Notes for Quantum Mechanics

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Lecture 15

Continuous spectra

Before we get to position an momentum, we will need to deal with continuous spectra, where the eigenvalues are not discreet but continuous. Before we had $\hat{A}\,|a_i\rangle = a_i|a_i\rangle$, where the a_i were discreet. Now lets do the continuous case. Now there is no index but we will assume the eigenvalue will serve as the continuous variable. For now we will use the variable x and the operator $\hat{X}$ so

$\hat{X}\,|x'\rangle = x'|x'\rangle$

We also have $\langle x'|x''\rangle = \delta(x'-x'')$ remember before we had $\langle a_i|a_j\rangle = \delta_{ij}$ $\delta(x'-x'')$ is the dirac delta function we saw before

$$\int dx'\,|\,x'\,\rangle\,\langle\,x'\,|\,=\hat{1} \quad \text{similar to} \sum_i |a_i\,\rangle\,\langle a_i\,|\,=\hat{1}$$

$$|\alpha\rangle = \int dx'\,|\,x'\,\rangle\,\langle x'|\alpha\rangle \quad \text{similar to} \quad |\,\alpha\,\rangle = \sum_i |a_i\,\rangle\,\langle a_i|\alpha\rangle$$

Normalization:

$$\int dx'\,|\,\langle\,x'\,|\,\alpha\,\rangle\,|^2 = 1 \quad \text{similar to} \sum_i |\,\langle\,a_i\,|\,\alpha\,\rangle\,|^2 = 1$$

$$\langle\beta|\alpha\rangle = \int dx'\,\langle\,\beta\,|\,x'\,\rangle\,\langle x'|\alpha\rangle \quad \text{similar to} \langle\,\beta\,|\,\alpha\,\rangle = \sum_i \langle\beta|a_i\,\rangle\,\langle a_i|\alpha\rangle$$

$$\langle x''\,|\,\hat{X}\,|\,x'\rangle = x'\,\delta(x'-x'') \text{ similar to } \langle a_j\,|\,\hat{A}\,|\,a_i\rangle = a'\,\delta_{ij}$$

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The position operator and eigenkets
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The position operator and eigenkets

We want to define $\hat{X}$ so

$\hat{X}\,|x'\rangle = x'|x'\rangle$

where x' is a position in space. What does this mean? If we take some ket $|\alpha\rangle$ then the probability of finding the particle at point x' is $|\langle x'|\alpha\rangle|^2$ dx. This makes some sense since the probability for finding it somewhere between -∞ and ∞ must be 1. i,e, $\int dx' \, |\langle x'|\alpha\rangle|^2 = 1$ and this is just the normalization requirement from above. Now for those who are used to dealing with wavefuntions, what is typically called $\psi_\alpha(x)=\langle x'|\alpha\rangle$. This is nice because $|\alpha\rangle$ is the ket. But in the position representation (or position basis - like the S_z basis) we can just write it $\langle x'|\alpha\rangle$

We are going to assume that the eigenkets of position are complete. Since they are eigenkets of the observable $\hat{X}$ they are orthogonal, i.e. $\langle x'|x''\rangle = \delta(x'-x'')$ This is a little weird but if you think about it a bit $\langle x'|x''\rangle$ is like asking if something is both at x' and at x''. Its true only if the two points are the same.

This notion can be expanded pretty easily to three dimensions, and we will just use ***x'* (boldface)** to represent (x',y',z') i.e.

