Notes for Quantum Mechanics

Richard Seto

```
Date[]
```

{2004, 11, 23, 11, 31, 28.3195952}

Lecture 17 - Time dependence

Lets go over how we got the space dependence of stuff first. We found a translation operator $\hat{\mathcal{T}}(\Delta x) = e^{-i \frac{\hat{P}_x}{\hbar} \Delta x}$ which translated a ket as follows $\hat{\mathcal{T}}(\delta x)|x\rangle=|x+\delta x\rangle$. We worked with an infinitesimal version of this thing $\hat{\mathcal{T}}(\delta x) =\hat{1}-i\delta x \frac{\hat{P}_x}{\hbar}$ and later applied this and infinite number of times to get the exponential version. We can also show that $e^{\frac{ia\hat{x}}{\hbar}}$ is a momentum boost operator i.e. $\hat{p}\, e^{\frac{ia\hat{x}}{\hbar}} |p'\rangle = (p'+a)\, e^{\frac{ia\hat{x}}{\hbar}} | p' \rangle$ so $e^{\frac{ia\hat{x}}{\hbar}} | p' \rangle= | p' +a\rangle$

We have not figured out how to get the time dependence of anything yet. One way, of course is to look at the time dependent Schroedinger eqn. which I gave to you before - As you recall, the way I got the Schroedinger eqn was a bit haphazard. Here we will use the idea of time evolution (or time translation) to get it.

What is it that we want? We will start out with a ket at t_0 $|\alpha, t_0\rangle$ and we want to know what this ket is at some later time t - that is $|\alpha, t\rangle$. Now its state at time t actually depends on the initial conditions at t_0 so for exactness we will call the ket at time t

$|\alpha, t; t_0\rangle$. Later we will drop the ; t_0 in our notation. Lets define an operator $\hat{U}$ which will do the job for us - so we have

$|\alpha, t; t_0\rangle \equiv \hat{U}(t, t_0)|\alpha,\hat{} t_0\rangle$

Now $\hat{U}$ should have several simple and obvious characteristics which we will use to deduce its form.

1) $\hat{U}$ is unitary - this will come about because we want to preserve the idea of probability-I will show this in a minute

2) $\hat{U}(t_2, t_0) =\hat{U}(t_2, t_1)\hat{U}(t_1, t_0)$ where $t_2 > t_1 > t_0$

3) lim (dt→0) $\hat{U}(t_0 + dt, t_0)\to 1$

First lets see why 1 is true if we want to preserve the idea of probability. If the ket is properly normalized then at t_0 $\langle\alpha, t_0 | \alpha, t_0\rangle=1$. We would like this normalization to be true also at later times so $\langle\alpha, t | \alpha, t\rangle = \langle\alpha, t_0 | \hat{U}^\dagger \hat{U} | \alpha, t_0\rangle=1$ and this will be true if $\hat{U}^\dagger \hat{U}=1$, meaning $\hat{U}$ is unitary.

Now let us first deal with infinitesimally small time intervals (just like we did before). Later we will look at finite times. This will turn out to cause complications. By construction we write $\hat{U}(t_0 + dt, t_0)=\hat{1}-i\hat{\Omega}dt$. This means that property 3 is satisfied trivially. Now if $\hat{U}$ is unitary this will mean that $\hat{\Omega}$ is hermitian.

proof: $1 = \hat{U}^\dagger \hat{U} = \left(\hat{1} + i\, \hat{\Omega}^\dagger dt\right)\left(\hat{1} - i\, \hat{\Omega}\, dt\right) = \hat{1} - i\, \hat{\Omega}\, dt + i\, \hat{\Omega}^\dagger dt + \hat{\Omega}^\dagger \hat{\Omega}\, (dt)^2$

The last term we take to be essentially zero to first order. This means that if this is to be true $\hat{\Omega} = \hat{\Omega}^\dagger$ *i.e.* $\hat{\Omega}$ is hermitian.

