

Last time we saw that the time dependent Schr. eqn. can be decomposed into two equations, one in time (t) and one in space (x):

$$\text{space} : \hat{H}\psi(x) = E\psi(x) \tag{1}$$

$$\text{time} : i\hbar \frac{\partial \phi(t)}{\partial t} = E\phi(t) \tag{2}$$

This time equation is easy: $\phi(t) = e^{-iEt/\hbar} \rightarrow \phi(t) = e^{-i\omega t}$, $\omega = \frac{E}{\hbar}$, or $E = \hbar\omega$. (Planck-Einstein relation.)

The spatial equation is harder. It is called the "time-independent Schrodinger equation." However difficult to solve, this equation is a special type of equation known as an *eigenvalue* problem, where "operator $\times \psi$ " = "constant $\times \psi$." Thus the Schr. eqn. reduces to an eigenvalue problem, which has a storied history in mathematics. To solve the Schr. eqn., one must find the set of wavefunctions $\{\psi_k(x)\}$ that return to themselves (times a constant) when acted on by \hat{H} : $\hat{H}\psi_k(x) = E_k\psi_k(x)$. Each solution ψ_k has an energy E_k associated with it. The states $\{\psi_k\}$ and only they have well-defined energies. The energies $\{E_k\}$ are the set of all physically allowed energies of the system.

The full time-dependent solution is $\psi(x,t) = \psi(x)\phi(t) = \psi_k(x)e^{-iE_k t/\hbar}$. Since these are linear equations we can add solutions, just as above for the free particle case. So, the most general solution to the Schrodinger equation is $\psi(x,t) = \sum_k A_k \psi_k(x)e^{-iE_k t/\hbar}$.

This tells us the rule for time evolution in quantum mechanics: if you want to know how a wave function evolves in time then you just break it down into energy eigenfunctions and multiply each one by a time-dependent phase factor whose frequency is proportional to its energy.

Example: Suppose at time $t=0$ we have $\psi(x) = A_1\psi_1(x) + A_2\psi_2(x) + A_3\psi_3(x)$ where $\hat{H}\psi_i(x) = E_i\psi_i(x)$. What is $\psi(x,t)$ for $t \neq 0$?

To solve this, we can just add in the phase factors:

$$\psi(x,t \neq 0) = A_1\psi_1(x)e^{-iE_1 t/\hbar} + A_2\psi_2(x)e^{-iE_2 t/\hbar} + A_3\psi_3(x)e^{-iE_3 t/\hbar} \tag{3}$$

Let's do another example: For a free particle $\hat{H} = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} \rightarrow \psi_k(x) = e^{ikx}$, $E_k = \frac{\hbar^2 k^2}{2m}$. Therefore, $\psi(x,t) = e^{ikx} e^{-i\frac{\hbar^2 k^2}{2m} t}$ as seen before.

In general $\hat{H}\psi(x) = E\psi(x)$ can be a very difficult differential equation to solve. Physicists and chemists spend a great deal of time solving this equation!

Note that we have already derived this time evolution earlier when analyzing the unitary evolution of a quantum state: $\psi(x,t \neq 0) = e^{-i\hat{H}t/\hbar}\psi(x,t = 0)$, with $e^{-i\hat{H}t/\hbar}$ the time evolution operator. Recall how we approached it before:

Any $\psi(x, t = 0)$ can be written $\psi(x, t = 0) = \sum_k A_k \psi_k(x)$, so:

$$\psi(x, t \neq 0) = e^{-i\hat{H}t/\hbar} \left(\sum_k A_k \psi_k(x) \right) = \sum_k A_k e^{-i\hat{H}t/\hbar} \psi_k(x) = \sum_k A_k \psi_k(x) e^{-iE_k t/\hbar} \quad (4)$$

which is the same as above, since $\psi_k(x)$ is an eigenfunction of \hat{H} with eigenvalue E_k .

