Quantum Dynamics, NWI-SM295, exercises week 8

Gerrit C. Groenenboom, June 9, 2019

Question 1: Angular momentum operators

The angular momentum operators $\hat{\boldsymbol{l}}$ for a single particle with position $\boldsymbol{r}$ and momentum $\hat{\boldsymbol{p}} = \frac{\hbar}{i}\boldsymbol{\nabla}$ are given by

$$\hat{\boldsymbol{l}} = \boldsymbol{r} \times \hat{\boldsymbol{p}}. \tag{1}$$

The position $\boldsymbol{r}$ expressed in spherical polar coordinates (r, θ, ϕ) is given by

$$\boldsymbol{r} = r \begin{pmatrix} \sin\theta\cos\phi \\ \sin\theta\sin\phi \\ \cos\theta \end{pmatrix}. \tag{2}$$

1a. Show that $\hat{l}_z$ in spherical polar coordinates is given by

$$\hat{l}_z = \frac{\hbar}{i}\frac{\partial}{\partial\phi}. \tag{3}$$

Answer: *In Cartesian coordinates:*

$$\hat{l}_z = \frac{\hbar}{i}\left(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}\right). \tag{4}$$

With the chain rule

$$\frac{\partial}{\partial\phi} = \frac{\partial y}{\partial\phi}\frac{\partial}{\partial y} + \frac{\partial x}{\partial\phi}\frac{\partial}{\partial x} \tag{5}$$

$$= r\sin\theta\cos\phi\frac{\partial}{\partial y} - r\sin\theta\sin\phi\frac{\partial}{\partial x} \tag{6}$$

$$= x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x} \tag{7}$$

and hence,

$$\frac{\hbar}{i}\frac{\partial}{\partial\phi} = \hat{l}_z. \tag{8}$$

Question 2: Rotations in $\mathbb{R}^3$

A rotation in $\mathbb{R}^3$ around a vector $\boldsymbol{n}$ with $|\boldsymbol{n}| = 1$ over an angle ϕ is given by

$$\boldsymbol{R}(\boldsymbol{n}, \phi) = e^{\phi\boldsymbol{N}}, \tag{9}$$

where $\boldsymbol{N}$ is an anti-Hermitian matrix, implicitly defined by

$$\boldsymbol{n} \times \boldsymbol{x} = \boldsymbol{N}\boldsymbol{x} \tag{10}$$

with

$$\boldsymbol{n} = \begin{pmatrix} n_1 \\ n_2 \\ n_3 \end{pmatrix}. \tag{11}$$

2a. Find the matrices $\boldsymbol{N}_1$, $\boldsymbol{N}_2$, and $\boldsymbol{N}_3$ such that

$$\boldsymbol{N} = n_1\boldsymbol{N}_1 + n_2\boldsymbol{N}_2 + n_3\boldsymbol{N}_3. \tag{12}$$

Answer:

$$\boldsymbol{n} \times \boldsymbol{x} = \begin{pmatrix} n_2 x_3 - n_3 x_2 \\ n_3 x_1 - n_1 x_3 \\ n_1 x_2 - n_2 x_1 \end{pmatrix} = \begin{pmatrix} 0 & -n_3 & n_2 \\ n_3 & 0 & -n_1 \\ -n_2 & n_1 & 0 \end{pmatrix} \boldsymbol{x} = \boldsymbol{N}\boldsymbol{x}, \tag{13}$$

so

$$\boldsymbol{N}_1 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -1 \\ 0 & 1 & 0 \end{pmatrix}, \quad \boldsymbol{N}_2 = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ -1 & 0 & 0 \end{pmatrix}, \quad \boldsymbol{N}_3 = \begin{pmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}. \tag{14}$$

2b. Show that

$$\boldsymbol{N}^T = -\boldsymbol{N}. \tag{15}$$

Answer:

$$\boldsymbol{N} = \begin{pmatrix} 0 & -n_3 & n_2 \\ n_3 & 0 & -n_1 \\ -n_2 & n_1 & 0 \end{pmatrix}. \tag{16}$$

