Quantum Basis for Quantum Computing

Schrödinger's Equation, Hilbert Space, and Dirac Notation

The physical world is governed by Schrödinger's equation:

$$\hat{H}\psi = i\hbar\frac{\partial\psi}{\partial t}$$

where $\hat{H}$ is the total energy of the system, written out in operator form according to the rules of quantum mechanics. All the information that can be known is contained in the wave function ψ.

As an example to get things going, if $\hat{H}$ corresponds to a linear harmonic oscillator problem on configuration space (a mass on a spring in real space), then

$$\hat{H} = \frac{\hat{P}^2}{2m} + \frac{1}{2}k\hat{x}^2$$

where k is the spring constant. P (the linear momentum) and x are conjugate variables and the hat means they are now quantum operators. The linear harmonic oscillator is a model that in fact serves as an approximation to many critical phenomena, though in general not quantum computing (The reason is that the linear harmonic oscillator is linear to all orders in the presence of a driving force. The basic quantum logic device must be highly nonlinear as seen below). In configuration space, according to the rules of quantum mechanics,

$$\hat{x} = x \text{ and } \hat{P} = -i\hbar\frac{\partial}{\partial x}$$

Since $\hat{H}$ is independent of time, we may use separation of variables to solve the PDE:

$$\hat{H}u(x) = Eu(x) \text{ and } i\hbar\frac{\partial g(t)}{\partial t} = Eg(t)$$

where $\psi = ug$, and E corresponds to an energy eigen value of the operator equation: $\hat{H}u = Eu$. There can be an infinite number of eigen functions and eigen values that solve this equation. The set of all solutions $\{u_n(x)\}$ form a complete ortho-normal (orthogonal and normalized) set that can be used to expand any arbitrary function, *defined on the same space*. In the above case, this means for an arbitrary $f(x)$,

$$f(x) = S_n c_n u_n(x)$$

where S_n is a discrete sum $S_n = \sum_n$. if n is discrete or $S_n = \int dn$ if n is continuous (not in the case of a linear harmonic oscillator.) If we know $f(x)$, then

$$c_n = \int_{space} g_n^*(x) f(x) dx$$

Dirac developed what looks like a short hand notation for this but is much more powerful and general. We simply suppress x and send $u_n(x) \to |n\rangle$ and $u_n^*(x) \to \langle n|$ (called a bra and ket, respectively). Then the expression for $f(x)$ becomes

$$|f\rangle = S_n c_n |n\rangle$$

Now, use your imagination. Suppose n took on only three values, which will call 1,2,3 or $\hat{x},\hat{y},\hat{z}$. Where the latter are unit vector for a Cartesian coordination system. Then, $|f\rangle$ would simply be the vector pointing off into space where the c_n's represent the projection of the vector $|f\rangle$ on to the 3 different axis. Then, of course, the c_n's are the inner vector product (dot product) between $|f\rangle$ and the different axis:

$c_n = \langle \psi_n^* | f \rangle$.

Now recognize the Hamiltonian need not necessarily be of the simple form in coordinate space that we used for the linear harmonic oscillator. It could be a more general operator, like a matrix. Then the eigen functions are indeed vectors (called eigen vectors) and the arbitrary function $f(x)$ becomes the state vector $|\psi\rangle$. We then say that the eigen functions of $\hat{H}$ ($\{|n\rangle\}$)span a Hilbert space (which may have an infinite number of dimensions).

Probability, Measurement and Wave Function Collapse

Notice that in the same sense that the coefficients of the sin's and cos's in a Fourier series present the fraction of wave form characterized by that specific frequency component, so to do the c_n's exactly correspond to the probability of finding the system described by a state $|\psi\rangle$ in an eigen state $|n\rangle$ of $\hat{H}$ when a measurement is made of the energy of the particle (or more general system).

After the measurement, the wave function collapses in the eigen state corresponding to the measured energy. In other words, if a measurement of energy of the system described by $|\psi\rangle$ is E_n, then after the measurement:

$|\psi\rangle = |n\rangle$

The measurement itself destroys the state of the system. This is why if you use quantum bits the way you use classical bits and make a measurement each time, you have no improvement with a quantum computer. The challenge has been to develop an algorithm which does not do this.