$|\boldsymbol{x}'\rangle \equiv |x',y',z,\rangle$ and we have $\hat{X}|\boldsymbol{x}'\rangle = x'|\boldsymbol{x}'\rangle$ $\hat{Y}|\boldsymbol{x}'\rangle = y'|\boldsymbol{x}'\rangle$ $\hat{Z}|\boldsymbol{x}'\rangle = z'|\boldsymbol{x}'\rangle$

We assume (unlike spin!) that we can measure all three components of the position vector simultaneously, i..e. we have $[\hat{X}_i,\hat{X}_j]=0$ where the components $\hat{X}_i$ are just $\hat{X}$, $\hat{Y}$, $\hat{Z}$ e.g. $[\hat{X},\hat{Y}]=0$ etc

Translation

Now I am going to do a little magic. Actually I am going to show you the fundamental relationship between momentum and the fact that space is homogeneous - i.e. that the rules of life do not change even if you move from California to Texas. [Actually they do, but doesn't that seem wrong? Physics is much more fair]

Just before we get into this, lets write out the taylor expansion for a function. To find the value of a function at a point x+h where h is a small number and f(x) is known you can use the following

$$f(x+h) = f(x) + h \frac{d}{dx} f(x) + \frac{h^2}{2!} \frac{d^2}{dx^2} f(x)....$$

Lets define a new operator - the translation operator $\hat{\vec{\mathcal{T}}}(\delta x)$ such that

$\hat{\vec{\mathcal{T}}}(\delta x)|x\rangle=|x+\delta x\rangle$ This DEFINES $\hat{\vec{\mathcal{T}}}$. This of course makes sense. It just moves the ket along by a distance δx.$\hat{\vec{\mathcal{T}}}(\delta x)$ is an infinitesimal translation which moves the ket along by a distance δx.

Now clearly $|x\rangle$ is not an eigenket of $\hat{\vec{\mathcal{T}}}$. We can use the taylor theorem to write $\langle x'-\delta x'|\alpha\rangle=\langle x'|\alpha\rangle-\delta x'\frac{d}{dx'}\langle x'|\alpha\rangle$ where we have taken $\langle x'|\alpha\rangle$ as the function we expand. Note that $\langle x'|\alpha\rangle$ is a function (or in some cases a number - it is NOT a ket anymore)

$$\hat{\vec{\mathcal{T}}}|\alpha\rangle=\vec{\mathcal{T}} \int d\boldsymbol{x}' \, |\boldsymbol{x}'\rangle\langle\boldsymbol{x}'|\alpha\rangle=\int d\boldsymbol{x}' \, \hat{\vec{\mathcal{T}}} \, |\boldsymbol{x}'\rangle\langle\boldsymbol{x}'|\alpha\rangle=\int d\boldsymbol{x}' \, |\boldsymbol{x}'+\delta\boldsymbol{x}'\rangle\langle\boldsymbol{x}'|\alpha\rangle=\int d\boldsymbol{x}' \, |\boldsymbol{x}'\rangle\langle\boldsymbol{x}'-\delta\boldsymbol{x}'|\alpha\rangle =$$

$$=\int d\boldsymbol{x}' \, |\boldsymbol{x}'\rangle(\langle\mathbf{x}'|\alpha\rangle-\delta\mathbf{x}'\frac{\boldsymbol{d}}{\mathbf{dx}'}\langle\mathbf{x}'|\alpha\rangle)=\int d\boldsymbol{x}' \, |\boldsymbol{x}'\rangle\langle\mathbf{x}'|\alpha\rangle-\int d\boldsymbol{x}' \, |\boldsymbol{x}'\rangle\delta\mathbf{x}'\frac{\boldsymbol{d}}{\mathbf{dx}'}\langle\mathbf{x}'|\alpha\rangle$$

where I have used the bold symbol $\frac{\boldsymbol{d}}{\mathbf{dx}'}$ in place of $\vec{\nabla}$ but you can also think of this in 1-D if you just forget the bolds

Now lets rewrite $\hat{\vec{\mathcal{T}}}(\delta\mathbf{x}')$ as $\hat{\vec{\mathcal{T}}}(\delta\mathbf{x}')=\hat{1}-i\delta\mathbf{x}'\cdot\hat{\boldsymbol{K}}$ where **K** is some operator related to $\hat{\vec{\mathcal{T}}}$. This sort of makes sense since $|x\rangle$ and $|x+\delta x\rangle$ can't be too different than one another.