Now before we use property 2, let us see what the units of $\hat{\Omega}$ must be. $\hat{\Omega}$t must be unitless so $\hat{\Omega}$ must have the units of 1/time or frequency - i.e. ω. Now recalling how $\hbar$ came into the picture in the case of momentum, lets look at the quantity $\hbar\omega$ which has units of energy. If we let $\hat{\Omega} = \frac{\hat{H}}{\hbar}$ where $\hat{H}$ is the hamiltonian operator with units of energy, this works out. It turns out that this is true. We have to deduce this from experiment. So now we have

$$\hat{U} = \left(\hat{1} - i\,\frac{\hat{H}}{\hbar}\,\mathrm{dt}\right)$$

Now lets use property number 2) - this will get us to the Schroedinger eqn.

$$\hat{U}(\mathrm{t+dt},\, t_0) = \hat{U}(\mathrm{t+dt},\, t)\hat{U}(\mathrm{t},\, t_0) = \left(\hat{1} - i\,\frac{\hat{H}}{\hbar}\,\mathrm{dt}\right)\hat{U}\,(t,\, t_0) \;\Rightarrow$$

$$\hat{U}(\mathrm{t+dt},\, t_0) - \hat{U}(\mathrm{t},\, t_0) = -i\,\frac{\hat{H}}{\hbar}\,\mathrm{dt}\hat{U}(\mathrm{t},\, t_0) \;\Rightarrow\; \frac{\hat{U}\,(t+\mathrm{dt},\, t_0) - \hat{U}\,(t,\, t_0)}{\mathrm{dt}} = -i\,\frac{\hat{H}}{\hbar}\hat{U}(\mathrm{t},\, t_0) \;\Rightarrow$$

$$i\hbar\,\frac{d}{\mathrm{dt}}\hat{U}\,(t,\, t_0) = \hat{H}\hat{U}\,(t,\, t_0) \quad \text{The Schroedinger eqn for } \hat{U}\,(t,\, t_0)\ !$$

Now lets operate on a ket $i\hbar\,\frac{d}{\mathrm{dt}}\,\hat{U}\,(t,\, t_0)\,|\alpha,\, t_0\rangle = \hat{H}\,\hat{U}\,(t,\, t_0)\,|\alpha,\, t_0\rangle$ and note that $|\alpha,\, t\rangle = \hat{U}\,(t,\, t_0)\,|\alpha,\, t_0\rangle$ so we have

$$i\hbar\,\frac{d}{\mathrm{dt}}\,|\alpha,\, t\rangle = \hat{H}|\alpha,t\rangle \quad \text{The Schroedinger eqn for a state ket}$$

One can now consider several cases of this, depending on the nature of $\hat{H}$ We will solve the eqn for $\hat{U}$

1) Suppose the Hamiltonian is independent of t, then $\hat{U}\,(t,\, t_0) = e^{-i\,\frac{\hat{H}}{\hbar}\,(t-t_0)}$

proof: to do this right, we really have to go to an expansion but we will sort of cheat and treat this thing like an ordinary eqn instead of the operator eqn which it is

$$i\hbar\,\frac{d}{\mathrm{dt}}\hat{U}\,(t,\, t_0) = i\hbar\,\frac{d}{\mathrm{dt}}\,e^{-i\,\frac{\hat{H}}{\hbar}\,(t-t_0)} = -i\hbar\mathrm{i}\,\frac{\hat{H}}{\hbar}\,e^{-i\,\hat{H}(t-t_0)} = \hat{H}e^{-i\,\hat{H}(t-t_0)} = \hat{H}\hat{U}\,(t,\, t_0)$$

another more correct way to do this is to start with the infinitesimal form of $\hat{U} = (1 - i\,\frac{\hat{H}}{\hbar}\mathrm{dt})$ and apply it many times so

$\hat{U}\,(t,\, t_0) = \lim_{N\to\infty}\left[\hat{1} - i\,\frac{\hat{H}}{\hbar}\,\frac{(t-t_0)}{N}\right]^N = e^{-i\,\frac{\hat{H}}{\hbar}\,(t-t_0)}$. Note that this form also has the property that as $t \to t_0$ then $\hat{U} \to 0$.

This is the form for $\hat{U}$ which will most often concern us in this class. I will list two other possibilities

2) Suppose the Hamiltonian depends on time, but the Hamiltonians at different times commute with one another, i.e. $[\hat{H}\,(t_1),\ \hat{H}\,(t_2)] = 0$. An example of this sort of Hamiltonian is spin magnetic resonance in which there is a B field whose strength varies with time, but whose direction is fixed. In this case

$$\hat{U}\,(t,\, t_0) = e^{-\left(\frac{i}{\hbar}\right)\int_{t_0}^{t}\hat{H}(t')\,\mathrm{dt'}}$$

proof: $\hat{U} = \hat{1} - \left(\frac{i}{\hbar}\right)\int_{t_0}^{t}\hat{H}(t')\,\mathrm{dt} + \left(\frac{-i}{2}\right)^2\left[\frac{\int_{t_0}^{t}\hat{H}(t')\,\mathrm{dt}}{\hbar}\right]^2 \ldots$

$$\frac{d\,\hat{U}}{\mathrm{dt}} = -\left(\frac{i}{\hbar}\right)\hat{H}(t) + \left(\frac{-i}{2}\right)^2 2\left[\frac{\int_{t_0}^{t}\hat{H}(t')\,\mathrm{dt}}{\hbar}\right]\hat{H}(t) \qquad \text{(If the H's at different times commute)}$$

$$= \hat{H}(\mathrm{t})[\hat{1} - \left(\frac{i}{\hbar}\right)\int_{t_0}^{t}\hat{H}(t')\,\mathrm{dt}]\left(\frac{-i}{\hbar}\right) = \hat{H}\hat{U}\left(\frac{-i}{\hbar}\right)$$