Time Dependence

Even if the Hamiltonian is time-independent, as it is for most systems of interest except for when the quantum computer is being driven, Schrödinger's equation is time dependent, and the wave function evolves in time. From above:

$\hat{H}|u_n\rangle = E_n|u_n\rangle$ *and* $i\hbar\frac{\partial g_n}{\partial t} = E_n g_n$

For every eigen state $|n\rangle$, there is an E_n. The right hand equation is readily integrated to give

$g_n = \exp -i\frac{E_n}{\hbar}t$

Then, in general, a wave function as a function of time is given by

$|\psi\rangle(t) = S_n c_n |u_n\rangle e^{-i\frac{E_n}{\hbar}t}$ where since Schrödinger's equation is first order in time (compared to classical equations of motion), we have only to specify the state of the system at t=0.

Measurement and Expectation Values

One of the critical postulates in quantum mechanics is that all classical observables are associated quantum mechanical operators. For the case above, we have $x \to \hat{x} = x \text{ and } p \to \hat{p} = -i\hbar\frac{\partial}{\partial x}$. If you make a measurement of the system, *the only values you are allowed to measure are eigen values of the corresponding eigen value equation for that operator*. For a system described by the state vector $|\psi\rangle(t)$, the average value for an operator, $\hat{O}$, is

$\langle O\rangle(t) = \langle\psi(t)|\hat{O}|\psi(t)\rangle$

For the case of the harmonic oscillator and momentum

$$\langle\hat{p}\rangle(t) = \langle\psi(x,t)|\hat{p}|\psi(x,t)\rangle = \int_{-\infty}^{\infty} dx\psi^*(x,t)\left(-i\hbar\frac{d}{dx}\right)\psi(x,t)$$

Spin, SU2 group, Two-Level Systems and Application to Quantum Computing

Of special importance to quantum computing is the concept of spin. Spin systems are important because they have been proposed for application to potential quantum devices. Perhaps more importantly, the formalism developed to describe spin systems is the backbone of the quantum computing literature, and there are many more systems, which can be characterized by so-called pseudo spin properties, have also been proposed for various quantum computing devices.

Spin is a new concept that has no classical analog. It's name sounds classical because experimentally spin was first observed in studies of angular momentum and is associated with what appears to be an *intrinsic* angular momentum. Indeed, the value of angular momentum is in fact $\frac{\hbar}{2}$. It is easy to see that this is non-classical by recognizing that the quantum mechanical operator for z-component of angular momentum is

$\hat{L}_z = -ih\frac{\partial}{\partial\theta}$. The corresponding eigen-value equation that determines the observables is

$\hat{L}_z u(\theta) = l_z u(\theta)$

with solution

$u(\theta) = e^{il_z\theta}$

To correspond to real world, we of course require $u(\theta) = u(\theta + 2\pi)$, i.e., the we must recover the function if we rotate the coordinate system 2π. This requires that l_z be $n\hbar$ where n is an integer. Clearly this is not satisfied with a half integer.

Since there is no classical analog, the usual quantum formalism does not work. We have to introduce a new kind of operator. Any operator will do, but the most convenient is a matrix operator. The full development of this formalism is beyond the time limits of this lecture, so we can at best simply write down the rules that result from following the very precise postulates of non-relativistic quantum mechanics.

Rules for Spin

Spin is vector, just like ordinary angular momentum, and the only two operators that can be associated with observables are S^2 corresponding the magnitude square of angular momentum and S_z. One of the critical postulates of quantum mechanics is that values for physical observables must come from the corresponding eigen value equation for their operators.

The result of the algebra is that the eigen functions, designated $|s, m_s\rangle$ give rise to eigen values for S^2 and S_z according to
$S^2|s,m_s\rangle = s(s+1)\hbar^2|s,m_s\rangle$ and
$S_z|s,m_s\rangle = m_z\hbar|s,m_s\rangle$
For the case of spin $\frac{1}{2}$ particles, $s=\frac{1}{2}$ and $m_z=\pm\frac{1}{2}$, corresponding to the "spin-up" state $\left|\frac{1}{2},\frac{1}{2}\right\rangle$, and "spin-down" state $\left|\frac{1}{2},-\frac{1}{2}\right\rangle$. The forms for the operators and eigen vectors are given below where the convention $\hat{\mathbf{S}}=\frac{\hbar}{2}\hat{\sigma}$ where the σ-operators are called the Pauli spin operators or matricies:
$\hat{\sigma}_x=\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix}$; $\hat{\sigma}_y=\begin{pmatrix}0 & -i\\ i & 0\end{pmatrix}$; $\hat{\sigma}_z=\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}$, $\hat{\sigma}^2=\begin{pmatrix}1 & 0\\ 0 & 1\end{pmatrix}$.
The corresponding eigen vectors are
$\left|\frac{1}{2},\frac{1}{2}\right\rangle=\begin{pmatrix}1\\0\end{pmatrix}\equiv|+\rangle\equiv|\uparrow\rangle$ and $\left|\frac{1}{2},-\frac{1}{2}\right\rangle=\begin{pmatrix}0\\1\end{pmatrix}\equiv|-\rangle\equiv|\downarrow\rangle$.