$$\hat{\vec{\mathcal{T}}}|\alpha\rangle=(\hat{1}-i\delta x'\hat{\boldsymbol{K}})\int dx' \, |x'\rangle\langle x'|\alpha\rangle= \int dx' \, |x'\rangle\langle x'|\alpha\rangle-(i\delta x\hat{\boldsymbol{K}})\int dx' \, |x'\rangle\langle x'|\alpha\rangle$$

Now comparing the two expressions for $\hat{\vec{\mathcal{T}}}|\alpha\rangle$ we get

$$(i\delta x\hat{\boldsymbol{K}})\int dx' \, |x'\rangle\langle x'|\alpha\rangle=\int d\boldsymbol{x}' \, |\boldsymbol{x}'\rangle\delta\mathbf{x}'\frac{\boldsymbol{d}}{\mathbf{dx}'}\langle\mathbf{x}'|\alpha\rangle \implies \hat{\boldsymbol{K}}\,|\alpha\rangle = \int d\boldsymbol{x}' \, |\boldsymbol{x}'\rangle \frac{1}{i}\frac{\boldsymbol{d}}{\mathbf{dx}'}\langle\mathbf{x}'|\alpha\rangle \implies$$

$$\langle x''|\,\hat{\boldsymbol{K}}\,|\alpha\rangle = \int d\boldsymbol{x}' \, \langle x''|\boldsymbol{x}'\rangle \frac{1}{i}\frac{\boldsymbol{d}}{\mathbf{dx}'}\langle\mathbf{x}'|\alpha\rangle \implies \langle x''|\,\hat{\boldsymbol{K}}\,|\alpha\rangle = \int d\boldsymbol{x}' \, \delta(x'-x'') \frac{1}{i}\frac{\boldsymbol{d}}{\mathbf{dx}'}\langle\mathbf{x}'|\alpha\rangle$$

$$\implies \langle x'|\,\hat{\boldsymbol{K}}\,|\alpha\rangle = \frac{1}{i}\frac{\boldsymbol{d}}{\mathbf{dx}'}\langle\mathbf{x}'|\alpha\rangle$$

So we get that $\langle x'|\,\hat{\boldsymbol{K}}\,|\,\alpha\rangle = \frac{1}{i}\frac{d}{dx'}\langle \mathbf{x}'|\alpha\rangle$ Now does this look familiar? See eqn 3.5. Remember when we first started the class that we had $\hat{\boldsymbol{P}} \to \frac{\hbar}{i}\frac{\partial}{\partial \mathbf{x}}$ We can associate $\hat{\boldsymbol{K}}$ with $\frac{\hat{P}}{\hbar}$ and $\langle \mathbf{x}'|\alpha\rangle$ with $\psi(\mathbf{x}')$. We will continue to write $\langle \mathbf{x}'|\alpha\rangle$, but we will replace $\hat{\boldsymbol{K}}$ with $\frac{\hat{\boldsymbol{p}}}{\hbar}$ so we get

$$\langle x'|\,\hat{\boldsymbol{p}}\,|\,\alpha\rangle = \frac{\hbar}{i}\frac{d}{dx'}\langle x'|\alpha\rangle$$

Now I had better be careful and tell you the $\hat{\boldsymbol{p}}$ here is in the position representation because the left hand side is $\langle x'|\,\hat{\boldsymbol{p}}\,|\,\alpha\rangle$. So the funny definition of momentum(in the position representation), naturally pops out of our understanding of the homogeneity of space and the translation operator. We will start to see what this definition of the momentum operator does.

Now I would like to show you the comuntator relationship between position and momentum, and of course from there we can get the standard Heisenberg uncertainty principle. For now I will do it in 1-D.

