Quantum Mechanics

Problem Sheet 4

Transformations & Orbital Angular Momentum

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Transformations

4.1 Reflection symmetry around a point $\mathbf{x}_0$

Let $|\mathbf{x}_0 + \mathbf{x}\rangle$ be a position eigenstate that yields $\mathbf{x}_0 + \mathbf{x}$ upon measurement of position. On physical grounds, reflecting the eigenstate about the point $\mathbf{x}_0$ should yield the eigenstate $|\mathbf{x}_0 - \mathbf{x}\rangle$:

$$\hat{P}_{\mathbf{x}_0} |\mathbf{x}_0 + \mathbf{x}\rangle = |\mathbf{x}_0 - \mathbf{x}\rangle \tag{1}$$

With this, consider the effect of $\hat{P}_{\mathbf{x}_0}\hat{x}\hat{P}_{\mathbf{x}_0}$ on a position eigenstate:

$$\begin{aligned} \hat{P}_{\mathbf{x}_0}\hat{x}\hat{P}_{\mathbf{x}_0} |\mathbf{x}_0 + \mathbf{x}\rangle &= \hat{P}_{\mathbf{x}_0}\hat{x} |\mathbf{x}_0 - \mathbf{x}\rangle \\ &= (\mathbf{x}_0 - \mathbf{x})\hat{P}_{\mathbf{x}_0} |\mathbf{x}_0 - \mathbf{x}\rangle \\ &= (\mathbf{x}_0 - \mathbf{x}) |\mathbf{x}_0 + \mathbf{x}\rangle \\ &= (2\mathbf{x}_0 - \mathbf{x}_0 - \mathbf{x}) |\mathbf{x}_0 + \mathbf{x}\rangle \\ &= (2\mathbf{x}_0\mathbb{I} - \hat{x}) |\mathbf{x}_0 + \mathbf{x}\rangle \end{aligned} \tag{2}$$

Further consider $\hat{P}_{\mathbf{x}_0}\hat{p}\hat{P}_{\mathbf{x}_0}$. Apparently $\hat{p}$ anticommutes with $\hat{P}_{\mathbf{x}_0}$ so that $\hat{p}\hat{P}_{\mathbf{x}_0} = -\hat{P}_{\mathbf{x}_0}\hat{p}$. Thus:

$$\begin{aligned} \hat{P}_{\mathbf{x}_0}\hat{p}\hat{P}_{\mathbf{x}_0} &= -\hat{P}_{\mathbf{x}_0}\hat{P}_{\mathbf{x}_0}\hat{p} \\ &= -\hat{p} \end{aligned} \tag{3}$$

since two successive reflections about the same point is equivalent to no reflection at all.

Consider the position wave function after the reflection:

$$\begin{aligned} \psi'(\mathbf{x}) &\equiv \langle \hat{x}|\hat{P}_{\mathbf{x}_0}|\psi\rangle \\ &= \int \langle \hat{x}|\hat{P}_{\mathbf{x}_0}|\mathbf{x}_0 + \mathbf{x}'\rangle \langle \mathbf{x}_0 + \mathbf{x}'|\psi\rangle \, \mathrm{d}^3x' \\ &= \int \langle \hat{x}|\mathbf{x}_0 - \mathbf{x}'\rangle \, \psi(\mathbf{x}_0 + \mathbf{x}') \, \mathrm{d}^3x' \\ &= \int (\mathbf{x}_0 - \mathbf{x}')\psi(\mathbf{x}_0 + \mathbf{x}') \, \mathrm{d}^3x' \end{aligned} \tag{4}$$

Consider the change of variable $\mathbf{x}' \to \mathbf{x}_0 - \mathbf{x}'$:

$$\psi'(\mathbf{x}) = \int \mathbf{x}'\psi(2\mathbf{x}_0 - \mathbf{x}') \, \mathrm{d}^3x' = \psi(2\mathbf{x}_0 - \mathbf{x}) \tag{5}$$

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4.2

For translation invariance, $\hat{H}$ must commute with $\hat{p}$. Since $\hat{x}$ and $\hat{p}$ generally do not commute, the only form $V(\hat{x})$ can take is a constant.