The time-independent Schr. eqn. sets a condition that determines what the allowed energies of a system are and what the states look like that have well-defined energy ("well-defined" means you'd get the same answer if you measured the energy of all of the members of an identically prepared ensemble of systems in that state). However, we can also construct states that have well-defined values of other physical quantities, like momentum, position, and angular momentum.

This is often called the basis of stationary states. Why? Because if $\psi = \psi_i(x)$ where $\hat{H}\psi_i = E_i\psi_i$ then $\psi(x, t) = \psi_i(x)e^{-iE_i t/\hbar}$. The probability density $P(x, t)$ is then given by

$$P(x, t) = |\psi(x, t)|^2 = \left(\psi_i(x)e^{-iE_i t/\hbar} \right)^* \left(\psi_i(x)e^{-iE_i t/\hbar} \right) = |\psi_i(x)|^2$$

Therefore the time dependence for the probability density dropped out and does not change in time.

But what does "well-defined" energy mean? It can mean two things: (1) A state ψ has well-defined energy if $\hat{H}\psi = C\psi$ where "C" = energy of state. (2) A state ψ has well defined energy if an ensemble (read, many copies) of systems all prepared in the state ψ give the same answer if you measure energy (i.e. $E = "C"$ if $\hat{H}\psi = E\psi$).

So let's discuss measurement. If $|\psi\rangle = a_1|\psi_{E_1}\rangle + a_2|\psi_{E_2}\rangle + a_3|\psi_{E_3}\rangle + \dots$, what is the result of a measurement of energy? One of the postulate of QM is that the result of the measurement must be an eigenvalue of \hat{H} . ψ will collapse onto one of these eigenstates with some probability. What's the probability of obtaining E_3 ? $P_3 = |\langle \psi_{E_3} | \psi \rangle|^2 = a_3^2$ And what is ψ after measurement? ψ is projected to ψ_3 upon an observation of E_3 . So, measurement is a random collapse onto one of the eig. states of the observable you are measuring!

The same holds for momentum: If we are discussing momentum then it's best to work with momentum eigenstates.

$$\hat{p}\psi_p = p\psi_p \Rightarrow \{\psi_p\}, \{p\}$$

Suppose $|\psi\rangle = b_1|\psi_{p_1}\rangle + b_2|\psi_{p_2}\rangle + b_3|\psi_{p_3}\rangle + \dots$ What is a result of a measurement of momentum? We will end up measuring an eigenvalue of momentum with some probability, and then collapse onto that eigenstate ($P_2 = |b_2|^2$).

The exact same thing happens for the observables \hat{x} , \hat{L} , etc. The eigenstates of these observables define bases, and measurement of that observable randomly collapses us onto one of those eigenstates.

Question: What if we take an ensemble of identically prepared states and measure the same physical quantity for each? How do we determine (theoretically) the average value of the measurements? This will lead us to the definition of an *expectation value*.

Example: ENERGY. Suppose we know states $\{\psi_E\}$, $\{E\}$. If an ensemble is prepared in $|\psi\rangle = |\psi_E\rangle$ then the situation is simple: $\langle E \rangle = E_0$. But what if we prepare an ensemble in a state $|\psi\rangle$ in a superposition

state which is not an eigenstate of \hat{H} , e.g. $|\psi\rangle = a_1|\psi_{E_1}\rangle + a_2|\psi_{E_2}\rangle + a_3|\psi_{E_3}\rangle + \dots$? What is $\langle E \rangle$ then?

$$\langle E \rangle = E_1 \text{Prob}[E_1] + E_2 \text{Prob}[E_2] + E_3 \text{Prob}[E_3] + \dots$$

where $\text{Prob}[E_i]$ is just

$$\text{Prob}[E_i] = |\langle \psi_{E_i} | \psi \rangle|^2 = |a_i|^2$$

This yields:

$$\langle E \rangle = |a_1|^2 E_1 + |a_2|^2 E_2 + |a_3|^2 E_3 + \dots$$

Our shorthand for this is given by:

$$\langle E \rangle = \langle \psi | \hat{H} | \psi \rangle$$

which is known as the expectation value of the Hamiltonian (or equivalently of the energy). Use completeness to show that $\langle E \rangle = \langle \psi | \hat{H} | \psi \rangle$ does indeed give you the same expression as above.