$[\hat{X},\hat{K}]=i$ (The 3-D version of this is $[\hat{X}_i, \hat{K}_j] = i\delta_{ij}$ whose proof is a little more confusing, because I have to use indices to consider the components separately)

Proof: note: $\hat{X}\hat{\mathcal{T}}(dx')|x'\rangle=\hat{X}|x'+dx'\rangle=(x'+dx')|x'+dx'\rangle$ and $\hat{\mathcal{T}}(dx')\hat{X}|x'\rangle=x'\hat{\mathcal{T}}(dx')|x'\rangle=x'|x'+dx'\rangle$

so $[\hat{X},\hat{\mathcal{T}}(dx')]|x'\rangle=dx'|x'+dx'\rangle \approx dx'|x'\rangle$ So now plugging in $\hat{\mathcal{T}}(dx') = \hat{1} - i dx'\,\hat{K}_x$ we now drop the ket and write just for the operators

$dx'=[\hat{X},\hat{\mathcal{T}}(dx')]=[\hat{X},\hat{1} - i dx'\,\hat{K}_x]=-i dx'[\hat{X},\hat{K}_x]$ so $[\hat{X},\hat{K}_x]=i$ and plugging in for $\hat{\boldsymbol{P}}_x$ we get $[\hat{X},\hat{P}_x]=i\hbar$

Now we can repeat the proof for the y and x components.

Now I need to do it for two components which are not the same i.e. I want to show e.g. $[\hat{X},\hat{K}_y]=0$

Proof: note: $\hat{X}\hat{\mathcal{T}}(dy')|x',y'\rangle=\hat{X}|x',y'+dy'\rangle=x'|x',y'+dy'\rangle$ and $\hat{\mathcal{T}}(dy')\hat{X}|x',y'\rangle=x'\hat{\mathcal{T}}(dy')|x',y'\rangle=x'|x',y'+dy'\rangle$

so $[\hat{X},\hat{\mathcal{T}}(dy')]|x',y'\rangle=dx'|x'+dx'\rangle=0$ so $0=[\hat{X},\hat{\mathcal{T}}(dy')]=[\hat{X},\hat{1} - i dy'\,\hat{K}_y]=-i dy'[\hat{X},\hat{K}_y]=0$

so for $\hat{P}_y$ we get $[\hat{X},\hat{P}_y]=0$

So summing up we get $[\hat{X}_i, \hat{P}_j] = i\delta_{ij}\hbar$ - The commuation relationship between position and momentum

Now lets start with the generalized Heisenberg principle from last time $\Delta\hat{A}\,\Delta\hat{B} \geq \frac{1}{2}\left|\langle\hat{C}\rangle\right|$ where $[\hat{A}, \hat{B}]=\hat{C}$

$\frac{1}{2}\left|\langle\hat{C}\rangle\right| = \frac{1}{2}\left|[\hat{X}_i, \hat{P}_j]\right| = \frac{1}{2}\left|i\delta_{ij}\,\hbar\right| = \frac{\hbar}{2}\delta_{ij}$ and finally plugging it in with $\hat{A} = \hat{X}_i$ and $\hat{B}=\hat{P}_j$

$\Delta\hat{X}_i\,\Delta\hat{P}_j \geq \frac{\hbar}{2}\delta_{ij}$ That's it. The Heiseberg Uncertainty principle - note that it is in operator form.

Now $\hat{\mathcal{T}}(\delta x)$ was a infinitesimal translation. Lets now move it along by by a finite amount. How do we do this? We have to do the infinitesimal translation many times. I will now go ahead and write $\hat{\mathcal{T}}(\delta\mathbf{x}) = \hat{1} - i\delta\mathbf{x}\cdot\frac{\hat{\boldsymbol{p}}}{\hbar}$ and for 1-D $\hat{\mathcal{T}}(\delta x) = \hat{1} - i\delta x\frac{\hat{\boldsymbol{P}}_x}{\hbar}$

So to translate a finite amount Δx

$\hat{\mathcal{T}}(\Delta x) = N \overset{\text{limit}}{\to} \infty \left(\hat{1} - i\,\frac{\hat{\boldsymbol{P}}_x}{\hbar}\,\frac{\Delta x}{N}\right)^N$ where $\frac{\Delta x}{N}=\delta x$ But if you look it up in some math tables