There are three other important operators associated with spin and pseudo spin $\frac{1}{2}$ systems. The first two are called raising and lower operators (or sometime creation and annilhilation operators) given by $\hat{\sigma}_\pm=\hat{\sigma}_x\pm i\hat{\sigma}_y$ where
$\hat{\sigma}_+=\begin{pmatrix}0 & 1\\ 0 & 0\end{pmatrix}$ and $\hat{\sigma}_-=\begin{pmatrix}0 & 0\\ 1 & 0\end{pmatrix}$.
They have the interesting algebraic features that
$\hat{\sigma}_+|-\rangle=|+\rangle,\ \hat{\sigma}_+|+\rangle=0$ and
$\hat{\sigma}_-|+\rangle=|-\rangle,\ \hat{\sigma}_-|-\rangle=0$.

In the sense that the spin has magnitude of $\frac{1}{2}$ which is fixed, changes in the direction of the spin amount to a rotation. In this algebra, it is possible to show that there exists a rotation operator that rotates the spin about the axis $\hat{\mathbf{n}}$ by an amount ϕ. The operator has the form
$\hat{U}_R=\exp\left(-\frac{i}{2}\phi\hat{\mathbf{n}}\cdot\hat{\sigma}\right)=\hat{I}\cos\frac{\phi}{2}-i\hat{\mathbf{n}}\cdot\hat{\sigma}\sin\frac{\phi}{2}$
This operator is special because it is a unitary operator and rotations are unitary transformations. It is special unitary operator characterized by a 2x2 matrix and is part of the SU2 group.

Generalization and Application to Quantum Computing

Spin is a particularly interesting physical observable to consider because, as we discuss below, a wave function given in as a *coherent superposition of two spin states* $\psi=c_+|+\rangle+c_-|-\rangle$ tends to be fairly robust against decoherence as described below. However, there are many other systems which can be characterized as having just two states (even when they may have an infinite number of states.) Such systems (atoms, semiconductor quantum dots, etc.) may have a large number of states, but in the laboratory, we can arrange to *interact* with only two of them, thus allowing us to make the *two-level approximation*. The two-level approximation allows us to

associate with this system a pseudo spin, where one state corresponds to "spin down" and the other state corresponds to "spin up".

The idea may have occurred to you now that a spin $\frac{1}{2}$ system can be associated with a single quantum bit (qubit), where, in analogy with classical computers, spin down is a "zero" and spin up is a "one." To get multiple qubits, it is important to have multiple spin systems. In the language of quantum mechanics, each spin defines a Hilbert space, and the system involving multiple qubits involves multiple Hilbert spaces formed by their product state.

To be more precise, if the systems are distinguishable (this is a complex issue in quantum mechanics), then let us call them 1 and 2, respectively, for a 2 qubit system. An eigen state of the combined Hilbert spaces is written as

$|s, m_s\rangle_1 |s' m_s'\rangle_2$ or for short hand $|m_s\rangle_1 |m_s'\rangle_2$. It easy to see that the binary numbers 00, 01, 10, and 11 can be written as

$|-\rangle_1|-\rangle_2, |-\rangle_1|+\rangle_2, |+\rangle_1|-\rangle_2 |+\rangle_1|+\rangle_2,$

respectively. More impressively is *that all four numbers can be written simultaneously in this quantum system as* :

$$|\psi\rangle_{ent.} = C_{00}|-\rangle_1|-\rangle_2 + C_{01}|-\rangle_1|+\rangle_2 + C_{10}|+\rangle_1|-\rangle_2 + C_{11}|+\rangle_1|+\rangle_2$$