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4.3

We define the orbital angular momentum operator $\hat{L}_i$ as:

$$\hat{L}_i \equiv \epsilon_{ijk}\hat{x}_j\hat{p}_k \tag{6}$$

Its Hermitian conjugate is:

$$\hat{L}_i^\dagger = \epsilon_{ijk}\hat{p}_k^\dagger\hat{x}_j^\dagger = \epsilon_{ijk}\hat{p}_k\hat{x}_j \tag{7}$$

On the other hand, from the canonical commutation relation:

$$[\hat{x}_j, \hat{p}_k] = i\hbar\delta_{jk}\mathbb{I} \tag{8}$$

which implies that $\hat{x}_j$ and $\hat{p}_k$ commute if $j \neq k$.

Therefore:

$$\hat{L}_i^\dagger = \epsilon_{ijk}\hat{p}_k\hat{x}_j = \epsilon_{ijk}\hat{x}_j\hat{p}_k = \hat{L}_i \tag{9}$$

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4.4

For a central potential, we write the Hamiltonian as:

$$\hat{H} = \frac{\hat{p}^2}{2m} + V(\hat{r}^2) \tag{10}$$

where we define the radial position operator $\hat{r}^2$ as:

$$\hat{r}^2 \equiv \hat{x}_1^2 + \hat{x}_2^2 + \hat{x}_3^2 \tag{11}$$

Let us write the potential as an expansion in terms of $\hat{r}^2$:

$$V(\hat{r}^2) = \sum_{n=0}^{\infty} a_n \hat{r}^{2n} \tag{12}$$

Consider the commutator $[\hat{H}, \hat{L}_i]$:

$$\begin{aligned}
[\hat{H}, \hat{L}_i] &= \frac{1}{2m}[\hat{p}^2, \hat{L}_i] + \sum_{n=0}^{\infty} a_n [\hat{r}^{2n}, \hat{L}_i] \\
&= \frac{1}{2m} \sum_{j=1,2,3} [\hat{p}_j^2, \hat{L}_i] + \sum_{n=0}^{\infty} a_n \sum_{j=1,2,3} [\hat{x}_j^{2n}, \hat{L}_i] \\
&= \frac{1}{2m} \epsilon_{ikl} \sum_{j=1,2,3} [\hat{p}_j^2, \hat{x}_k \hat{p}_l] + \sum_{n=0}^{\infty} a_n \epsilon_{ikl} \sum_{j=1,2,3} [\hat{x}_j^{2n}, \hat{x}_k \hat{p}_l]
\end{aligned} \tag{13}$$

Let us consider the commutators separately. Note the following commutation relations:

$$\begin{aligned}
[AB, C] &= A[B, C] + [A, C]B \\
[A, BC] &= [A, B]C + B[A, C]
\end{aligned} \tag{14}$$

For $[\hat{p}_j^2, \hat{x}_k \hat{p}_l]$:

$$\begin{aligned}
[\hat{p}_j^2, \hat{x}_k \hat{p}_l] &= \hat{p}_j [\hat{p}_j, \hat{x}_k \hat{p}_l] + [\hat{p}_j, \hat{x}_k \hat{p}_l] \hat{p}_j \\
&= \hat{p}_j [\hat{p}_j, \hat{x}_k] \hat{p}_l + \hat{p}_j \hat{x}_k [\hat{p}_j, \hat{p}_l] + [\hat{p}_j, \hat{x}_k] \hat{p}_l \hat{p}_j + \hat{x}_k [\hat{p}_j, \hat{p}_l] \hat{p}_j \\
&= \hat{p}_j [\hat{p}_j, \hat{x}_k] \hat{p}_l + [\hat{p}_j, \hat{x}_k] \hat{p}_l \hat{p}_j
\end{aligned} \tag{15}$$

where we have used the fact that $\hat{p}_j$ and $\hat{p}_l$ commute.

This commutator is nonzero only when $k = j$, in which case:

$$[\hat{p}_j^2, \hat{x}_k \hat{p}_l] = -2i\hbar \hat{p}_j \hat{p}_l \tag{16}$$

Then the first term in the commutator $[\hat{H}, \hat{L}_i]$ becomes:

$$\frac{1}{2m} \epsilon_{ijl} \sum_{j=1,2,3} (-2i\hbar \hat{p}_j \hat{p}_l) = \frac{1}{im} \epsilon_{ijl} \hat{p}_j \hat{p}_l \tag{17}$$