3) General case - this is called the Dyson Series

$$\hat{U}\,(t,\, t_0) = \hat{1} + \sum_{n=1}^{\infty}\left(\frac{-i}{\hbar}\right)^n\int_{t_0}^{t}\mathrm{dt}_1\int_{0}^{t_1}\mathrm{dt}_2\int_{0}^{t_2}\mathrm{dt}_3 \ldots \int_{0}^{t_{n-1}}\mathrm{dt}_n\ \hat{H}(t_1)\hat{H}(t_2)\hat{H}(t_3) \ldots \hat{H}(t_n)$$

$t_1 > t_2 > t_{3...} > t_n$

Time Dependence of Energy Eigenkets

The task is to find the time dependence for any ket $|\alpha\rangle$. Let's first do it for an energy eigenket |a'⟩ where $\hat{H}|a'\rangle = E_{a'}|a'\rangle$. We start with |a'⟩ ket at $t_0 = 0$ and then evolve it with the $\hat{U} = e^{-i \frac{\hat{H}}{\hbar} t}$. We can write

$\hat{U} = e^{-i \frac{\hat{H}}{\hbar} t} = \sum_{a''} |a''\rangle \langle a''| e^{-i \frac{\hat{H}}{\hbar} t} \sum_{a'} |a'\rangle \langle a'| = \sum_{a''a'} |a''\rangle\langle a''| e^{-i \frac{\hat{H}}{\hbar} t} |a'\rangle\langle a'| = \sum_{a''a'} |a''\rangle\langle a''| e^{-i \frac{E_{a'}}{\hbar} t} |a'\rangle\langle a'| =$
$\sum_{a''a'} |a''\rangle\langle a''|a'\rangle e^{-i \frac{E_{a'}}{\hbar} t} \langle a'| = \sum_{a'} |a'\rangle e^{-i \frac{E_{a'}}{\hbar} t} \langle a'|$

So $\hat{U} = \sum_{a'} |a'\rangle e^{-i \frac{E_{a'}}{\hbar} t} \langle a'|$

So now we can find $|\alpha,t\rangle$ if we know $|\alpha, t_0\rangle$. We first expand it in energy eigenkets then apply $\hat{U}$

$|\alpha, t_0\rangle = \sum_{a'} |a'\rangle \langle a' \,|\, \alpha, t_0\rangle = \sum_{a'} c_{a'} |a'\rangle$

$|\alpha, t\rangle = \hat{U} \,|\, \alpha, t_0\rangle = \sum_{a'} |a'\rangle e^{-i \frac{E_{a'}}{\hbar} t} \langle a' \,|\, \alpha, t_0\rangle = \sum_{a'} c_{a'} e^{-i \frac{E_{a'}}{\hbar} t} |a'\rangle$ and we can consider

$c_{a'}(t) = c_{a'} e^{-i \frac{E_{a'}}{\hbar} t}$

Now if $|\alpha, t_0\rangle = |a''\rangle$ then $|\alpha,t\rangle = |a'\rangle e^{-i \frac{E_{a'}}{\hbar} t}$ *i.e.* only *a* phase is added and the probability $\langle\alpha,t|\alpha,t\rangle = \langle\alpha, t_0|\alpha, t_0\rangle$ is unchanged

Quantum Dynamics

Before starting, I would like to remind you of a very important theorem from lecture 13 - that is

Theorem : Suppose that Â and B̂ are compatible observables (i.e. $[\hat{A}, \hat{B}] = 0$)
and the eigenvalues of Â are non – degenerate.
Then the matrix elements $\langle a_i \,|\, \hat{B} \,|\, a_j\rangle$ are all diagonal. (Recall that the matrix elements of $\hat{A}$ are already diagonal if $|a_i\rangle$ are used as eigenkets)

A simple way to think about this for now, is to assume that commuting observables have the same eigenkets This is a very important fact. It means that if we have a complete set of eigenkets for an observable which spans the relevant space - then any state in that space can be expanded in those eigenkets - in particular - if one has a initial ket $|\alpha, t_0\rangle$, then $|\alpha, t\rangle$ can be expanded in those eigenkets. So we can set up *a* way to solve for the time dependence of *a* ket.