Such a state is said to be *quantum mechanically entangled* and it is this quantum mechanical entanglement which allows for the algebraic speedup in quantum computing. Recall that to see this speedup, it is essential not to make a measurement on the system until the calculation is completed because a measurement will collapse the wave function to one of the eigenstates, destroying the information contained in the probability amplitudes (the C's) associated with the other states. It is necessary for a system to be entangled that it *not* be in a production state of the two spins; i.e.,

$$|\psi\rangle_{ent.} \neq (C_a|-\rangle_1 + C_b|+\rangle_2)(C_a'|-\rangle_1 + C_2'|+\rangle_2)$$

Time Dependent Interactions and Rabi Oscillations

Up to this point, we have taken the Hamiltonian to be time independent. However, a quantum computer characterized by a time independent Hamiltonian is one that is "turned off": not very interesting. There are many variations in the details of how this might be done for various systems, but all of these proposals have a similar outcome, namely that it is important to be able to drive the system between one state and anther.

To understand this, we start with Schrödinger's equation

$$\hat{H}\psi = i\hbar\frac{\partial\psi}{\partial t}$$

where $\hat{H} = \hat{H}_0 + \hat{V}(t)$

and H_0 is the Hamiltonian for a simple two spin system and $\hat{V}(t)$ is some kind of interaction that we apply to the system (for example, an electromagnetic coupling by a laser, say). We assume that the two spin states (up and down) are separated in energy, and that the spin down is at energy E_- and spin up is at energy E_+. In a real spin system, this can be done by applying a simple magnetic field. The Hamiltonian for this system is

$$\hat{H}_0 = \begin{pmatrix} E_+ & 0 \\ 0 & E_- \end{pmatrix}$$

The Hamiltonian for the time independent system is diagonal. Notice that the spin states are eigen states of the Hamiltonian (as they needed to be)

$$\hat{H}_0|+\rangle = \begin{pmatrix} E_+ & 0 \\ 0 & E_- \end{pmatrix}\begin{pmatrix} 1 \\ 0 \end{pmatrix} = E_+\begin{pmatrix} 1 \\ 0 \end{pmatrix} = E_+|+\rangle \text{ and}$$

$$\hat{H}_0|-\rangle = \begin{pmatrix} E_+ & 0 \\ 0 & E_- \end{pmatrix}\begin{pmatrix} 0 \\ 1 \end{pmatrix} = E_-\begin{pmatrix} 0 \\ 1 \end{pmatrix} = E_-|-\rangle$$

We now consider the idea that we can "drive this system. To imagine this, we take $\hat{V}(t)$ to be of the form:

$$\hat{V}(t) = -\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}\Omega_R \cos\omega t = -(\hat{\sigma}_+ + \hat{\sigma}_-)\Omega_R \cos\omega t$$

We now consider the exact solution of Schrödinger's equation (within the to-be-defined rotating wave approximation.)

In general, the wave function is given by

$$|\psi\rangle(t) = C_+(t)e^{-i\omega_+ t}|+\rangle + C_-(t)e^{-i\omega_- t}|-\rangle$$

where $\hbar\omega_\pm = E_\pm$

We now insert this into Schrödinger's equation, and use the fact that the eigenstates of the spin operator are orthonormal (i.e., $\langle i|j\rangle = \delta_{ij}$). The algebra follows:

$\hat{H}\psi = i\hbar\frac{\partial\psi}{\partial t}$ becomes

$$\hat{H}\left[C_+(t)e^{-i\omega_+ t}|+\rangle + C_-(t)e^{-i\omega_- t}|-\rangle\right] = i\hbar\frac{\partial}{\partial t}\left[C_+(t)e^{-i\omega_+ t}|+\rangle + C_-(t)e^{-i\omega_- t}|-\rangle\right]$$

$$\left[C_+(t)e^{-i\omega_+ t}\omega_+|+\rangle + C_-(t)e^{-i\omega_- t}\omega_-|-\rangle - \Omega_R\cos\omega t\left[e^{-i\omega_+ t}|-\rangle + e^{-i\omega_- t}|+\rangle\right]\right] =$$

$$\left[\left[C_+(t)\omega_+ + i\dot{C}_+(t)\right]e^{-i\omega_+ t}|+\rangle + \left[C_-(t)\omega_- + i\dot{C}_-(t)\right]e^{-i\omega_- t}|-\rangle\right]$$

