CSE 389D: Mathematical Modeling **Spring 2025**

Problem Set 3

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Problem 3.1

Part a

Recall that the angular momentum operator of a particle is given by

$$\hat{L} = \hat{r} \times \hat{p} = (\hat{r}_y\hat{p}_z - \hat{r}_z\hat{p}_y)u_x + (\hat{r}_z\hat{p}_x - \hat{r}_x\hat{p}_z)u_y + (\hat{r}_x\hat{p}_y - \hat{r}_y\hat{p}_x)u_z$$

then we have that

$$\begin{aligned}
[\hat{L}_x, \hat{L}_y] &= [\hat{r}_y\hat{p}_z - \hat{r}_z\hat{p}_y, \hat{r}_z\hat{p}_x - \hat{r}_x\hat{p}_z] \\
&= [\hat{r}_y\hat{p}_z, \hat{r}_z\hat{p}_x] - [\hat{r}_y\hat{p}_z, \hat{r}_x\hat{p}_z] - [\hat{r}_z\hat{p}_y, \hat{r}_z\hat{p}_x] + [\hat{r}_z\hat{p}_y, \hat{r}_x\hat{p}_z] \\
&= [\hat{r}_y\hat{p}_z, \hat{r}_z]\hat{p}_x + \hat{r}_z[\hat{r}_y\hat{p}_z, \hat{p}_x] - [\hat{r}_y\hat{p}_z, \hat{r}_x]\hat{p}_z \\
&\quad - \hat{r}_x[\hat{r}_y\hat{p}_z, \hat{p}_z] - [\hat{r}_z\hat{p}_y, \hat{r}_z]\hat{p}_x - \hat{r}_z[\hat{r}_z\hat{p}_y, \hat{p}_x] + [\hat{r}_z\hat{p}_y, \hat{r}_x]\hat{p}_z + \hat{r}_x[\hat{r}_z\hat{p}_y, \hat{p}_z]
\end{aligned}$$

then we see that

$$\begin{aligned}
[\hat{r}_y\hat{p}_z, \hat{r}_z] &= \hat{r}_y[\hat{p}_z, \hat{r}_z] + [\hat{r}_y, \hat{r}_z]\hat{p}_z = -i\hbar\hat{r}_y \\
[\hat{r}_y\hat{p}_z, \hat{p}_x] &= \hat{r}_y[\hat{p}_z, \hat{p}_x] + [r_y, \hat{p}_x]\hat{p}_y = 0 \\
[\hat{r}_y\hat{p}_z, \hat{r}_x] &= 0 \\
[\hat{r}_y\hat{p}_z, \hat{p}_z] &= 0 \\
[\hat{r}_z\hat{p}_y, \hat{r}_z] &= 0 \\
[\hat{r}_z\hat{p}_y, \hat{p}_x] &= 0 \\
[\hat{r}_z\hat{p}_y, \hat{r}_x] &= 0 \\
[\hat{r}_z\hat{p}_y, \hat{p}_z] &= i\hbar\hat{p}_y
\end{aligned}$$

and hence

$$[\hat{L}_x, \hat{L}_y] = -i\hbar\hat{r}_y\hat{p}_x + i\hbar\hat{r}_x\hat{p}_y = i\hbar\hat{L}_z$$

as desired.

Part b

We have that

$$\begin{aligned}
[\hat{L}_z, \hat{L}^2] &= [\hat{L}_z, \hat{L}_x^2 + \hat{L}_y^2 + \hat{L}_z^2] = [\hat{L}_z, \hat{L}_x^2] + [\hat{L}_z, \hat{L}_y^2] + [\hat{L}_z, \hat{L}_z^2] \\
&= [\hat{L}_z, \hat{L}_x]\hat{L}_x + \hat{L}_x[\hat{L}_z, \hat{L}_x] + [\hat{L}_z, \hat{L}_y]\hat{L}_y + \hat{L}_y[\hat{L}_z, \hat{L}_y] + [\hat{L}_z, \hat{L}_z]\hat{L}_z + \hat{L}_z[\hat{L}_z, \hat{L}_z] \\
&= 2i\hbar\hat{L}_x\hat{L}_y - 2i\hbar\hat{L}_y\hat{L}_x = 0
\end{aligned}$$

Part c

Suppose that $|\epsilon\rangle$ is an eigenstate of $\hat{L}_z$, then we have that

$$\hat{L}_z |\epsilon\rangle = \epsilon |\epsilon\rangle$$

and notice that from part b, we showed that $[\hat{L}_z, \hat{L}^2] = 0$ and hence we have that

$$\hat{L}^2 \hat{L}_z |\epsilon\rangle = \epsilon \hat{L}^2 |\epsilon\rangle = \hat{L}_z \hat{L}^2 |\epsilon\rangle$$

an hence $\hat{L}^2 |\epsilon\rangle = K |\epsilon\rangle$ and hence $|\epsilon\rangle$ is also an eigenstate of $\hat{L}^2$.