1) Find an observable Â that commutes with $\hat{H}$ (very often it will be $\hat{H}$ itself), and its eigenkets

2) expand the initial ket $|\alpha, t_0\rangle$ in those eigenkets

3) apply the time evolution operator $\hat{U} = \sum_{a'} |a'\rangle e^{-i \frac{E_{a'}}{\hbar} t} \langle a'|$

Now before I do some examples, let's find out how the expectation value changes with time.

Lets find $\langle\hat{B}\rangle$ where $\hat{B}$ does not necessarily have to commute with $\hat{H}$ (or Â), with respect to the energy eigenstates. That is we want to find $\langle a',t|\hat{B}|a',t\rangle$

$\langle a',t|\hat{B}|a',t\rangle = \langle a'|\hat{U}^\dagger \hat{B}\hat{U}|a'\rangle = \langle a'|e^{+i \frac{\hat{H}}{\hbar} t} \hat{B} e^{-i \frac{\hat{H}}{\hbar} t}|a'\rangle = \langle a'|e^{+i \frac{E_{a'}}{\hbar} t} \hat{B} e^{-i \frac{E_{a'}}{\hbar} t}|a'\rangle = \langle a'|\hat{B}|a'\rangle$ independent of time!

Since the expectation of any operator with respect to an energy eigenvalue, is independent of time, we call energy eigenkets - stationary kets.

Now lets find the expectation value of $\hat{B}$ with respect to some more complicated state $|\alpha,t=0\rangle=\sum_{a'} c_{a'}\,|a'\rangle$

$\langle \alpha, t \mid \hat{B} \mid \alpha, t\rangle = (\sum_{a'} c_{a'}{}^{*}\,\langle a'\,|)e^{+i\frac{\hat{H}}{\hbar}t}\hat{B}e^{-i\frac{\hat{H}}{\hbar}t}(\sum_{a''} c_{a''}\,|a''\rangle)=(\sum_{a'} c_{a'}{}^{*}\,\langle a'\,|e^{+i\frac{E_{a'}}{\hbar}t})\hat{B}(\sum_{a''} c_{a''}e^{-i\frac{E_{a''}}{\hbar}t}|a''\rangle)=\sum_{a'\,a''} c_{a'}{}^{*}\,c_{a''}\,\langle a'\,|$ $\hat{B}\,|a''\rangle e^{-i\frac{(E_{a''}-E_{a'})}{\hbar}t}=\sum_{a'\,a''} c_{a'}{}^{*}\,c_{a''}\,\langle a'\,|\hat{B}\,|a''\rangle e^{-i\omega t}$ where $\omega = \frac{(E_{a''}-E_{a'})}{\hbar}$

Example - particle in a box

Let's now try to find the time dependence of the particle in a box. First $\hat{H} = \frac{\hat{p}^2}{2m}$+V(x) where V(x)=$\begin{cases} 0 & 0<x<a \\ \infty & x = 0 \text{ or } a \end{cases}$

This is time independent so $\hat{U}\,(t, t_0) = e^{-i\frac{\hat{H}}{\hbar}(t-t_0)}$

The eigenfunctions in the x representation are $\varphi_n(x)=\langle x|n\rangle=\sqrt{\frac{2}{a}}\,\sin(\frac{n\pi x}{a})$ and the energy eigenvalues are $E_n = n^2\,\frac{\hbar^2\,\pi^2}{2\,ma^2}$

First lets find the energy dependence of the n=2 eigenfunction |2⟩, which means that at time=0 the state of the particle in the box is $\langle x|2\rangle=\sqrt{\frac{2}{a}}\,\sin(\frac{2\pi x}{a})$ and the energy eigenvalue is $4\frac{\hbar^2\,\pi^2}{2\,ma^2}$

$|2,t\rangle=\hat{U}\,|2\rangle=e^{-i\frac{\hat{H}}{\hbar}t}|2\rangle=e^{-i\frac{E_2}{\hbar}t}|2\rangle$ So $\langle x|2,t\rangle=\sqrt{\frac{2}{a}}\,\sin(\frac{2\pi x}{a})e^{-i\omega_2 t}$ where $\omega_2=\frac{E_2}{\hbar}=\frac{2\,\hbar\pi^2}{ma^2}$

So as we saw before, all that happens is that there is an extra phase factor $e^{-i\omega_2 t}$ in the wave function. The probabilities don't change. What about the expectation value of $\hat{H}$

$\langle 2, t \mid \hat{H} \mid 2, t\rangle = \left\langle 2 \left| e^{+i\frac{\hat{H}}{\hbar}t}\,\hat{H}\,e^{-i\frac{\hat{H}}{\hbar}t} \right| 2\right\rangle = \left\langle 2 \left| e^{+i\frac{E_2}{\hbar}t}\,\hat{H}\,e^{-i\frac{E_2}{\hbar}t} \right| 2\right\rangle = \langle 2 \mid \hat{H} \mid 2\rangle = \langle 2 \mid E_2 \mid 2\rangle = E_2$ independent of time as we expected.