We now project out the two different eigenstates by multiplying first by $\langle+|$ and then by $\langle-|$ and then simplifying the exponential parts by set $\omega = \omega_+ - \omega_-$ which we note is a positive number by our convention:

$$\left[C_+(t)e^{-i\omega_+ t}\omega_+ - C_-(t)\Omega_R\cos\omega t e^{-i\omega_- t}\right] = i\left[C_+(t)\omega_+ + \dot{C}_+(t)\right]e^{-i\omega_+ t}$$

giving

$$\dot{C}_+(t) = iC_-(t)\Omega_R\cos\omega t e^{i\omega_0 t} = iC_-(t)\frac{\Omega_R}{2}\left(e^{i\omega t} + e^{-i\omega t}\right)e^{i\omega_0 t}$$

and

$$\left[C_-(t)e^{-i\omega_- t}\omega_- - C_+(t)\Omega_R\cos\omega t e^{-i\omega_+ t}\right] = \left[C_-(t)\omega_- + \dot{C}_-(t)\right]e^{-i\omega_- t}$$

giving

$$\dot{C}_-(t) = iC_+(t)\Omega_R\cos\omega t e^{-i\omega_0 t} = iC_+(t)\frac{\Omega_R}{2}\left(e^{i\omega t} + e^{-i\omega t}\right)e^{-i\omega_0 t}$$

We have made no approximations so far. Now however, we note that on the right hand side, there are two exponentials of the form $e^{i(\omega\pm\omega_0)t}$. We will retain on the difference frequency, since that changes relatively slowly. The equations of motion become

$\dot{C}_+(t) = iC_-(t)\frac{\Omega_R}{2}e^{-i\Delta t}$ and

$\dot{C}_-(t) = iC_+(t)\frac{\Omega_R}{2}e^{i\Delta t}$ where

$\Delta = \omega - \omega_0$. Integration of these equations is straight forward. We find for example that $|C_+(t)|^2 = \sin^2\left[\frac{\Omega_R t}{2}\right]$ if we are on resonance, i.e., $\Delta = 0$ and we assume that at t=0, the system starts in the $|-\rangle$or "zero qubit" state (i.e., $C_-(t=0)=1$. The system oscillates in time at the Rabi frequency. We note that the end of a time where $\Omega_R t = \pi$ (we created a square wave pulse at the resonant frequency), the probability of being in the $|+\rangle$ or "one qubit" state goes from zero to 1. Hence, we have now found a way to drive our quantum computer from one state to another.

Decoherence

When a system is in a coherent superposition of two or more states, there exists a definite phase relationship between these states. It may even vary in time, but the phase relationship is deterministic. For an arbitrary two level system represented by a spin notation we can write:

$|\psi\rangle(t) = C_-(t)e^{-i\omega_- t}|-\rangle + C_+(t)e^{-i\omega_+ t}|+\rangle$

When we make a measurement of an observable that couples the states, like say, in the case of spin, something associated with the magnetization, we end up having to take expectation values of operators. A typical operator is $\hat{\sigma}_\pm$. In the case say of $\hat{\sigma}_+$,

$\langle\hat{\sigma}_+\rangle(t) = \langle\psi(t)|\hat{\sigma}_+|\psi(t)\rangle = C_-^*(t)C_+(t)e^{-i\omega_0 t}$

There is a problem with this result. Namely, it assumes the system is fully isolated from the rest of the universe, including what we call *vacuum field fluctuations*. This coupling to other modes of the bigger system results in a rather remarkable and, for quantum computing disasterous, time evolution. It is straight forward to show that unless you can turn off the vacuum field fluctuations:

$|C_+|^2(t) = |C_+|^2(t=0)e^{-\gamma_{dec}t}$ and

$\langle\hat{\sigma}_+\rangle(t) = C_-^*(t)C_+(t)e^{-i\omega_0 t-\left(\frac{\gamma_{dec}}{2}+\gamma_{ph}\right)t}$

where γ_{dec} represents the decay of $|\sigma_+\rangle$ to $|\sigma_-\rangle$ and γ_{ph} represents the rate of loss of phase coherence between the two states. A fully rigorous description of this problem is possible and results, after considerable algebra, in this simple exponential decay. The decay of the coherence leads to error in the quantum computation.

There is a language that is historical in this context. The inverse rate of γ_{dec} is often referred to as T_1 while the inverse rate of $\left(\frac{\gamma_{dec}}{2}+\gamma_{ph}\right)$ is called T_2.

There is a figure of merit in quantum computing that in order to do error correction, we require 10^4 operations in a time less than T_2. This translates to $\Omega_R T_2 >> 10^4$.