We can do this for *any* observable! Consider arbitrary observable \hat{A} . The average value of this quantity for ensemble of systems prepared in $|\psi\rangle$ is $\langle A \rangle = \langle \psi | \hat{A} | \psi \rangle$.

It should be noted that it is sometimes hard to evaluate the expectation value. Take the continuous basis for example ($|x\rangle$). Suppose $\psi(x) = \langle x | \psi \rangle = A e^{-x^2}$. What is the average value of measured momentum for an ensemble of systems?

$$\langle \hat{p} \rangle = \langle \psi | \hat{p} | \psi \rangle = \int_{-\infty}^{\infty} \psi^*(x) \hat{p} \psi(x) dx = \int_{-\infty}^{\infty} (A^* e^{-x^2}) \left(\frac{\hbar}{i} \frac{\partial}{\partial x} \right) (A e^{-x^2}) dx = 0$$

So, in this instance the expectation value is zero. It is left as an exercise to evaluate $\langle p^2 \rangle$ (symmetry analysis will immediately tell you if it zero or not).

1 Particle-in-a-box model for atomic qubit

Let's do an example now! Let's consider a situation where we want to use the electrons inside atoms as qubits. How do we describe the physical details of these qubits? What are their allowed energies? How do they change in time? *What do we do???* We solve the Schr. equation, that's what.

As is the case in most QM problems, we must find the Hamiltonian \hat{H} . \hat{H} in this case is the energy operator for an electron in an atom. To know this then we must make some assumptions about how electrons behave in an atom.

Let's assume that atoms are very tiny ($\approx 10^{-10}$ meter) 1-D boxes with very hard walls. The walls are located at position $x = 0$ and $x = l$. This model works surprisingly well. Inside the box \hat{H} is given by the free particle

Hamiltonian $\hat{H} = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2}$. Outside the box we model the very hard walls as regions where the potential energy $V \rightarrow \infty$. This has the effect of *disallowing* any ψ to be nonzero outside the box. If it did exist in this region its energy (obtained, as always, by applying the Hamiltonian) would also go to infinity. That's too much energy for our little electrons, so we can say that we will restrict our wavefunctions $\psi(x)$ to functions which vanish at $x \leq 0$ and $x \geq l$.

$$\psi(x=0) = \psi(x=l) = 0$$

Strictly speaking, we mean that $\psi(x \leq 0) = \psi(x \geq l) = 0$. We will see that this will allow us to construct wavefunctions which are normalized over our restricted box space $x \in \{0, l\}$. The system as we've described it can be sketched in Figure 2.

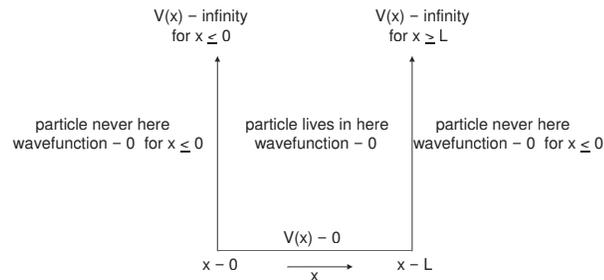


Figure 1: Particle in a box

The first thing to note is that we've done this problem before! For a free particle we know that we have solutions $\psi_E(x) = Ae^{ikx} + Be^{-ikx}$ with energies $E_k = \frac{\hbar^2 k^2}{2m}$. Are we done? No, because we need to impose our *boundary condition* that $\psi(x=0) = \psi(x=l) = 0$ since those walls are hard and do not allow particles to exist outside of the free particle box we've constructed.