Problem 3.2

Part a

Suppose we have the Hamilton operator of a certain quantum system in Dirac's notation

$$\hat{H} = E_0 = \sum_{n=1}^{\infty} n^2 |n\rangle \langle n|$$

then we see that

$$\begin{aligned}
\hat{H} |m\rangle &= E_0 \sum_{n=1}^{\infty} n^2 |n\rangle \langle n| |m\rangle \\
&= E_0 \sum_{n=1}^{\infty} n^2 |n\rangle \delta_{nm} \\
&= E_0 m^2 |m\rangle
\end{aligned}$$

thus $|m\rangle$ is an eigenstate of $\hat{H}$ with eigenvalue $E_0 m^2$, where m is a positive integer.

Part b

We can define a square root operator of $\hat{H}$ as

$$\hat{H}^{1/2} = \sqrt{E_0} \sum_{n=1}^{\infty} n |n\rangle \langle n|$$

since each of the $|n\rangle$ are orthogonal, we have that each of the off-diagonal terms are zero and hence we are left with the diagonal terms and hence get the form above.

Part c

Note that using the form of $\hat{H}^{1/2}$ above, we can see that

$$\hat{H}^{1/2} = \sqrt{E_0} \sum_{n=1}^{\infty} (-1)^{mn} n |n\rangle \langle n|$$

for any choice $m \in \mathbb{Z}$, are also square-root operators of $\hat{H}$, and thus there are infinitely many square-root operators of $\hat{H}$.

Part d

Looking at the eigenvalue spectrum of the Hamiltonian in part a, we see that this system describes a particle in the one-dimensional infinite square well potential

$$V(x) = \begin{cases} -V_0 & |x| < a \\ \infty & |x| > a \end{cases}$$

the square-root operator, $\hat{H}$, is associated with the magnitude of the momentum of the particle.

Problem 3.3

Part a

Suppose that we have the one-dimensional quartic anharmonic oscillator

$$\hat{H} = \frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega^2\hat{x}^2 + \kappa\frac{m^2\omega^3}{\hbar}\hat{x}^4$$

recall that

$$\hat{a} = \sqrt{\frac{m\omega}{2\hbar}}\left(\hat{x} + i\frac{\hat{p}}{m\omega}\right)$$
$$\hat{a}^\dagger = \sqrt{\frac{m\omega}{2\hbar}}\left(\hat{x} - i\frac{\hat{p}}{m\omega}\right)$$

and we compute that

$$\begin{aligned}
\hat{a}^\dagger\hat{a} &= \frac{m\omega}{2\hbar}\left(\hat{x} - i\frac{\hat{p}}{m\omega}\right)\left(\hat{x} + i\frac{\hat{p}}{m\omega}\right) \\
&= \frac{m\omega}{2\hbar}\left(\hat{x}^2 + i\frac{\hat{x}\hat{p}}{m\omega} - i\frac{\hat{p}\hat{x}}{m\omega} + \frac{\hat{p}^2}{m^2\omega^2}\right) \\
&= \frac{m\omega}{2\hbar}\left(\hat{x}^2 + i\frac{[\hat{x},\hat{p}]}{m\omega} + \frac{\hat{p}^2}{m^2\omega^2}\right) \\
&= \frac{m\omega}{2\hbar}\left(\hat{x}^2 - \frac{\hbar}{m\omega} + \frac{\hat{p}^2}{m^2\omega^2}\right) \\
&= -\frac{1}{2} + \frac{m\omega}{2\hbar}\hat{x}^2 + \frac{\hat{p}^2}{2\hbar m\omega}
\end{aligned}$$

and

$$\hat{a} + \hat{a}^\dagger = \sqrt{\frac{m\omega}{2\hbar}}2\hat{x}$$

then we see that

$$\begin{aligned}
\frac{1}{2} + \hat{a}^\dagger \hat{a} + \frac{\kappa}{4}(\hat{a} + \hat{a}^\dagger)^4 &= \frac{1}{2} + \left(-\frac{1}{2} + \frac{m\omega}{2\hbar}\hat{x}^2 + \frac{\hat{p}^2}{2\hbar m\omega}\right) + \frac{\kappa}{4}\left(\frac{4m^2\omega^2}{\hbar^2}\hat{x}^4\right) \\
&= \left(\frac{m\omega}{2\hbar}\hat{x}^2 + \frac{\hat{p}}{2\hbar m\omega} + \frac{\kappa m^2\omega^2}{\hbar^2}\hat{x}^4\right) \\
&= \frac{1}{\hbar\omega}\left(\frac{m\omega^2}{2}\hat{x}^2 + \frac{\hat{p}}{2m} + \kappa\frac{m^2\omega^3}{\hbar}\hat{x}^4\right) \\
&= \frac{\hat{H}}{\hbar\omega}
\end{aligned}$$

Part b

Consider

$$(\hat{a} + \hat{a}^\dagger)^4 = (\hat{a} + \hat{a}^\dagger)^2(\hat{a} + \hat{a}^\dagger)^2$$

