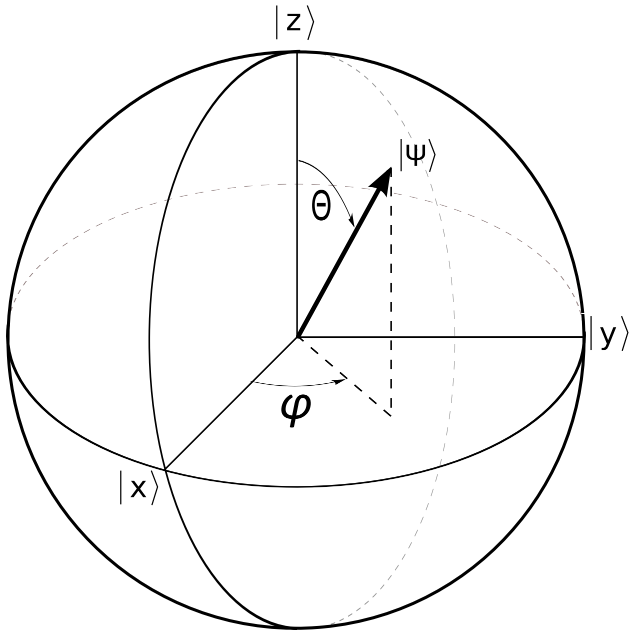

Figure 6: Bloch sphere representation of a qubit state.

We'll see a lot more of the Bloch Sphere representation over the next few lectures, so you'll have time to get accustomed to it.