This is zero since $\hat{p}_j$ and $\hat{p}_l$ commute. We then consider the second commutator $[\hat{x}_j^{2n}, \hat{x}_k \hat{p}_l]$:

$$[\hat{x}_j^{2n}, \hat{x}_k\hat{p}_l] = [\hat{x}_j^{2n}, \hat{x}_k]\hat{p}_l + \hat{x}_k[\hat{x}_j^{2n}, \hat{p}_l] \tag{18}$$

where the first term is always zero since $\hat{x}_j^{2n}$ and $\hat{x}_k$ commute and the second term is nonzero only when $l = j$, in which case:

$$\begin{aligned}
[\hat{x}_j^{2n}, \hat{p}_l] &= \hat{x}_k[\hat{x}_j^{2n}, \hat{p}_j] \\
&= \hat{x}_k\left\{\hat{x}_j^{2n-1}[\hat{x}_j, \hat{p}_j] + [\hat{x}_j^{2n-1}, \hat{p}_j]\hat{x}_j\right\} \\
&= \hat{x}_k\left\{\hat{x}_j^{2n-1}[\hat{x}_j, \hat{p}_j] + x_j^{2n-2}[\hat{x}_j, \hat{p}_j]\hat{x}_j + \cdots + [\hat{x}_j, \hat{p}_j]\hat{x}_j^{2n-1}\right\} \\
&= i\hbar(2n)\hat{x}_k\hat{x}_j^{2n-1}
\end{aligned} \tag{19}$$

Therefore the second term in the commutator $[\hat{H}, \hat{L}_i]$ becomes:

$$\sum_{n=0}^{\infty} a_n\epsilon_{ikj}\sum_{j=1,2,3} i\hbar(2n)\hat{x}_k\hat{x}_j^{2n-1} \tag{20}$$

which is always zero since $\hat{x}_k$ and $\hat{x}_j^{2n-1}$ commute.

Therefore $[\hat{H}, \hat{L}_i] = 0$ for a central potential and the angular momentum is conserved.

Furthermore, consider a potential that has azimuthal symmetry, i.e. $V(\mathbf{x}) = V(\hat{x}_1^2 + \hat{x}_2^2)$. In this case, we can write the potential as:

$$V = \sum_{n=0}^{\infty} a_n(\hat{x}_1^2 + \hat{x}_2^2)^n \tag{21}$$

The change from previous results occurs on the second term, where we only let j run over 1 and 2. Due to the presence of the ϵ_{ikj} term, the sum is zero only for $i = 3$, since for the other two cases we will miss one term in the sum due to $j = 3$ missing. Therefore, the Hamiltonian only commutes with $\hat{L}_3$, which is the z-component of the angular momentum. The x- and y-components of the angular momentum are not conserved.

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4.5

Let us expand the expression using binomial theorem:

$$
\begin{aligned}
\lim_{N\to\infty}\left(1+\frac{x}{N}\right)^N &= \lim_{N\to\infty}\sum_{n=0}^{N}\binom{N}{n}\left(\frac{x}{N}\right)^n \\
&= \lim_{N\to\infty}\sum_{n=0}^{N}\frac{N!}{n!(N-n)!}\frac{1}{N^n}x^n \\
&= \lim_{N\to\infty}\sum_{n=0}^{N}\frac{N(N-1)(N-2)\cdots(N-n+1)}{N^n}\frac{1}{n!}x^n \\
&= \lim_{N\to\infty}\sum_{n=0}^{N}\frac{1}{n!}x^n \\
&= e^x
\end{aligned}
\tag{22}
$$

where at the last step we have used the fact that the sum is the Taylor series of e^x.

This can in some way be viewed as a definition of e^x. Indeed, the definition of exponential for an operator is just this limit:

$$
\exp\left(\hat{A}\right) \equiv \lim_{N\to\infty}\left(1+\frac{\hat{A}}{N}\right)^N = \left(1+\frac{\hat{A}}{N}\right)\left(1+\frac{\hat{A}}{N}\right)\cdots\left(1+\frac{\hat{A}}{N}\right)
\tag{23}
$$

which can be viewed as applying the operator $(1+\hat{A}/N)$ to the state N times.

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4.6 Heisenberg equations of motion for the SHO

Orbital Angular Momentum

4.7

(a)

$$\begin{aligned}
[\hat{L}_i, \hat{x}_j] &= \epsilon_{ikl}[\hat{x}_k\hat{p}_l, \hat{x}_j] \\
&= \epsilon_{ikl}\hat{x}_k[\hat{p}_l, \hat{x}_j] + \epsilon_{ikl}[\hat{x}_k, \hat{x}_j]\hat{p}_l \\
&= -i\hbar\epsilon_{ikl}\hat{x}_k \\
&= i\hbar\epsilon_{ijk}\hat{x}_k
\end{aligned} \tag{24}$$

$$\begin{aligned}
[\hat{L}_i, \hat{p}_j] &= \epsilon_{ikl}[\hat{x}_k\hat{p}_l, \hat{p}_j] \\
&= \epsilon_{ikl}\hat{x}_k[\hat{p}_l, \hat{p}_j] + \epsilon_{ikl}[\hat{x}_k, \hat{p}_j]\hat{p}_l \\
&= i\hbar\epsilon_{ijl}\hat{p}_l \\
&= i\hbar\epsilon_{ijk}\hat{p}_k
\end{aligned} \tag{25}$$