2c. Derive the commutation relations

$$[\boldsymbol{N}_1, \boldsymbol{N}_2] = \boldsymbol{N}_3. \tag{17}$$

Answer: *Using the answer of* **2a***:*

$$\boldsymbol{N}_1\boldsymbol{N}_2 - \boldsymbol{N}_2\boldsymbol{N}_1 = \boldsymbol{N}_3. \tag{18}$$

Question 3: Wigner rotation matrices

A rotation operator acting on the $(2l+1)$ dimensional linear space

$$\{|lm\rangle,\ m = -l, -l+1, \dots, l\} \tag{19}$$

is given by

$$\hat{R}(\boldsymbol{n}, \phi) = e^{-\frac{i}{\hbar}\phi\, \boldsymbol{n}\cdot\hat{\boldsymbol{l}}}. \tag{20}$$

Wigner rotation matrices $\boldsymbol{D}^{(l)}(\boldsymbol{n}, \phi)$ are defined by

$$\hat{R}(\boldsymbol{n}, \phi)|lm\rangle = \sum_{m'=-l}^{l} |lm'\rangle D^{(l)}_{m',m}(\boldsymbol{n}, \phi). \tag{21}$$

We will use the short-hand notation $\boldsymbol{D}^{(l)}(\hat{R}) \equiv \boldsymbol{D}^{(l)}(\boldsymbol{n}, \phi)$.

3a. Show that $\boldsymbol{D}^{(l)}$ is a *representation* of $\hat{R}$, i.e.,

$$\boldsymbol{D}^{(l)}(\hat{R}_1\hat{R}_2) = \boldsymbol{D}^{(l)}(\hat{R}_1)\boldsymbol{D}^{(l)}(\hat{R}_2). \tag{22}$$

Answer: *By definition,*

$$(\hat{R}_1\hat{R}_2)|lm\rangle \equiv \hat{R}_1(\hat{R}_2|lm\rangle) \tag{23}$$

The left-hand-side gives

$$(\hat{R}_1\hat{R}_2)|lm\rangle = \sum_{m'=-l}^{l} |lm'\rangle D^{(l)}_{m',m}(\hat{R}_1\hat{R}_2). \tag{24}$$

The right-hand-sie gives

$$\begin{aligned}\hat{R}_1(\hat{R}_2|lm\rangle) &= \hat{R}_1 \sum_{m''=-l}^{l} |lm''\rangle D^{(l)}_{m'',m}(\hat{R}_2) &(25)\\ &= \sum_{m''=-l}^{l}\sum_{m'=-l}^{l} |lm'\rangle D^{(l)}_{m',m''}(\hat{R}_1) D^{(l)}_{m'',m}(\hat{R}_2) &(26)\\ &= \sum_{m'=-l}^{l} |lm'\rangle \sum_{m''=-l}^{l} D^{(l)}_{m',m''}(\hat{R}_1) D^{(l)}_{m'',m}(\hat{R}_2). &(27)\end{aligned}$$

Combining these results gives

$$D^{(l)}_{m',m}(\hat{R}_1\hat{R}_2) = \sum_{m''=-l}^{l} D^{(l)}_{m',m''}(\hat{R}_1) D^{(l)}_{m'',m}(\hat{R}_2), \tag{28}$$

or

$$\boldsymbol{D}^{(l)}(\hat{R}_1\hat{R}_2) = \boldsymbol{D}^{(l)}(\hat{R}_1)\boldsymbol{D}^{(l)}(\hat{R}_2). \tag{29}$$

3b. Show that rotation over $\phi = 0$ is represented by the $(2l+1)\times(2l+1)$ identity matrix:

$$\boldsymbol{D}^{(l)}(\boldsymbol{n}, 0) = \boldsymbol{I}_{(2l+1)\times(2l+1)}. \tag{30}$$

Answer: *Since* $e^0 = 1$ *we have*

$$D^{(l)}_{m'm}(\boldsymbol{n}, 0) = \langle lm'|e^0|lm\rangle = \langle lm'|lm\rangle = \delta_{m'm}. \tag{31}$$

3c. Use the representation property to show that

$$\boldsymbol{D}^{(l)}(\hat{R}^\dagger) = \boldsymbol{D}^{(l)}(\hat{R})^\dagger. \tag{32}$$

