# Notes for Quantum Mechanics

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## Lecture 18

**Time dependece of Expecation Values**

$\frac{d\langle\hat{A}\rangle}{\mathrm{dt}}=\frac{d\langle\alpha,t|\hat{A}|\alpha,t\rangle}{\mathrm{dt}}=\frac{d\langle\alpha,t_0|\hat{U}^\dagger(t,t_0)\hat{A}\,U(\hat{t},t_0)|\alpha,t_0\rangle}{\mathrm{dt}}$ Now we know that $|\alpha, t_0\rangle$ is independent of time (by definition). Lets also assume that $\hat{A}$ does not have an explicit time dependence (e.g. it could be momentum, angular momentum-which we will learn about later, spin, position-watch it though, position does not commute with $\hat{H}$)

and we remember the Schroedinger eqn for $\hat{U}$ $i\hbar\frac{d}{\mathrm{dt}}\hat{U}(t, t_0)=\hat{H}\hat{U}(t, t_0)$ and the hermitian conjugate of this eqn $-i\hbar\frac{d}{\mathrm{dt}}\hat{U}^\dagger(t, t_0)=\hat{U}^\dagger(t, t_0)\hat{H}$ (remember that $\hat{H}$ is hermitian)

$\frac{d\langle\hat{A}\rangle}{\mathrm{dt}}=\langle\alpha, t_0\left|\frac{d\hat{U}^\dagger(t,t_0)}{\mathrm{dt}}\hat{A}\,\hat{U}(t, t_0)+\hat{U}^\dagger(t, t_0)\hat{A}\frac{\mathrm{dU}(\hat{t},t_0)}{\mathrm{dt}}\right|\alpha, t_0\rangle=$

$\frac{1}{i\hbar}\langle\alpha, t_0\left|-\hat{U}^\dagger\hat{H}\hat{A}\hat{U}+\hat{U}^\dagger\hat{A}\hat{H}\hat{U}\right|\alpha, t_0\rangle=$

$\frac{i}{\hbar}\langle\alpha, t_0\left|\hat{U}^\dagger(\hat{H}\hat{A}-\hat{A}\hat{H})\hat{U}\right|\alpha, t_0\rangle=\frac{i}{\hbar}\langle\alpha, t\left|\left[\hat{H},\hat{A}\right]\right|\alpha, t\rangle$ So finally we have

$$\frac{d\langle\hat{A}\rangle}{\mathrm{dt}}=\frac{i}{\hbar}\left\langle\left[\hat{H},\hat{A}\right]\right\rangle$$

This is an important theorem. It means that if any observable $\hat{A}$ commutes with $\hat{H}$ then its expectation value does not change with time - that is - it is a constant of motion.

**Symmetry and conservation laws (an important aside)**

This then leads to the connection between the properties of space and conservation laws. As I will show you, the homogeneity of space will lead to momentum conservation - i.e physics doesnt change depending on where you are, simillarly the fact that physics doesn't change when you rotate things leads to angular momentum conservation, and the fact that physics doesnt change with time will lead to energy conservation. There are other symmetry principles which lead to other conservation laws as well. Here I will show you these three.

Lets think about translation. We will deal with infinitesimal translations for ease, but we can always generalize to finite translations. Remember we has that $\hat{\mathcal{T}}(\delta\mathrm{x})|\mathrm{x}\rangle=|\mathrm{x}+\delta\mathrm{x}\rangle$ and that $\hat{\mathcal{T}}(\delta\mathrm{x})=\hat{1}-i\delta\mathrm{x}\frac{\hat{p}_x}{\hbar}$. Now lets take some ket $|\alpha\rangle$. What does it mean that physics is the same everywhere - that is, that it is translationaly invariant? Well it means that if we get some answer for one of our invariant observables (lets take $\hat{H}$) then if we figure out that observable somwhere else, it should give the same answer. So for example, lets assume that $\hat{H}$ is the free particle Hamiltonian which is just $\hat{p}^2/2m$. It has no dependence on position. This means that if we take a ket $|\alpha\rangle$ and calculate $\langle\hat{H}\rangle$ and then move the ket somewhere else using the translation operator, it should give the same answer. How do we move the ket $\hat{\mathcal{T}}$?

$\hat{\mathcal{T}}|\alpha\rangle=\hat{\mathcal{T}}\int dx'|x'\rangle\langle x'|\alpha\rangle=\int dx'\hat{\mathcal{T}}|x'\rangle\langle x'|\alpha\rangle$ etc.