(b)

$$\begin{aligned}
[\hat{L}_x, \hat{L}_y] &= [\hat{L}_x, \hat{z}\hat{p}_x - \hat{x}\hat{p}_z] \\
&= [\hat{L}_x, \hat{z}\hat{p}_x] - [\hat{L}_x, \hat{x}\hat{p}_z] \\
&= [\hat{L}_x, \hat{z}]\hat{p}_x + \hat{z}[\hat{L}_x, \hat{p}_x] - [\hat{L}_x, \hat{x}]\hat{p}_z - \hat{x}[\hat{L}_x, \hat{p}_z] \\
&= i\hbar(\hat{x}\hat{p}_y - \hat{y}\hat{p}_x) \\
&= i\hbar\hat{L}_z
\end{aligned} \tag{26}$$

which can be generalised to:

$$[\hat{L}_i, \hat{L}_j] = i\hbar\epsilon_{ijk}\hat{L}_k \tag{27}$$

(c) In position representation, the angular momentum operator have the form:

$$\begin{aligned}
\langle \mathbf{x}|\hat{L}_i|\psi\rangle &= \epsilon_{ijk}\langle \mathbf{x}|\hat{x}_j\hat{p}_k|\psi\rangle \\
&= \epsilon_{ijk}x_j\langle \mathbf{x}|\hat{p}_k|\psi\rangle \\
&= -i\hbar\epsilon_{ijk}x_j\frac{\partial}{\partial x_k}\psi(\mathbf{x})
\end{aligned} \tag{28}$$

(d) Consider the commutator $[\hat{L}_i, \hat{L}^2]$:

$$
\begin{aligned}
[\hat{L}_i, \hat{L}^2] &= \sum_{r=1,2,3} [\hat{L}_i, \hat{L}_r^2] \\
&= \sum_{r=1,2,3} \left([\hat{L}_i, \hat{L}_r]\hat{L}_r + \hat{L}_r[\hat{L}_i, \hat{L}_r]\right) \\
&= i\hbar\epsilon_{jir}(\hat{L}_j\hat{L}_r + \hat{L}_r\hat{L}_j) \\
&= 0
\end{aligned}
\tag{29}
$$

•

4.8

We have the expression of $\hat{L}^2$ in spherical coordinates:

$$
\hat{L}^2 = -\hbar^2 \left[\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right] \tag{30}
$$

(a) The following calculations follow:

$$
\begin{aligned}
\hat{L}^2(\cos\theta) &= -\hbar^2\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(-\sin^2\theta\right) \\
&= 2\hbar^2\cos\theta \\
\hat{L}^2\left(\sin\theta e^{\pm i\phi}\right) &= -\hbar^2\left[\frac{e^{\pm i\phi}}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\sin\theta\right) + \frac{1}{\sin\theta}\frac{\partial}{\partial\phi}\left(\frac{\partial}{\partial\phi}e^{\pm i\phi}\right)\right] \\
&= -\hbar^2\left[\frac{e^{\pm i\phi}}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\cos\theta\right) + \frac{1}{\sin\theta}\frac{\partial}{\partial\phi}\left(\pm ie^{\pm i\phi}\right)\right] \\
&= -\hbar^2\left[\frac{e^{\pm i\phi}}{\sin\theta}\left(\cos^2\theta - \sin^2\theta\right) - \frac{1}{\sin\theta}e^{\pm i\phi}\right] \\
&= 2\hbar^2 e^{\pm i\phi}
\end{aligned}
\tag{31}
$$

$$
\begin{aligned}
\hat{L}_z(\cos\theta) &= -i\cos\theta \\
\hat{L}_z\left(\sin\theta e^{\pm i\phi}\right) &= \mp i\sin\theta e^{\pm i\phi}
\end{aligned}
\tag{32}
$$

(b) For Y_1^0, the normalisation condition is:

$$
|N|^2\int_0^{2\pi}\int_0^{\pi}\cos^2\theta\sin\theta\,\mathrm{d}\theta\,\mathrm{d}\phi = 1 \tag{33}
$$

which gives $N = \pm\sqrt{3/4\pi}$.

