Notes for Quantum Mechanics

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

Lecture 25 work - calculus and transforming coordinates

x'=rsinθcosϕ y'=rsinθsinϕ z'=rcosθ r=$\sqrt{x'^2+y'^2+z'^2}$ θ= acos$\left(\frac{z'}{r}\right)$= acos$\left(\frac{z'}{\sqrt{x'^2+y'^2+z'^2}}\right)$ ϕ = atan$\left(\frac{y'}{x'}\right)$

a couple of derivatives you might have forgotten $\frac{d}{\mathrm{dx}}$acos(x)= $\frac{-1}{\sqrt{1-x^2}}$ and $\frac{d}{\mathrm{dx}}$atan(x)= $\frac{1}{1+x^2}$

$\frac{\mathrm{dr}}{\mathrm{dx}} = 2\,\frac{x}{r} = \sin\theta\cos\phi$ $\frac{\mathrm{d}\theta}{\mathrm{dx}} = \frac{\cos\theta\cos\phi}{r}$ $\frac{\mathrm{d}\phi}{\mathrm{dx}} = -\frac{\sin\phi}{r\sin\theta}$

$\frac{\mathrm{dr}}{\mathrm{dy}} = 2\,\frac{y}{r} = \sin\theta\sin\phi$ $\frac{\mathrm{d}\theta}{\mathrm{dy}} = \frac{\cos\theta\sin\phi}{r}$ $\frac{\mathrm{d}\phi}{\mathrm{dy}} = \frac{\cos\phi}{r\sin\theta}$

$\frac{\mathrm{dr}}{\mathrm{dz}} = 2\,\frac{z}{r} = \cos\theta$ $\frac{\mathrm{d}\theta}{\mathrm{dz}} = -\frac{\sin\theta}{r}$ $\frac{\mathrm{d}\phi}{\mathrm{dz}} = 0$

Now remember the chain rule when you have several variables!

$$\frac{d}{\mathrm{dx}} = \frac{\mathrm{dr}}{\mathrm{dx}}\frac{d}{\mathrm{dr}} + \frac{\mathrm{d}\theta}{\mathrm{dx}}\frac{d}{\mathrm{d}\theta} + \frac{\mathrm{d}\phi}{\mathrm{dx}}\frac{d}{\mathrm{d}\phi} = \sin\theta\cos\phi\,\frac{d}{\mathrm{dr}} + \frac{\cos\theta\cos\phi}{r}\,\frac{d}{\mathrm{d}\theta} - \frac{\sin\phi}{r\sin\theta}\,\frac{d}{\mathrm{d}\phi}$$

$$\frac{d}{\mathrm{dy}} = \frac{\mathrm{dr}}{\mathrm{dy}}\frac{d}{\mathrm{dr}} + \frac{\mathrm{d}\theta}{\mathrm{dy}}\frac{d}{\mathrm{d}\theta} + \frac{\mathrm{d}\phi}{\mathrm{dy}}\frac{d}{\mathrm{d}\phi} = \sin\theta\sin\phi\,\frac{d}{\mathrm{dr}} + \frac{\cos\theta\sin\phi}{r}\,\frac{d}{\mathrm{d}\theta} + \frac{\cos\phi}{r\sin\theta}\,\frac{d}{\mathrm{d}\phi}$$

$$\frac{d}{\mathrm{dz}} = \frac{\mathrm{dr}}{\mathrm{dz}}\frac{d}{\mathrm{dr}} + \frac{\mathrm{d}\theta}{\mathrm{dz}}\frac{d}{\mathrm{d}\theta} + \frac{\mathrm{d}\phi}{\mathrm{dz}}\frac{d}{\mathrm{d}\phi} = \cos\theta\,\frac{d}{\mathrm{dr}} - \frac{\sin\theta}{r}\,\frac{d}{\mathrm{d}\theta}$$

so $\hat{L}_z=\hat{x}\,\hat{p}_y - \hat{y}\,\hat{p}_x = \frac{\hbar}{i}\hat{x}\,\frac{d}{\mathrm{dy}} - \frac{\hbar}{i}\,\hat{y}\,\frac{d}{\mathrm{dx}} =$