So lets first look at $\langle\hat{H}\rangle$ and the original location $\langle\alpha\mid\hat{H}\mid\alpha\rangle$. Now if space is homogeneous the this should be the same as the expectation value for $\hat{\mathcal{T}}\,|\alpha\rangle$, that is $\langle\alpha\,|\,\hat{\mathcal{T}}^{\dagger}\,\hat{H}\,\hat{\mathcal{T}}\,|\,\alpha\rangle$. So if $\langle\alpha\,|\,\hat{\mathcal{T}}^{\dagger}\,\hat{H}\,\hat{\mathcal{T}}\,|\,\alpha\rangle=\langle\alpha\mid\hat{H}\mid\alpha\rangle$, this means that $\hat{\mathcal{T}}^{\dagger}\,\hat{H}\,\hat{\mathcal{T}}=\hat{H}$, so $\hat{H}\,\hat{\mathcal{T}}=\hat{\mathcal{T}}\,\hat{H}$ (since $\hat{\mathcal{T}}$ is unitary) $\rightarrow[\hat{H},\,\hat{\mathcal{T}}]=0\rightarrow[\hat{H},\,\hat{p}_x]=0$

But using the theorem above we get that $\frac{d\langle\hat{p}_x\rangle}{dt}=[\hat{H},\,\hat{p}_x]=0$ and momentum is conserved.

We can do the same where we replace $\hat{\mathcal{T}}$ with the unitary time evolution operator and get $\frac{d\langle E\rangle}{dt}=0$ , the conservation of energy. Later we will have a rotation operator which will lead to the conservation of angular momentum.

**Free particle states**

We now want to look at free particle states. What does this mean? It means where we start with a Hamiltonian that has no potential, i,e $\hat{H}=\,\hat{p}^2/2\,m$ . Lets now find eigenkets and eigenvalues of this hamiltonian

$\frac{\hat{p}^2}{2\,m}|E\rangle=E|E\rangle$ where the eigenvalues are the energies E, and we label the states with E.

Now we can put this in the x representation. I will do it slowly here. Remember $\langle x'|\,\hat{\boldsymbol{p}}\mid\alpha\rangle=\frac{\hbar}{i}\,\frac{\boldsymbol{d}}{\mathbf{dx'}}\langle x'|\alpha\rangle$ and $\langle x'|\,\hat{\boldsymbol{p}}\mid x''\rangle=\frac{\hbar}{i}\,\frac{\boldsymbol{d}}{\mathbf{dx'}}\langle x'|x''\rangle=\frac{\hbar}{i}\,\frac{\boldsymbol{d}}{\mathbf{dx'}}\delta(x'-x'')$

$\langle x'|\frac{\hat{p}^2}{2\,m}|E\rangle=E\langle x'|E\rangle\quad\rightarrow\quad\frac{1}{2\,m}\int dx''\langle x'|\hat{p}\,|x''\rangle\,\langle x''|\,\hat{p}|E\rangle=\frac{1}{2\,m}\,\int dx''\frac{\hbar}{i}\,\frac{\boldsymbol{d}}{\mathbf{dx'}}\delta(x'-x'')\frac{\hbar}{i}\,\frac{\boldsymbol{d}}{\mathbf{dx''}}\langle x''|E\rangle=\frac{-\hbar^2}{2\,m}\,\frac{\boldsymbol{d}}{\mathbf{dx'}}\,\frac{\boldsymbol{d}}{\mathbf{dx'}}\langle x'|E\rangle$ $=\frac{-\hbar^2}{2\,m}\,\frac{\boldsymbol{d}^2}{\mathbf{dx'}^2}\langle x'|E\rangle=E\langle x'|E\rangle\quad\rightarrow\quad\frac{\boldsymbol{d}^2}{\mathbf{dx'}^2}\langle x'|E\rangle=-\frac{2\,mE}{\hbar^2}\langle x'|E\rangle$ The solutions for this are $\langle x'\mid E\rangle=e^{\pm ikx}$ where $k=\sqrt{\frac{2\,mE}{\hbar^2}}$ or $E=\frac{\hbar^2\,k^2}{2\,m}$. Note that these eigenkets are normalized. Now we could have just as easily chosen sines and cosines as the basic solutions but this will have a drawback as we will see now. This is a case where there is a degeneracy. i.e. there are two eigenkets with the same eigenvalue E. Remember we want to break this degeneracy, by finding some other operator which commutes with $\hat{H}$ which we can use to distinguish the states. If we look around for some likely operator, we might guess that it is $\hat{\boldsymbol{p}}$, the momentum. Lets see if the eigenkets we chose $\langle x'\mid E\rangle=e^{\pm ikx}$ are eigenkets of $\hat{\boldsymbol{p}}$. $\frac{\hbar}{i}\,\frac{\boldsymbol{d}}{\mathbf{dx'}}\langle x'|\alpha\rangle=p\langle x'|E\rangle$ $\rightarrow\quad\frac{\hbar}{i}(\pm ikx)e^{\pm ikx}=pe^{\pm ikx}$ So $p=\pm\hbar k$. Notice that if we chose sine's and cosines these would not be eigenkets of $\hat{\boldsymbol{p}}$. So now lets label the states with k instead of E

i.e. the eigenkets of the free particle hamiltonian $\hat{H}=\frac{\hat{p}^2}{2\,m}$ are $|k\rangle$ and $|-k\rangle$ where $\langle x|k\rangle=e^{+ikx}$ $\langle x|-k\rangle=e^{-ikx}$ and $E=\frac{\hbar^2\,k^2}{2\,m}$ and $p=\pm\hbar k$ (maybe we should have labeled these $|E,k\rangle$ and $|E,-k\rangle$ but that sort of redundant dont you think?)