Our previous solution $\psi_E(x) = Ae^{ikx} + Be^{-ikx}$ is fine, but we can also write another general solution as follows:

$$\psi_E(x) = C \sin(kx) + D \cos(kx)$$

As we will see, this is a convenient choice. If we now impose our first boundary conditions:

$$\psi_E(x=0) = 0 = C \sin[k(x=0)] + D \cos[k(x=0)] = C(0) + D(1) = D$$

So $D = 0$ and we can forget about the cosine solution. The second boundary condition tells us:

$$\psi_E(x=l) = 0 = C \sin(kl) = 0$$

This is satisfied for all $kl = n\pi$, where n is an integer. Therefore, we have $k_n = \frac{n\pi}{l}$ which gives us our *quantized* eigenfunction set. The energy eigenvalues are

$$E_n = \frac{\hbar^2 k_n^2}{2m} = \frac{\hbar^2 n^2 \pi^2}{2m}$$

with eigenfunctions

$$\psi_n(x) = C \sin\left(\frac{n\pi}{l}x\right)$$

Are we done? No, because we must normalize.

$$\langle \psi_n | \psi_n \rangle = \int_0^l |\psi_n(x)|^2 dx = 1 \Rightarrow \int_0^l C^2 \sin^2\left(\frac{n\pi}{l}x\right) dx = 1 \Rightarrow C = \sqrt{\frac{2}{l}}$$

So normalization has given us our proper set of energy eigenfunctions and eigenvalues:

$$\psi_n(x) = \sqrt{\frac{2}{l}} \sin\left(\frac{n\pi}{l}x\right), E_n = \frac{\hbar^2 n^2 \pi^2}{2ml^2}$$

Higher energy states have more nodes. Some of the wavefunctions can be sketched as follows:

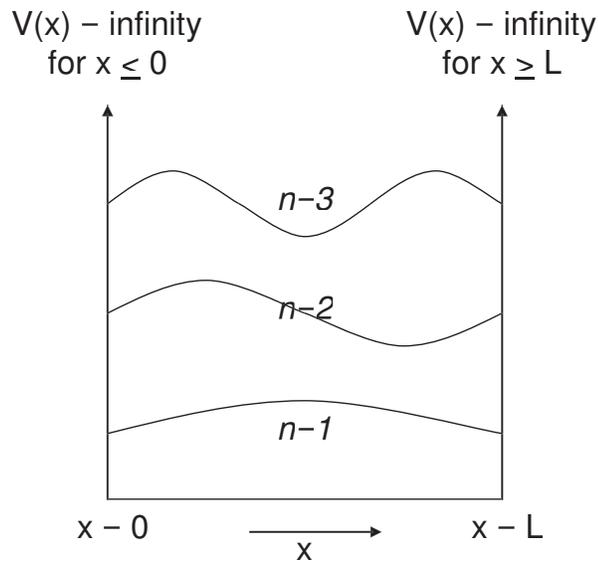


Figure 2: The first three eigenfunctions of the particle in a box system.

What does this have to do with the discrete quantum state picture as described in the context of qubits? To obtain a qubit from this system, we can construct our standard basis $|0\rangle$ and $|1\rangle$ by just restricting our state space to the bottom two eigenstates:

$$|0\rangle = \psi_1(x) = \sqrt{\frac{2}{l}} \sin\left(\frac{\pi}{l}x\right), E_{n=0} = \frac{\hbar^2 \pi^2}{2ml^2}$$

$$|1\rangle = \psi_2(x) = \sqrt{\frac{2}{l}} \sin\left(\frac{2\pi}{l}x\right), E_{n=1} = \frac{4\hbar^2 \pi^2}{2ml^2}$$

Physically this would mean forcing the total energy of the system to be less than E_2 , meaning that the particle could never have any overlap with ψ_n for $n \geq 2$.

What about the energies of qubit states? Suppose I take 10^6 qubits prepared in state $|0\rangle = \psi_1$ and measure their energy and make a histogram. What does the histogram look like? See Figure 1(a).