Answer: *According to the representation property of D-matrices we have*

$$\hat{R}|lm\rangle = \sum_{m'} |lm'\rangle D^{(l)}_{m'm}(\hat{R}). \tag{33}$$

Taking the Hermitian conjugate gives

$$\langle lm|\hat{R}^\dagger = \sum_{m'} D^{(l)}_{m'm}(\hat{R})^* \langle lm'| \tag{34}$$

Taking the scalar product with $|lm'\rangle$ *give*

$$\langle lm|\hat{R}^\dagger|lm'\rangle = D^{(l)}_{m'm}(\hat{R})^*, \tag{35}$$

so

$$D^{(l)}_{mm'}(\hat{R}^\dagger) = D^{(l)}_{m'm}(\hat{R})^* = \left[\boldsymbol{D}^{(l)}(\hat{R})^\dagger\right]_{m'm}. \tag{36}$$

Question 4: Euler angles

A rotation may be expressed in zyz Euler angles by

$$\hat{R}(\alpha,\beta,\gamma) = \hat{R}(\boldsymbol{e}_z,\alpha)\hat{R}(\boldsymbol{e}_y,\beta)\hat{R}(\boldsymbol{e}_z,\gamma). \tag{37}$$

4a. Show that

$$D^{(l)}_{m,k}(\alpha,\beta,\gamma) \equiv \langle lm|\hat{R}(\alpha,\beta,\gamma)|lk\rangle = e^{-im\alpha}d^{(l)}_{m,k}(\beta)e^{-ik\gamma} \tag{38}$$

with

$$\boldsymbol{d}^{(l)}(\beta) \equiv \boldsymbol{D}^{(l)}(\boldsymbol{e}_y,\beta). \tag{39}$$

Note: the matrix $\boldsymbol{d}^{(l)}(\beta)$ is real.

Answer: *For the* γ *dependent factor:*

$$\hat{R}(\boldsymbol{e}_z,\gamma)|lk\rangle = e^{-\frac{i}{\hbar}\gamma\boldsymbol{e}_z\cdot\hat{\boldsymbol{l}}}|lk\rangle = e^{-\frac{i}{\hbar}\gamma\hat{l}_z}|lk\rangle = e^{-\frac{i}{\hbar}\gamma\hbar k}|lk\rangle = |lk\rangle e^{-ik\gamma}. \tag{40}$$

For the α *dependent factor:*

$$\left[e^{i\alpha\hat{l}_z}|lm\rangle\right]^\dagger = \left[e^{i\alpha m}|lm\rangle\right]^\dagger \tag{41}$$

so

$$\langle lm|e^{-i\alpha\hat{l}_z} = \langle lm|e^{-im\alpha}. \tag{42}$$

Question 5: Spherical harmonic addition theorem

Two normalized vectors $\hat{\boldsymbol{r}}$ and $\hat{\boldsymbol{k}}$ are defined by rotations of $\boldsymbol{e}_z$,

$$\hat{\boldsymbol{r}} = \boldsymbol{R}_1\boldsymbol{e}_z, \tag{43}$$

$$\hat{\boldsymbol{k}} = \boldsymbol{R}_2\boldsymbol{e}_z. \tag{44}$$

The angle between $\hat{\boldsymbol{r}}$ and $\hat{\boldsymbol{k}}$ is θ,

$$\hat{\boldsymbol{r}}\cdot\hat{\boldsymbol{k}} = \cos\theta. \tag{45}$$

The scalar product can be written as

$$\hat{\boldsymbol{r}}\cdot\hat{\boldsymbol{k}} = (\boldsymbol{R}_1\boldsymbol{e}_z)\cdot(\boldsymbol{R}_2\boldsymbol{e}_z) = \boldsymbol{e}_z\cdot\boldsymbol{R}_1^\dagger\boldsymbol{R}_2\boldsymbol{e}_z. \tag{46}$$

The rotation $\boldsymbol{R}_1^\dagger\boldsymbol{R}_2$ can be expressed in zyz Euler angles (α,β,γ)

$$\boldsymbol{R}_1^\dagger\boldsymbol{R}_2 = \boldsymbol{R}(\alpha,\beta,\gamma) = \boldsymbol{R}(\boldsymbol{e}_z,\alpha)\boldsymbol{R}(\boldsymbol{e}_y,\beta)\boldsymbol{R}(\boldsymbol{e}_z,\gamma) \tag{47}$$