$$\frac{\hbar}{i}[\mathrm{r}\sin\theta\cos\phi(\sin\theta\sin\phi\,\frac{d}{\mathrm{dr}} + \frac{\cos\theta\sin\phi}{r}\,\frac{d}{\mathrm{d}\theta} + \frac{\cos\phi}{r\sin\theta}\,\frac{d}{\mathrm{d}\phi}) - \mathrm{r}\sin\theta\sin\phi(\sin\theta\cos\phi\,\frac{d}{\mathrm{dr}} + \frac{\cos\theta\cos\phi}{r}\,\frac{d}{\mathrm{d}\theta} - \frac{\sin\phi}{r\sin\theta}\,\frac{d}{\mathrm{d}\phi})]$$

$$= \frac{\hbar}{i}(\mathrm{r}\sin^2\theta\cos\phi\sin\phi\,\frac{d}{\mathrm{dr}} + \cos\theta\sin\theta\cos\phi\sin\phi\,\frac{d}{\mathrm{d}\theta} + \cos^2\phi\,\frac{d}{\mathrm{d}\phi} - \mathrm{r}\sin^2\theta\cos\phi\sin\phi\,\frac{d}{\mathrm{dr}} - \cos\theta\sin\theta\sin\phi\cos\phi\,\frac{d}{\mathrm{d}\theta} + \sin^2\phi\,\frac{d}{\mathrm{d}\phi})$$

$$= \frac{\hbar}{i}(\cos^2\phi + \sin^2\phi)\frac{d}{\mathrm{d}\phi} = \frac{\hbar}{i}\,\frac{d}{\mathrm{d}\phi}$$

Similarly we can find (and after some work converting to spherical coordinates)

$\hat{L}_z=\hat{x}\,\hat{p}_y - \hat{y}\,\hat{p}_x$ $\hat{L}_x=\hat{y}\,\hat{p}_z - \hat{z}\,\hat{p}_y$ $\hat{L}_y=\hat{z}\,\hat{p}_x - \hat{y}\,\hat{p}_x$

$\langle \mathrm{x'},\mathrm{y'},\mathrm{z'}|\hat{L}_z|\alpha\rangle = \langle \mathrm{x'}+\mathrm{y'}\delta\phi,\ \mathrm{y'}-\mathrm{x'}\delta\phi,\ \mathrm{z'}|\alpha\rangle = \frac{\hbar}{i}\,\frac{d}{\mathrm{d}\phi}\langle \mathbf{x}|\alpha\rangle$

$\langle \mathrm{x'},\mathrm{y'},\mathrm{z'}|\hat{L}_x|\alpha\rangle = \langle \mathrm{x'},\ \mathrm{y'}+\mathrm{z'}\delta\phi,\ \mathrm{z'}-\mathrm{y'}\delta\phi|\alpha\rangle = \frac{\hbar}{i}\left(-\sin\phi\,\frac{d}{\mathrm{d}\theta} - \cot\theta\cos\phi\,\frac{d}{\mathrm{d}\phi}\right)\langle \mathbf{x}|\alpha\rangle$

$\langle \mathrm{x'},\mathrm{y'},\mathrm{z'}|\hat{L}_y|\alpha\rangle = \langle \mathrm{x'}-\mathrm{z'}\delta\phi,\ \mathrm{y'},\ \mathrm{z'}+\mathrm{x'}\delta\phi|\alpha\rangle = \frac{\hbar}{i}(-\cos\phi\,\frac{d}{\mathrm{d}\theta} - \cot\theta\sin\phi\,\frac{d}{\mathrm{d}\phi})\langle \mathbf{x}|\alpha\rangle$

Then we can figure out the raising and lowering operators

$\hat{L}_{\pm} = \hat{L}_x \pm i\,\hat{L}_y \;=\; \frac{\hbar}{i}\, e^{\pm i\phi}(\pm i\,\frac{d}{d\theta} - \cot\theta\,\frac{d}{d\phi})\langle \mathbf{x}|\alpha\rangle$ and

$$L^2 = {L_z}^2 + \frac{1}{2}\,(L_+\,L_- + L_-\,L_+)$$

$$= -\hbar^2\left\{\left(\frac{d^2}{d\phi^2}\right) + \frac{1}{2}\left[e^{i\phi}\left(+i\,\frac{d}{d\theta} - \cot\theta\,\frac{d}{d\phi}\right)e^{-i\phi}\left(-i\,\frac{d}{d\theta} - \cot\theta\,\frac{d}{d\phi}\right) + e^{-i\phi}\left(-i\,\frac{d}{d\theta} - \cot\theta\,\frac{d}{d\phi}\right)e^{i\phi}\left(+i\,\frac{d}{d\theta} - \cot\theta\,\frac{d}{d\phi}\right)\right]\right\}$$