Now suppose that I prepare 10^6 qubits in the superposition state $\psi' = \sqrt{\frac{3}{5}}|0\rangle + \sqrt{\frac{2}{5}}|1\rangle$, measure *their* energies, and make a histogram. How does it look? See Figure 1(b)

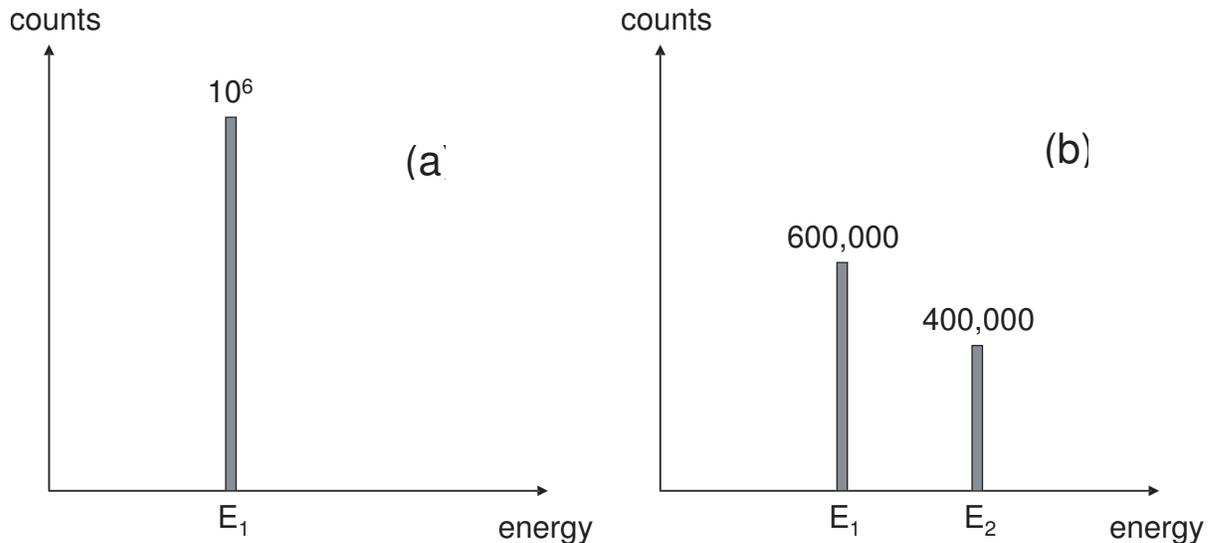


Figure 3: Histograms of particle energy measurements.

Ask yourself, is ψ' a state with well-defined energy? *NO*. Why not? ψ' is not an eigenstate of the Hamiltonian operator. Let's check this:

$$\hat{H}\psi' = \hat{H}\left(\sqrt{\frac{3}{5}}\psi_1 + \sqrt{\frac{2}{5}}\psi_2\right) = \sqrt{\frac{3}{5}}E_1\psi_1 + \sqrt{\frac{2}{5}}E_2\psi_2$$

Does this equal (constant) $\times(\psi')$? No, because as stated E_1 and E_2 are not equal. Therefore ψ' is not an eigenstate of the energy operator and has no well-defined energy. However it is a perfectly valid superposition state of the qubit.

This extremely simple model of a confined particle is actually very useful physically, and pops up in many real-world applications. In fact, the particle-in-a-box model provides one of the simplest meaningful descriptions of an atom. In an atom the confined particle is an electron and the box is created by the Coulomb