Lets look at the expectation value of momentum. Remember in the x representation $\langle x'|\,\hat{\boldsymbol{p}}\,|\,\alpha\rangle=\frac{\hbar}{i}\,\frac{\boldsymbol{d}}{\mathbf{dx'}}\langle x'|\alpha\rangle$

$\langle 2, t \mid \hat{p} \mid 2, t\rangle = \left\langle 2 \left| e^{+i\frac{\hat{H}}{\hbar}t}\,\hat{p}\,e^{-i\frac{\hat{H}}{\hbar}t} \right| 2\right\rangle = \left\langle 2 \left| e^{+i\frac{E_2}{\hbar}t}\,\hat{p}\,e^{-i\frac{E_2}{\hbar}t} \right| 2\right\rangle = \langle 2 \mid \hat{p} \mid 2\rangle = \int dx'\langle 2 \mid x'\rangle\,\langle x' \mid \hat{p} \mid 2\rangle=$
$=\int dx'\langle 2 \mid x'\rangle\,\frac{\boldsymbol{d}}{\mathbf{dx'}}\,\langle x' \mid 2\rangle=\frac{\hbar}{i}\,\frac{2}{a}\int dx'\sin(\frac{2\pi x'}{a})\frac{\boldsymbol{d}}{\mathbf{dx'}}\sin(\frac{2\pi x'}{a})=\frac{\hbar}{i}\,\frac{2}{a}\,\frac{2\pi}{a}\int dx'\sin(\frac{2\pi x'}{a})\cos(\frac{2\pi x'}{a})=0$ and again it is time independent.

So now lets try a more complicated initial condition. $\langle x|\alpha,t=0\rangle=\sqrt{\frac{2}{a}}\,\frac{\sin(2\pi x/a)+2\sin(\pi x/a)}{\sqrt{5}}$

The first thing we have to do is to expand in terms of the energy eigenkets. The right way to do this is to do a fourier transform and find the expansion coefficients. This initial condition here is such that it is easy to figure out the expansion so $\langle x \mid \alpha, t = 0\rangle = \sqrt{\frac{2}{a}}\,\frac{\sin(2\pi x/a)+2\sin(\pi x/a)}{\sqrt{5}} = \frac{1}{\sqrt{5}}\langle x|2\rangle+\frac{2}{\sqrt{5}}\langle x|1\rangle$ Note that this is normalized correctly.

Now we will evolve it in time. start with $|\alpha,t=0\rangle=\frac{1}{\sqrt{5}}|2\rangle+\frac{2}{\sqrt{5}}|1\rangle$

$|\,\alpha, t\rangle = \hat{U}\,(\frac{1}{\sqrt{5}}|2\rangle+\frac{2}{\sqrt{5}}|1\rangle)=\frac{1}{\sqrt{5}}e^{-i\frac{\hat{H}}{\hbar}t}|2\rangle+\frac{2}{\sqrt{5}}e^{-i\frac{\hat{H}}{\hbar}t}|1\rangle=\frac{1}{\sqrt{5}}e^{-i\frac{E_2}{\hbar}t}|2\rangle+\frac{2}{\sqrt{5}}e^{-i\frac{E_1}{\hbar}t}|1\rangle$

$\langle x|\alpha,t\rangle=\frac{1}{\sqrt{5}}e^{-i\frac{E_2}{\hbar}t}\langle x|2\rangle+\frac{2}{\sqrt{5}}e^{-i\frac{E_1}{\hbar}t}\langle x|1\rangle=\frac{1}{\sqrt{5}}e^{-i\frac{E_2}{\hbar}t}\sqrt{\frac{2}{a}}\,\sin(\frac{2\pi x}{a})+\frac{2}{\sqrt{5}}e^{-i\frac{E_1}{\hbar}t}\sqrt{\frac{2}{a}}\,\sin(\frac{\pi x}{a})=$
$\frac{1}{\sqrt{5}}\sqrt{\frac{2}{a}}\,[e^{-i\omega_2 t}\sin(2\pi x/a)+2e^{-i\omega_1 t}\sin(\pi x/a)]$