Now look at the term as follows so we can figure out the position representation of L^2 in spherical coordinates :

$$2\frac{d^2}{d\phi^2} + \; e^{i\phi}\left(+i\,\frac{d}{d\theta} - \cot\theta\,\frac{d}{d\phi}\right)e^{-i\phi}\left(-i\,\frac{d}{d\theta} - \cot\theta\,\frac{d}{d\phi}\right) + e^{-i\phi}\left(-i\,\frac{d}{d\theta} - \cot\theta\,\frac{d}{d\phi}\right)e^{i\phi}\left(+i\,\frac{d}{d\theta} - \cot\theta\,\frac{d}{d\phi}\right)=$$

$$2\frac{d^2}{d\phi^2} + \; e^{i\phi}\left(+i\,\frac{d}{d\theta}\right)e^{-i\phi}\left(-i\,\frac{d}{d\theta}\right) + e^{-i\phi}\left(-i\,\frac{d}{d\theta}\right)e^{i\phi}\left(+i\,\frac{d}{d\theta}\right)+$$
$$e^{i\phi}\left(+i\,\frac{d}{d\theta}\right)e^{-i\phi}\left(-\cot\theta\,\frac{d}{d\phi}\right) + e^{-i\phi}\left(-i\,\frac{d}{d\theta}\right)e^{i\phi}\left(-\cot\theta\,\frac{d}{d\phi}\right)+$$
$$e^{i\phi}\left(-\cot\theta\,\frac{d}{d\phi}\right)e^{-i\phi}\left(-i\,\frac{d}{d\theta}\right) + e^{-i\phi}\left(-\cot\theta\,\frac{d}{d\phi}\right)e^{i\phi}\left(+i\,\frac{d}{d\theta}\right)+$$
$$e^{i\phi}\left(-\cot\theta\,\frac{d}{d\phi}\right)e^{-i\phi}\left(-\cot\theta\,\frac{d}{d\phi}\right) + e^{-i\phi}\left(-\cot\theta\,\frac{d}{d\phi}\right)e^{i\phi}\left(-\cot\theta\,\frac{d}{d\phi}\right)=$$

$$2\frac{d^2}{d\phi^2} + e^{i\phi}\left(\frac{d}{d\theta}\right)e^{-i\phi}\left(\frac{d}{d\theta}\right) + e^{-i\phi}\left(\frac{d}{d\theta}\right)e^{i\phi}\left(\frac{d}{d\theta}\right)+$$
$$-i\,e^{i\phi}\left(\frac{d}{d\theta}\right)e^{-i\phi}\left(\cot\theta\,\frac{d}{d\phi}\right) + i\;e^{-i\phi}\left(\frac{d}{d\theta}\right)e^{i\phi}\left(\cot\theta\,\frac{d}{d\phi}\right)$$
$$+i\,e^{i\phi}\left(\cot\theta\,\frac{d}{d\phi}\right)e^{-i\phi}\left(\frac{d}{d\theta}\right) - i\,e^{-i\phi}\left(\cot\theta\,\frac{d}{d\phi}\right)e^{i\phi}\left(\frac{d}{d\theta}\right)+$$
$$e^{i\phi}\left(\cot\theta\,\frac{d}{d\phi}\right)e^{-i\phi}\left(\cot\theta\,\frac{d}{d\phi}\right) + e^{-i\phi}\left(\cot\theta\,\frac{d}{d\phi}\right)e^{i\phi}\left(\cot\theta\,\frac{d}{d\phi}\right)=$$