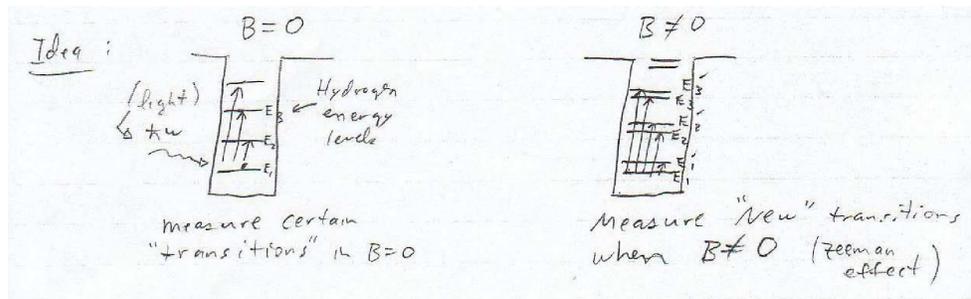
attraction between the negatively charged electron and the positively charged nucleus. Most atoms have a lot of electrons, but all atoms behave (at some level) in a manner that is very similar to the simplest atom which is hydrogen. Hydrogen has just one electron that circles around one proton. Solving the exact Schroedinger equation for the motion of an electron around a proton involves some complexities that we don't want to worry about right now, but suffice to say that the energy is determined most strongly by the radial motion of electron. (i.e. the electron's radial distance from the proton). The "radial Schroedinger Equation of the electron then looks very much like the simple "particle-in-a-box model that we have just solved. The ground state and quantized excited states of hydrogen look like standing waves in much the same way as the particle-in-a-box wave-functions. Higher energy states of hydrogen have more nodes just like the particle-in-a-box states.

Spin

Qubit systems can always be mapped onto an effective spin 1/2 system so it is important to understand what this is and where it comes from.

Elementary particles and composite particles carry an intrinsic angular momentum called spin. For our purposes, the most important particles are electrons and protons. To each of these is associated an angular momentum vector that can point up $|\uparrow\rangle$ or down $|\downarrow\rangle$. The quantum mechanical spin state of an electron or proton is thus $|\psi\rangle = \alpha|\uparrow\rangle + \beta|\downarrow\rangle$. Therefore, spins can be used as qubits with $|0\rangle = |\uparrow\rangle$, $|1\rangle = |\downarrow\rangle$.

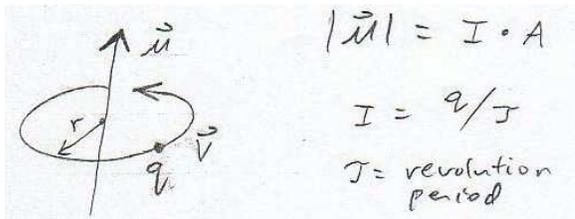
The spin angular momentum is intrinsic and signals the presence of an intrinsic magnetic moment. Uhlenbeck and Goudsmit introduced the concept of 'spin' in 1925 to explain the behavior of hydrogen atoms in a magnetic field:



The extra transitions can be explained if an electron has an *intrinsic* magnetic moment $\vec{\mu}$, since a magnetic moment in a magnetic field \vec{B} has an energy $E = -\vec{\mu} \cdot \vec{B}$. In the context of QM, new energy levels can derive from $\vec{\mu}$ being oriented parallel or anti-parallel to \vec{B} .

Where does $\vec{\mu}$ come from?

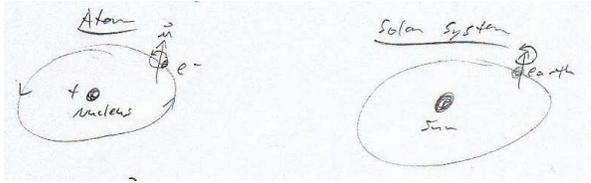
The simplest explanation is "classical": classically, a magnetic moment $\vec{\mu}$ comes from a loop of current.



The energy $E = -\vec{\mu} \cdot \vec{B}$ comes from $\vec{I} \times \vec{B}$ force of current in a B-field (Lorentz force). The lowest energy, and thereby the place where "the system wants to go", is obtained when the magnetic moment and B-field

line up.