5a. Show that

$$\boldsymbol{e}_z\cdot\boldsymbol{R}(\alpha,\beta,\gamma)\boldsymbol{e}_z = \cos\beta \tag{48}$$

Answer: *First note that* $\boldsymbol{e}_z$ *is invariant under rotations around* $\boldsymbol{e}_z$

$$\boldsymbol{R}(\boldsymbol{e}_z,\gamma)\boldsymbol{e}_z = \boldsymbol{e}_z \tag{49}$$

so

$$\boldsymbol{e}_z \cdot \boldsymbol{R}(\alpha,\beta,\gamma)\boldsymbol{e}_z = \boldsymbol{e}_z \cdot \boldsymbol{R}(\boldsymbol{e}_y,\beta)\boldsymbol{e}_z \tag{50}$$

and

$$\boldsymbol{R}(\boldsymbol{e}_y,\beta)\begin{pmatrix}0\\0\\1\end{pmatrix} = \begin{pmatrix}\sin\beta\\0\\\cos\beta\end{pmatrix}, \tag{51}$$

i.e., the z *component is* $\cos\beta$.

5b. Show that $\cos\beta = \cos\theta$.

Answer: *From the definitions we have*

$$\cos\theta = \hat{\boldsymbol{r}}\cdot\hat{\boldsymbol{k}} = \boldsymbol{e}_z\cdot\boldsymbol{R}_1^\dagger\boldsymbol{R}_2\boldsymbol{e}_z = \boldsymbol{e}_z\cdot\boldsymbol{R}(\alpha,\beta,\gamma)\boldsymbol{e}_z = \cos\beta. \tag{52}$$

We now have established that

$$P_l(\cos\theta) \equiv d^{(l)}_{0,0}(\theta) = \boldsymbol{D}^{(l)}_{0,0}(\boldsymbol{R}_1^\dagger\boldsymbol{R}_2). \tag{53}$$

Spherical harmonics Y_{lm}, Racah normalized spherical harmonics C_{lm}, and Legendre polynomials P_l may be expressed as special cases of Wigner rotations matrices by

$$C_{lm}(\theta,\phi) \equiv D^{(l)}_{m,0}(\phi,\theta,0)^* \tag{54}$$
$$P_l(\cos\theta) \equiv C_{l,0}(\theta,0) \tag{55}$$
$$Y_{lm}(\theta,\phi) \equiv \sqrt{\frac{2l+1}{4\pi}}C_{lm}(\theta,\phi). \tag{56}$$

5c. Derive the spherical harmonics addition theorem

$$P_l(\cos\theta) = \frac{4\pi}{2l+1}\sum_{m=-1}^{l} Y_{lm}(\hat{\boldsymbol{r}})Y_{lm}(\hat{\boldsymbol{k}})^*. \tag{57}$$

Answer: *The representation property of D-matrices (22) and the result of (32) give*

$$\boldsymbol{D}^{(l)}(\boldsymbol{R}_1^\dagger\boldsymbol{R}_2) = \boldsymbol{D}^{(l)}(\boldsymbol{R}_1^\dagger)\boldsymbol{D}^{(l)}(\boldsymbol{R}_2) = \boldsymbol{D}^{(l)}(\boldsymbol{R})^\dagger\boldsymbol{D}^{(l)}(\boldsymbol{R}_2). \tag{58}$$

The $(0,0)$ *component:*

$$D^{(l)}_{0,0}(\boldsymbol{R}_1^\dagger\boldsymbol{R}_2) = \sum_{m=-l}^{l}\left[D^{(l)}(\boldsymbol{R}_1)^\dagger\right]_{0,m} D^{(l)}_{m,0}(\boldsymbol{R}_2) = \sum_{m=-l}^{l} D^{(l)}_{m,0}(\boldsymbol{R}_1)^* D^{(l)}_{m,0}(\boldsymbol{R}_2), \tag{59}$$

so

$$P_l(\cos\theta) = \sum_{m=-l}^{l} C_{lm}(\hat{r})C_{lm}(\hat{k})^* = \frac{4\pi}{2l+1}\sum_{m=-1}^{l} Y_{lm}(\hat{\boldsymbol{r}})Y_{lm}(\hat{\boldsymbol{k}})^*. \tag{60}$$