$$2\frac{d^2}{d\phi^2} + \left(\frac{d}{d\theta}\right)\left(\frac{d}{d\theta}\right) + \left(\frac{d}{d\theta}\right)\left(\frac{d}{d\theta}\right)+$$
$$-i\left(\frac{d}{d\theta}\right)\left(\cot\theta\,\frac{d}{d\phi}\right) + i\;\left(\frac{d}{d\theta}\right)\left(\cot\theta\,\frac{d}{d\phi}\right)$$
$$+i\,e^{i\phi}\left(\cot\theta\,\frac{d}{d\phi}\right)e^{-i\phi}\left(\frac{d}{d\theta}\right) - i\,e^{-i\phi}\left(\cot\theta\,\frac{d}{d\phi}\right)e^{i\phi}\left(\frac{d}{d\theta}\right)+$$
$$e^{i\phi}\left(\cot\theta\,\frac{d}{d\phi}\right)e^{-i\phi}\left(\cot\theta\,\frac{d}{d\phi}\right) + e^{-i\phi}\left(\cot\theta\,\frac{d}{d\phi}\right)e^{i\phi}\left(\cot\theta\,\frac{d}{d\phi}\right)=$$

$$2\frac{d^2}{d\phi^2} + 2\frac{d^2}{d\theta^2} \;+i\,e^{i\phi}\cot\theta\left(\frac{d}{d\phi}\right)e^{-i\phi}\left(\frac{d}{d\theta}\right) - i\,e^{-i\phi}\cot\theta\left(\frac{d}{d\phi}\right)e^{i\phi}\left(\frac{d}{d\theta}\right)+e^{i\phi}\cot^2\theta\left(\frac{d}{d\phi}\right)e^{-i\phi}\left(\frac{d}{d\phi}\right) + e^{-i\phi}\cot^2\theta\left(\frac{d}{d\phi}\right)e^{i\phi}\left(\frac{d}{d\phi}\right)=$$

Now let it operate on ψ

$$2\frac{d^2\psi}{d\phi^2} + 2\frac{d^2\psi}{d\theta^2} + i\,e^{i\phi}\cot\theta\left(\frac{d}{d\phi}\;e^{-i\phi}\;\frac{d\psi}{d\theta}\right) - i\,e^{-i\phi}\cot\theta\left(\frac{d}{d\phi}\;e^{i\phi}\;\frac{d\psi}{d\theta}\right)+e^{i\phi}\cot^2\theta\left(\frac{d}{d\phi}\;e^{-i\phi}\;\frac{d\psi}{d\phi}\right) + e^{-i\phi}\cot^2\theta\left(\frac{d}{d\phi}\;e^{i\phi}\;\frac{d\psi}{d\phi}\right)=$$

$$2\frac{d^2\psi}{d\phi^2} + 2\frac{d^2\psi}{d\theta^2} + i\,e^{i\phi}\cot\theta\left((-i)\,e^{-i\phi}\;\frac{d\psi}{d\theta} \;+ e^{-i\phi}\;\frac{d}{d\phi}\;\frac{d\psi}{d\theta}\right) - i\,e^{-i\phi}\cot\theta\left(i\,e^{i\phi}\;\frac{d\psi}{d\theta} \;+ e^{i\phi}\;\frac{d}{d\phi}\;\frac{d\psi}{d\theta}\right)$$
$$+e^{i\phi}\cot^2\theta\left((-i)\,e^{-i\phi}\;\frac{d\psi}{d\phi} \;+ e^{-i\phi}\;\frac{d}{d\phi}\;\frac{d\psi}{d\phi}\right) + e^{-i\phi}\cot^2\theta\left(i\,e^{i\phi}\;\frac{d\psi}{d\phi} \;+ e^{i\phi}\;\frac{d}{d\phi}\;\frac{d\psi}{d\phi}\right)=$$

$$2\frac{d^2\psi}{d\phi^2} + 2\frac{d^2\psi}{d\theta^2}$$

$$+i\cot\theta\left((-i)\frac{d\psi}{d\theta}+\frac{d}{d\phi}\frac{d\psi}{d\theta}\right)-i\cot\theta\left(i\frac{d\psi}{d\theta}+\frac{d}{d\phi}\frac{d\psi}{d\theta}\right)+\cot^2\theta\left((-i)\frac{d\psi}{d\phi}+\frac{d}{d\phi}\frac{d\psi}{d\phi}\right)+\cot^2\theta\left(i\frac{d\psi}{d\phi}+\frac{d}{d\phi}\frac{d\psi}{d\phi}\right)=$$