If an isolated electron has “intrinsic” $\vec{\mu}$ then the simplest explanation for this is that electron spins about some axis. This is independent of its orbital motion in an atom, just like the Earth’s ”spin” about the north pole is independent of its orbit around the sun.



Since $\vec{\mu}$ is associated with a “spinning” charge, then we can write $\vec{\mu}$ in terms of angular momentum. Anything that spins has angular momentum!

The simplest way to see this is classically for a spinning charge. For an electron the charge q is equal to $-e$. Angular momentum is given by $\vec{L} = \vec{r} \times \vec{p} = \vec{r} \times m\vec{v}$. $L = mvr$ for a charge of mass $= m$ moving in a circle with velocity $= v$. The magnetic moment can be obtained as follows:

$$\mu = (\text{current}) (\text{Area}) = \frac{q}{\tau} \cdot \pi r^2$$

But the revolution period $\tau = \frac{2\pi r}{v}$. Substituting for τ and v in terms of L , we obtain

$$\vec{\mu} = \frac{q}{2m} \vec{L}$$

Now comes the tricky part. *The electron is not actually spinning about some axis!* It only acts as though it is. Electrons are point particles which, as far as we know, have no ”size” in the traditional sense. Therefore the r in the previous discussion of spinning charge is not meaningful. The *intrinsic* angular momentum of an electron has nothing to do with ”orbital” motion, but it does lead to an intrinsic $\vec{\mu}$. This is a relativistic effect that can be derived from the Dirac Equation (Relativistic Schrodinger equation for spin- $\frac{1}{2}$ particles), but it holds for electrons that are not moving fast.

This intrinsic angular momentum is called “spin” $= \vec{S}$.

For an electron, classically: $\vec{\mu} = -\frac{e}{2m} \vec{L}$, while quantum mechanically: $\vec{\mu} = -\frac{ge}{2m} \vec{S}$.

What is g ? g is called the g-factor and it is a unitless correction factor due to QM. For electrons, $g \approx 2$. For protons, $g \approx 5.6$. You should also note that $\frac{m_{\text{proton}}}{m_{\text{electron}}} \approx 2000$, so we conclude that $\mu_{\text{proton}} \ll \mu_{\text{electron}}$.

So, to understand behavior of the electron’s intrinsic magnetic moment $\vec{\mu}$ (which is an observable we can measure) then we must understand the behavior of its intrinsic angular momentum $= \vec{S}$. This is why spin is important. Since the electron is small, \vec{S} must be described by QM.

See also notes “electrons in atoms” (look for “spin” section) on the web page Science Trek at <http://www.colorado.edu/phy>

1.1 The Bloch Sphere

A very nice way to think of the quantum states of qubits is via the ”Bloch Sphere.” This is a convenient mapping for all possible single-qubit states. See Figure 1 below.

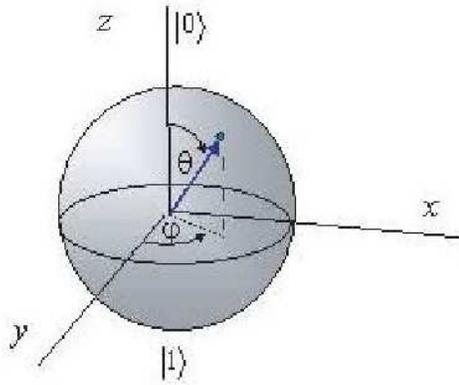


Figure 4: The Bloch sphere. $|0\rangle$ is at the North pole, $|1\rangle$ at the South pole.

θ and ϕ are the usual spherical coordinates, with $0 \leq \theta \leq \pi, 0 < \phi \leq 2\pi$. Every point on the sphere represents a possible qubit. All possible qubits (within an overall multiplicative phase factor) can be thought of as vectors on this unit sphere. A vector on the Bloch Sphere represents this qubit:

$$|\psi\rangle = \cos\frac{\theta}{2}|0\rangle + e^{i\phi}\sin\frac{\theta}{2}|1\rangle$$