Lets look at the time dependence of ⟨E⟩

$\langle\alpha,t|\hat{H}|\alpha,t\rangle=(\frac{1}{\sqrt{5}}e^{+i\frac{E_2}{\hbar}t}\langle 2|+\frac{2}{\sqrt{5}}e^{+i\frac{E_1}{\hbar}t}\langle 1|\,)\hat{H}(\frac{1}{\sqrt{5}}e^{-i\frac{E_2}{\hbar}t}|2\rangle+\frac{2}{\sqrt{5}}e^{-i\frac{E_1}{\hbar}t}|1\rangle)=$
$(\frac{1}{\sqrt{5}}e^{+i\frac{E_2}{\hbar}t}\langle 2|+\frac{2}{\sqrt{5}}e^{+i\frac{E_1}{\hbar}t}\langle 1|\,)(\frac{1}{\sqrt{5}}e^{-i\frac{E_2}{\hbar}t}\,\hat{H}|2\rangle+\frac{2}{\sqrt{5}}e^{-i\frac{E_1}{\hbar}t}\hat{H}|1\rangle)=$
$(\frac{1}{\sqrt{5}}e^{+i\frac{E_2}{\hbar}t}\langle 2|+\frac{2}{\sqrt{5}}e^{+i\frac{E_1}{\hbar}t}\langle 1|\,)(\frac{1}{\sqrt{5}}e^{-i\frac{E_2}{\hbar}t}\,E_2|2\rangle+\frac{2}{\sqrt{5}}e^{-i\frac{E_1}{\hbar}t}E_1|1\rangle)=$

$\frac{1}{\sqrt{5}}\, e^{+i\,\frac{E_2}{\hbar}\,t}\, \frac{1}{\sqrt{5}}\, e^{-i\,\frac{E_2}{\hbar}\,t}\, E_2 + \frac{2}{\sqrt{5}}\, e^{+i\,\frac{E_1}{\hbar}\,t}\, \frac{2}{\sqrt{5}}\, e^{-i\,\frac{E_1}{\hbar}\,t}\, E_1 = \frac{1}{5} E_2 + \frac{4}{5}\, E_1$ which as we know is independent of time.

How about the time dependence of $\hat{p}$

$=(\frac{1}{\sqrt{5}} e^{+i\,\frac{E_2}{\hbar}\,t}\langle 2| + \frac{2}{\sqrt{5}} e^{+i\,\frac{E_1}{\hbar}\,t}\langle 1|\,)\hat{p}(\frac{1}{\sqrt{5}} e^{-i\,\frac{E_2}{\hbar}\,t}|2\rangle + \frac{2}{\sqrt{5}} e^{-i\,\frac{E_1}{\hbar}\,t}|1\rangle)=$

$(\frac{1}{\sqrt{5}} e^{+i\,\frac{E_2}{\hbar}\,t}\langle 2| + \frac{2}{\sqrt{5}} e^{+i\,\frac{E_1}{\hbar}\,t}\langle 1|\,)(\frac{1}{\sqrt{5}} e^{-i\,\frac{E_2}{\hbar}\,t}\,\hat{p}|2\rangle + \frac{2}{\sqrt{5}} e^{-i\,\frac{E_1}{\hbar}\,t}\,\hat{p}|1\rangle)=$

$(\frac{1}{\sqrt{5}} e^{+i\,\frac{E_2}{\hbar}\,t}\langle 2|\,)(\frac{1}{\sqrt{5}} e^{-i\,\frac{E_2}{\hbar}\,t}\,\hat{p}|2\rangle)+(\frac{1}{\sqrt{5}} e^{+i\,\frac{E_2}{\hbar}\,t}\langle 2|)(\frac{2}{\sqrt{5}} e^{-i\,\frac{E_1}{\hbar}\,t}\,\hat{p}|1\rangle)+(\frac{2}{\sqrt{5}} e^{+i\,\frac{E_1}{\hbar}\,t}\langle 1|\,)(\frac{1}{\sqrt{5}} e^{-i\,\frac{E_2}{\hbar}\,t}\,\hat{p}|2\rangle)+$

$(\frac{2}{\sqrt{5}} e^{+i\,\frac{E_1}{\hbar}\,t}\langle 1|\,)(\frac{2}{\sqrt{5}} e^{-i\,\frac{E_1}{\hbar}\,t}\,\hat{p}|1\rangle)=$