$$2\frac{d^2\psi}{d\phi^2}+2\frac{d^2\psi}{d\theta^2}+\cot\theta\frac{d\psi}{d\theta}+i\cot\theta\frac{d}{d\phi}\frac{d\psi}{d\theta}+\cot\theta\frac{d\psi}{d\theta}-i\cot\theta\frac{d}{d\phi}\frac{d\psi}{d\theta}$$
$$-i\cot^2\theta\frac{d\psi}{d\phi}+\cot^2\theta\frac{d^2\psi}{d\phi^2}+i\cot^2\theta\frac{d\psi}{d\phi}+\cot^2\theta\frac{d^2\psi}{d\phi^2}=$$

$$+2\frac{d^2\psi}{d\phi^2}+\cot^2\theta\frac{d^2\psi}{d\phi^2}+\cot^2\theta\frac{d^2\psi}{d\phi^2}$$
$$+\cot\theta\frac{d\psi}{d\theta}+\cot\theta\frac{d\psi}{d\theta}$$
$$+2\frac{d^2\psi}{d\theta^2}$$
$$+i\cot\theta\frac{d}{d\phi}\frac{d\psi}{d\theta}$$
$$-i\cot\theta\frac{d}{d\phi}\frac{d\psi}{d\theta}$$
$$-i\cot^2\theta\frac{d\psi}{d\phi}$$
$$+i\cot^2\theta\frac{d\psi}{d\phi}$$

$$=(2+2\cot^2\theta)\frac{d^2\psi}{d\phi^2}+2\cot\theta\frac{d\psi}{d\theta}+2\frac{d^2\psi}{d\theta^2}\qquad \text{note: } 1+\cot^2=\frac{1}{\sin^2}$$

So $L^2=-\hbar^2[(1+\cot^2\theta)\frac{d^2}{d\phi^2}+\cot\theta\frac{d}{d\theta}+\frac{d^2}{d\theta^2}]=-\hbar^2\left[\frac{1}{\sin^2\theta}\frac{d^2}{d\phi^2}+\cot\theta\frac{d\psi}{d\theta}+\frac{d^2\psi}{d\theta^2}\right]$

Now

$$-\hbar^2\left[\frac{1}{\sin^2\theta}\frac{d^2\psi}{d\phi^2}+\frac{1}{\sin\theta}\frac{d}{d\theta}\left(\sin\theta\frac{d\psi}{d\theta}\right)\right]=-\hbar^2\left[\frac{1}{\sin^2\theta}\frac{d^2\psi}{d\phi^2}+\frac{1}{\sin\theta}\left(\cos\theta\frac{d\psi}{d\theta}+\sin\theta\frac{d}{d\theta}\frac{d\psi}{d\theta}\right)\right]=-\hbar^2\left[\frac{1}{\sin^2\theta}\frac{d^2\psi}{d\phi^2}+\cot\theta\frac{d\psi}{d\theta}+\frac{d^2\psi}{d\theta^2}\right]$$

So finally we have

$$\langle \boldsymbol{x}|\hat{\boldsymbol{L}}^2|\alpha\rangle=-\hbar^2\left[\frac{1}{\sin^2\theta}\frac{d^2}{d\phi^2}+\frac{1}{\sin\theta}\frac{d}{d\theta}\left(\sin\theta\frac{d}{d\theta}\right)\right]\langle \boldsymbol{x}|\alpha\rangle$$

Note that this is the angular part of laplacian in spherical coordinates apart from $\frac{1}{r^2}$ You can derive the Laplacian in spherical coordinates: $\nabla^2=\left(\frac{d^2}{dx^2}+\frac{d^2}{dy^2}+\frac{d^2}{dz^2}\right)=\frac{1}{r^2}\left[\frac{d}{dr}\left(r^2\frac{d}{dr}\right)+\frac{1}{\sin^2\theta}\frac{d^2}{d\phi^2}+\frac{1}{\sin\theta}\frac{d}{d\theta}\left(\sin\theta\frac{d}{d\theta}\right)\right]$