For $Y_1^{\pm 1}$, the normalisation condition is:

$$|N|^2 \int_0^{2\pi} \int_0^{\pi} \sin^2\theta \sin\theta \,\mathrm{d}\theta \,\mathrm{d}\phi = 1 \tag{34}$$

which gives $N = \pm\sqrt{3/8\pi}$.

(c) In Cartesian coordinates, the above spherical harmonics are:

$$\begin{aligned} Y_1^0 &= \sqrt{\frac{3}{4\pi}} \frac{z}{\sqrt{x^2+y^2+z^2}} \\ Y_1^{\pm 1} &= \mp\sqrt{\frac{3}{8\pi}} \frac{\sqrt{x^2+y^2}}{\sqrt{x^2+y^2+z^2}} \exp\left[\pm i \tan^{-1}\left(\frac{y}{x}\right)\right] \end{aligned} \tag{35}$$

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4.9

The wave function cna be identified as:

$$\langle\theta,\phi|\psi\rangle \propto \sqrt{2}\sqrt{\frac{4\pi}{3}} Y_1^0 + \sqrt{\frac{8\pi}{3}} Y_1^1 + \sqrt{\frac{8\pi}{3}} Y_1^{-1} \tag{36}$$

so that $\hat{L}^2$ always yields $2\hbar^2$ and $\hat{L}_z$ yields zero with probability 1/3 and $\pm\hbar$ with probability 1/3.

The expectation of $\hat{L}_z$ is zero.

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4.10

We recognise $\sin^2\theta e^{2i\phi}$ as Y_2^2 up to a constant factor. Therefore, $\hat{L}^2$ yields $6\hbar^2$ and $\hat{L}_z$ yields $2\hbar$ each with probability 1.

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4.11

Consider the the wave function $\langle\theta,\phi|\psi\rangle = A\sin^2\theta$:

$$
\begin{aligned}
\langle\theta,\phi|\psi\rangle &= A\sin^2\theta \\
&= A(1-\cos^2\theta) \\
&= A\left(1-\frac{\sqrt{16\pi/5}Y_2^0+1}{3}\right) \\
&= A\left(-\sqrt{\frac{16\pi}{45}}Y_2^0+\frac{2}{3}\right) \\
&= A\left(-\sqrt{\frac{16\pi}{45}}Y_2^0+\frac{2\sqrt{4\pi}}{3}Y_0^0\right)
\end{aligned}
\tag{37}
$$

where we have made use of the following spherical harmonics:

$$
\begin{aligned}
Y_2^0 &= \sqrt{\frac{5}{16\pi}}(3\cos^2\theta-1) \\
Y_0^0 &= \frac{1}{\sqrt{4\pi}}
\end{aligned}
\tag{38}
$$

Therefore, measurement with $\hat{L}_z$ always yields 0 and measurement with $\hat{L}^2$ yields $6\hbar^2$ with probability 1.

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4.12

(a) The term $-e\varepsilon\hat{x}$ in the Hamiltonian suggests some kind of position dependent (linear) potential. In light of the charge factor, this can be interpreted as the potential due to a uniform electric field of strength ε in the x-direction.

(b) The Hamiltonian of the form:

$$
\hat{H} = -\frac{\hbar^2}{2m}\nabla^2 - \frac{e^2}{4\pi\epsilon_0 r} - e\varepsilon\hat{x}
\tag{39}
$$

is spherically symmetrical if $\varepsilon = 0$ and symmetrical only about the x-axis if $\varepsilon \neq 0$.

Therefore, in the case of $\varepsilon = 0$, $\hat{L}^2$ and $\hat{L}_i$ are conserved. In the case of $\varepsilon \neq 0$, only $\hat{L}_x$ is conserved.

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4.13

$$
\begin{aligned}
[\hat{L}_i, \hat{x} \cdot \hat{p}] &= \sum_{r=1,2,3} [\hat{L}_i, \hat{x}_r \hat{p}_r] \\
&= \sum_{r=1,2,3} \Big([\hat{L}_i, \hat{x}_r]\hat{p}_r + \hat{x}_r [\hat{L}_i, \hat{p}_r] \Big) \\
&= i\hbar \sum_{r=1,2,3} \left(\epsilon_{irl} \hat{x}_l \hat{p}_r + \epsilon_{irl} \hat{x}_r \hat{p}_l \right) \\
&= 0
\end{aligned} \tag{40}
$$

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