$\frac{1}{5}\langle 2|\hat{p}|2\rangle + \frac{2}{5} e^{+i\,\frac{E_2-E_1}{\hbar}\,t}\langle 2|\hat{p}|1\rangle + \frac{2}{5} e^{+i\,\frac{E_1-E_2}{\hbar}\,t}\langle 1|\hat{p}|2\rangle + \frac{4}{5}\langle 1|\hat{p}|1\rangle=$

$\frac{1}{5}\langle 2|\hat{p}|2\rangle + \frac{2}{5} e^{+i\omega t}\langle 2|\hat{p}|1\rangle + \frac{2}{5} e^{-i\omega t}\langle 1|\hat{p}|2\rangle + \frac{4}{5}\langle 1|\hat{p}|1\rangle=$ where $\omega=\frac{E_2-E_1}{\hbar}$

Now $\langle n|\hat{p}|n\rangle=\int dx'\langle n\mid x'\rangle\,\langle x'\mid \hat{p}\mid n\rangle = =\int dx'\langle n\mid x'\rangle\,\frac{d}{dx'}\,\langle x'\mid n\rangle = \frac{\hbar}{i}\,\frac{2}{a}\int dx'\sin(\frac{n\pi x'}{a})\frac{d}{dx'}\sin(\frac{n\pi x'}{a})=$

$\frac{\hbar}{i}\,\frac{2}{a}\,\frac{n\pi}{a}\int dx'\sin(\frac{n\pi x'}{a})\cos(\frac{n\pi x'}{a})=0$

$\langle m|\hat{p}|n\rangle=\int dx'\langle m\mid x'\rangle\,\langle x'\mid \hat{p}\mid n\rangle = =\int dx'\langle m\mid x'\rangle\,\frac{d}{dx'}\,\langle x'\mid n\rangle = \frac{\hbar}{i}\,\frac{2}{a}\int dx'\sin(\frac{m\pi x'}{a})\frac{d}{dx'}\sin(\frac{n\pi x'}{a})=$

$\frac{\hbar}{i}\,\frac{2}{a}\,\frac{n\pi}{a}\int_0^a dx'\sin(\frac{m\pi x'}{a})\cos(\frac{n\pi x'}{a}) = \frac{\hbar}{i}\,\frac{2}{a}\,n\int_0^a \frac{\pi}{a}\,dx'\sin(\frac{m\pi x'}{a})\cos(\frac{n\pi x'}{a}) = \frac{\hbar}{i}\,\frac{2}{a}\,n\int_0^{\pi} dy\sin(my)\cos(ny)=$

$\frac{\hbar}{i}\,\frac{2}{a}\,n[\frac{\sin(n-m)\,x}{2\,(n-m)} + \frac{\sin(n+m)\,x}{2\,(n+m)}]\ \{0,\pi\}=0$

So $\langle\hat{p}\rangle=0$ always which makes sense since there is no external momentum to change it, and we have momentum conservation.

Example: Spin Precession in a magnetic field

For an electron in a magnetic field the hamiltonian is

$\hat{H} = \vec{\mu}\cdot\vec{B} = -(\frac{e}{mc})\vec{S}\cdot\vec{B}$ (e is negative) Now lets let $\vec{B}$ be a static magnetic field in the z direction so

$\hat{H} = -(\frac{eB}{mc})\hat{S}_z = -(\frac{eB\hbar}{2\,mc})\sigma_z = -\frac{\hbar\omega}{2}\sigma_z$ where $\omega=\frac{|e|B}{mc}$

Now $\hat{H}$ and $\hat{S}_z$ (or σ_z) commute so lets use the eigenkets of $\hat{S}_z$ as the kets we will use to expand i.e. $|+\rangle$ and $|-\rangle$.

There have eigenvalues of $\hat{H}$ of $E_\pm = \mp\frac{\hbar\omega}{2}$

Now we can write $\hat{H}=\omega\hat{S}_z$ so the time evolution operator is $\exp(-\frac{i\hat{H}t}{\hbar})=\exp(-\frac{i\omega\hat{S}t}{\hbar})$

We will have some intial ket $|\alpha\rangle = c_+\,|+\rangle + c_-|-\rangle$

$\hat{U}\,|\alpha\rangle = |\alpha,\,t\rangle = c_+\,\exp(-\frac{i\omega\hat{S}\,t}{\hbar})\,|+\rangle + c_-\,\exp(-\frac{i\omega\hat{S}\,t}{\hbar})|-\rangle = c_+\,\exp(-\frac{i\omega t}{2})\,|+\rangle + c_-\,\exp(\frac{i\omega t}{2})|-\rangle$