$(1-x)^n = 1 - \mathrm{nx} + \frac{n(n-1)}{2!} x^2 \ldots$ so $\left(1 - \frac{x}{N}\right)^N = 1 - x + \frac{(N-1)}{2!\,N} x^2 \ldots \sim 1 - x + \frac{1}{2!} x^2 = e^x$

$\hat{\vec{\mathcal{T}}}(\Delta\mathrm{x}) \quad = e^{-i \frac{\hat{\boldsymbol{P}}_{\boldsymbol{x}}}{\hbar} \Delta\mathrm{x}}$ Where we define the exponential of an operator in terms of the expansion $e^x = 1 + x + \frac{x^2}{2!} + \ldots$

Next we will require that translations in x, y, and z directions all commute with each other. This of course makes sense on a flat world, but not on a curved one. [think about a world globe - the world is 25000 miles around - pretend its 24000 miles. Start on the equator. Go 6000 miles in the x direction then 6000 miles in the y direction -if you define x and y like I do you should be at the north pole. Then start at the same place but reverse the order. Go 6000 miles y direction and then 6000 miles in the x direction. you will be back at the equator - welcome to curved space and general relativity - No one has figured out how to do Quantum General Relativity - so lets go back to a flat world]

Translations in the x,y, and z all commute with one another. This will meam that e.g.

$[\hat{\vec{\mathcal{T}}}(\Delta\mathrm{x}) \;, \hat{\vec{\mathcal{T}}}(\Delta\mathrm{y}) \;] = [(\hat{1} - i \frac{\hat{\boldsymbol{P}}_{\boldsymbol{x}}}{\hbar} \frac{\Delta\mathrm{x}}{N} \ldots.),(\hat{1} - i \frac{\hat{\boldsymbol{P}}_{\boldsymbol{y}}}{\hbar} \frac{\Delta\mathrm{y}}{N} \ldots.)]=0$ Work this out and you will get

$[\hat{P}_{\boldsymbol{x}}, \hat{P}_{\boldsymbol{y}}] = 0$

So lets summarize all the commutation relationships

$[\hat{X}_i, \hat{X}_j]=0 \quad [\hat{P}_{\boldsymbol{i}}, \hat{P}_{\boldsymbol{j}}] = 0 \quad [\hat{X}_i, \hat{P}_j] = \mathrm{i}\delta_{\mathrm{ij}}\hbar$

Finally lets now think about eigenkets of $\hat{P}_{\boldsymbol{i}}$ which we will call $|p_i'\rangle$ so that

$\hat{P}_{\boldsymbol{i}}|p_i'\rangle = p_i'|p_i'\rangle$ and i=1,2,3 or x,y,z

What does translation do to this? Lets try it

$\mathcal{T}(\delta\mathrm{x})|p_x'\rangle = \left(\hat{1} - i \frac{\hat{\boldsymbol{P}}_{\boldsymbol{x}}}{\hbar} \delta\mathrm{x}\right)|p_x'\rangle = \left(1 - i \frac{\boldsymbol{p}_{\boldsymbol{x}}'}{\hbar} \delta\mathrm{x}\right)|p_x'\rangle$ so $|p_x'\rangle$ is an eigenket of $\mathcal{T}(\delta\mathrm{x})$ with an eigenvalue $\left(1 - i \frac{\boldsymbol{p}_{\boldsymbol{x}}'}{\hbar} \delta\mathrm{x}\right)$ so the eigenvalue is not real. This means that $\mathcal{T}$ is unitary but not Hermitain (since Hermitian operators have real eigenvalues) Also one can see that $[\hat{\vec{\mathcal{T}}}(\delta\mathrm{x}), \hat{\boldsymbol{P}}_{\boldsymbol{x}}] = [\left(\hat{1} - i \frac{\hat{\boldsymbol{P}}_{\boldsymbol{x}}}{\hbar} \delta\mathrm{x}\right), \hat{\boldsymbol{P}}_{\boldsymbol{x}}]=0$ that is momentum commutes with translation.