Now lets take a look at the characteristics of these eigenstates. First, lets look at how they evolve with time.

$|\pm k,\,t\rangle=\hat{U}\,|\pm k\rangle=e^{-\frac{i\hat{H}\,t}{\hbar}}\,|\pm k\rangle=e^{-\frac{i\hbar^2\,k^2\,t}{2\,m\hbar}}\,|\pm k\rangle=e^{-i\omega t}|\pm k\rangle$ $\omega=\frac{\hbar^2\,k^2}{2\,m\hbar}=\frac{E}{\hbar}$ as we know, it gets a phase. Now lets put it in position representation

$\langle x'\mid\pm k,\,t\rangle=e^{-i\omega t}\,e^{\pm ikx}=e^{i(\pm kx-\omega t)}$ again, it is normalized correctly. It is a plane wave. If you follow the peak of the function, and increase t, x increases for k positive, and x must decrease for k negative. i.e. we have a wave that moves forward and backward as we might expect. So this "particle" just moves as you might guess, forward or backward depending on the momentum.

Let's figure out $\frac{d\langle\hat{p}\rangle}{dt}$ which should be zero and $\frac{d\langle\hat{x}\rangle}{dt}$ which should be a constant - the velocity

$\frac{d\langle\hat{p}\rangle}{dt}=\;\frac{i}{\hbar}\,\langle[\hat{H},\,\hat{p}]\rangle\;=\frac{i}{\hbar}\,\langle[\frac{\hat{p}^2}{2\,m},\,\hat{p}]\rangle=0$ so $\langle\hat{p}\rangle$ is a constant as should be

$\frac{d\langle\hat{x}\rangle}{\mathrm{dt}} = \frac{i}{\hbar}\left\langle\left[\hat{H},\hat{x}\right]\right\rangle = \frac{i}{2\,\mathrm{m}\hbar}\left\langle\left[\hat{p}^2,\hat{x}\right]\right\rangle = \frac{i}{2\,\mathrm{m}\hbar}\left(\left\langle\hat{p}[\hat{p},\hat{x}]\right\rangle + \left\langle[\hat{p},\hat{x}]\,\hat{p}\right\rangle\right) = \frac{i}{2\,\mathrm{m}\hbar}\left\langle\hat{p}\right\rangle(-2\,\mathrm{i}\hbar) = \frac{\langle\hat{p}\rangle}{m}$=constant since $\langle\hat{p}\rangle$ is a constant. We can then write $\langle\hat{x}\rangle = \langle\hat{x}\rangle_0 + \frac{\langle\hat{p}\rangle}{m}\mathrm{t}$ where $\langle\hat{x}\rangle_0 = \langle k,\, t=0\,|\,\hat{x}\,|\,k,\, t=0\rangle$

Now just how particle like is this thing? The common notion of a particle is something that occupies a finite extent in space. Lets see what the dispersion is in x.

$\langle\hat{x}\rangle = \int_{-\infty}^{\infty} dx\, e^{-i(\pm\mathrm{kx}-\omega\mathrm{t})}\, x\, e^{-i(\pm\mathrm{kx}-\omega\mathrm{t})} = 0$

$\langle\hat{x}^2\rangle = \int_{-\infty}^{\infty} dx\, e^{-i(\pm\mathrm{kx}-\omega\mathrm{t})}\, x^2 e^{-i(\pm\mathrm{kx}-\omega\mathrm{t})} = \infty$

$(\Delta\mathrm{x})^2 = \langle\hat{x}^2\rangle - \langle\hat{x}\rangle^2 = \infty$ i.e. it covers all of space - its not particle like at all. This thing will satisfy the Heisenbergy because $\Delta$p=0 (figure it out!)

Now we can look at something much more particle like, but more complicated - that is a particle which is localized in x (which of course must have a corresponding spread in momentum) This is a gaussian wave packet whose initial condition in x representation is

$\langle x\,|\alpha,\, t=0\rangle = \frac{1}{\sqrt{a}\,(2\pi)^{1/4}}\, e^{-x^2/4a^2}\, e^{\mathrm{ik}_0 x}$ . We can then do a fourier transform of this to see what the spread in momentum is. Then we can evolve it in time. The integrals are a pain. For the moment I will not do them here. They are in Liboff.

 