So now lets try some specific intial conditions

First let $|\alpha\rangle=|+\rangle$ so $c_+ = 1$ and $c_-=0$ $|\alpha,t\rangle=\exp(-\frac{i\omega t}{2})\,|+\rangle$ and as before, there is just a phase

Now lets let $|\alpha\rangle = |S_x +\rangle = \frac{1}{\sqrt{2}}\,|+\rangle + \frac{1}{\sqrt{2}}\,|-\rangle$ then $|\alpha,\,t\rangle = \frac{1}{\sqrt{2}}\,e^{-\frac{i\omega t}{2}}\,|+\rangle + \frac{1}{\sqrt{2}}\,e^{\frac{i\omega t}{2}}|-\rangle$

Now its interesting to figure out the probability that the state is in $|S_x \pm\rangle$ later.

$|\,\langle S_x \pm|\,\alpha,\,t\rangle\,|^2 = [(\frac{1}{\sqrt{2}}\,\langle +| + \frac{1}{\sqrt{2}}\,\langle -|)(\frac{1}{\sqrt{2}}\,e^{-\frac{i\omega t}{2}}\,|+\rangle + \frac{1}{\sqrt{2}}\,e^{\frac{i\omega t}{2}}\,|-\rangle)]^2 =$

$\left[\frac{1}{2}\, e^{-\frac{i\omega t}{2}} \pm \frac{1}{2}\, e^{\frac{i\omega t}{2}}\right]^2 = \begin{cases} \cos^2 \frac{\omega t}{2} \text{ for } S_x + \\ \sin^2 \frac{\omega t}{2} \text{ for } S_x - \end{cases}$

Now lets figure out the expection value of $\hat{S}_x$, $\hat{S}_y$ and $\hat{S}_z$

There are two ways to do this. The first is just to figure it out, the second is to use a formula from before, i.e. $\langle \hat{A} \rangle = \sum_{a'} a' \mid \langle a' | \alpha \rangle \mid^2$. We will do it both ways. First we will use the formula

$\langle \hat{S}_x \rangle = \frac{\hbar}{2} \cos^2 \frac{\omega t}{2} + (-\frac{\hbar}{2}) \sin^2 \frac{\omega t}{2} = \frac{\hbar}{2} \cos \omega t$

to figure out $\langle \hat{S}_y \rangle$ we will use $\hat{S}_y = \frac{1}{2i} (\hat{S}_+ - \hat{S}_-)$

$\langle \hat{S}_y \rangle = \langle \alpha, t \mid \hat{S}_y \mid \alpha, t \rangle = \left(\frac{1}{\sqrt{2}}\, e^{+\frac{i\omega t}{2}} \langle + | + \frac{1}{\sqrt{2}}\, e^{-\frac{i \omega t}{2}} \langle - | \right) \frac{1}{2i} (\hat{S}_+ - \hat{S}_-) \left(\frac{1}{\sqrt{2}}\, e^{-\frac{i\omega t}{2}} | + \rangle + \frac{1}{\sqrt{2}}\, e^{\frac{i \omega t}{2}} | - \rangle \right) =$

$\frac{1}{2i} (\frac{\hbar}{2}\, e^{+i\omega t} - \frac{\hbar}{2}\, e^{-i \omega t}) = \frac{\hbar}{2} \sin \omega t$

$\langle \hat{S}_z \rangle = \left(\frac{1}{\sqrt{2}}\, e^{+\frac{i\omega t}{2}} \langle + | + \frac{1}{\sqrt{2}}\, e^{-\frac{i \omega t}{2}} \langle - | \right) \hat{S}_z \left(\frac{1}{\sqrt{2}}\, e^{-\frac{i\omega t}{2}} | + \rangle + \frac{1}{\sqrt{2}}\, e^{\frac{i \omega t}{2}} | - \rangle \right) =$

$\frac{\hbar}{2} \left(\frac{1}{\sqrt{2}}\, e^{+\frac{i\omega t}{2}} \langle + | + \frac{1}{\sqrt{2}}\, e^{-\frac{i \omega t}{2}} \langle - | \right) \left(\frac{1}{\sqrt{2}}\, e^{-\frac{i\omega t}{2}} | + \rangle - \frac{1}{\sqrt{2}}\, e^{\frac{i \omega t}{2}} | - \rangle \right) = \frac{\hbar}{2}\, \frac{1}{2} [1-1] = 0$

So summing up $\langle \hat{S}_x \rangle = \frac{\hbar}{2} \cos \omega t$ $\langle \hat{S}_y \rangle = \frac{\hbar}{2} \sin \omega t$ $\langle \hat{S}_z \rangle = 0$ So it looks like the electron spin just goes around in a circle - i.e. spin precession!