Then for

$$\begin{aligned}
(\hat{a} + \hat{a}^\dagger)^2 &= (\hat{a}^2 + \hat{a}\hat{a}^\dagger + \hat{a}^\dagger\hat{a} + \hat{a}^{\dagger^2}) \\
&= (\hat{a}^2 + 1 + 2\hat{a}^\dagger\hat{a} + \hat{a}^{\dagger^2}) \\
&= (\hat{a}^2 + 1 + 2\hat{N} + \hat{a}^{\dagger^2})
\end{aligned}$$

thus

$$(\hat{a} + \hat{a}^\dagger)^4 = (\hat{a}^2 + \hat{a}^{\dagger^2})^2 + (\hat{a}^2 + \hat{a}^{\dagger^2})(1 + 2\hat{N}) + (1 + 2\hat{N})(\hat{a}^2 + \hat{a}^{\dagger^2}) + (1 + 2\hat{N})^2$$

and we have that

$$\begin{aligned}
(\hat{a}^2 + \hat{a}^{\dagger^2}) &= \hat{a}^4 + \hat{a}^2\hat{a}^{\dagger^2} + \hat{a}^{\dagger^2}\hat{a}^2 + \hat{a}^{\dagger^2} \\
(\hat{a}^2 + \hat{a}^{\dagger^2})(1 + 2\hat{N}) &= \hat{a}^2 + 2\hat{a}^2\hat{N} + \hat{a}^{\dagger^2} + 2\hat{a}^{\dagger^2}\hat{N} \\
(1 + 2\hat{N})(\hat{a}^2 + \hat{a}^{\dagger^2}) &= \hat{a}^2 + 2\hat{N}\hat{a}^2 + \hat{a}^{\dagger^2} + 2\hat{N}\hat{a}^{\dagger^2} \\
(1 + 2\hat{N})^2 &= 1 + 4\hat{N} + 4\hat{N}^2
\end{aligned}$$

and hence

$$(\hat{a}+\hat{a}^\dagger)^4 = \hat{a}^4 + \hat{a}^{\dagger^2} + 2(\hat{a}^2 + \hat{a}^{\dagger^2}) + 2\left[\hat{N}(\hat{a}^2 + \hat{a}^{\dagger^2}) + (\hat{a}^2 + \hat{a}^{\dagger^2})\hat{N}\right] + \hat{a}^2\hat{a}^{\dagger^2} + \hat{a}^{\dagger^2}\hat{a}^2 + 4\hat{N} + 4\hat{N}^2 + 1$$

then we have

$$\begin{aligned}
\hat{a}^2\hat{a}^{\dagger^2} &= 2 + 3\hat{N} + \hat{N}^2 \\
\hat{a}^{\dagger^2}\hat{a}^2 &= \hat{N}^2 - \hat{N}
\end{aligned}$$

and so we have that

$$(\hat{a} + \hat{a}^\dagger)^4 = \hat{a}^4 + \hat{a}^{\dagger^4} + 2(\hat{a}^2 + \hat{a}^{\dagger^2}) + 2\left[\hat{N}(\hat{a}^2 + \hat{a}^{\dagger^2}) + (\hat{a}^2 + \hat{a}^{\dagger^2})\hat{N}\right] + 3 + 6\hat{N} + 6\hat{N}^2$$

Part c

Let $\kappa = 0$, and let $|n\rangle$ be an eigenstate of $\hat{H}$, then we have that

$$\hat{a}\,|n\rangle = \sqrt{n}\,|n-1\rangle \implies \hat{a}^2\,|n\rangle = \sqrt{n(n-1)}\,|n-2\rangle$$

and thus

$$\langle n|\,\hat{a}^2\,|n\rangle = \sqrt{n(n-1)}\,\langle n|n-2\rangle = 0$$

since $|n\rangle$ and $|n-2\rangle$ are orthogonal. Now we consider,

$$\hat{a}^\dagger\,|n\rangle = \sqrt{n+1}\,|n+1\rangle \implies \hat{a}^{\dagger^2}\,|n\rangle = \sqrt{(n+1)(n+2)}\,|n+2\rangle$$

then we have that

$$\langle n|\,\hat{a}^{\dagger^2}\,|n\rangle = \sqrt{(n+1)(n+2)}\,\langle n|n+2\rangle = 0$$

since $|n\rangle$ and $|n+2\rangle$ are orthogonal. Lastly we have that

$$\begin{aligned}\langle n|\,\hat{a}^4\,|n\rangle &= \sqrt{n(n-1)(n-2)(n-3)}\,\langle n|n-4\rangle = 0\\ \langle n|\,\hat{a}^{\dagger^4}\,|n\rangle &= \sqrt{(n+1)(n+2)(n+3)(n+4)}\,\langle n|n+4\rangle = 0\end{aligned}$$

Part d

$$\begin{aligned}\langle n|\,\hat{N}\hat{a}^2\,|n\rangle &= \sqrt{n(n-1)}\,\langle n|\,\hat{N}\,|n-2\rangle = (n-2)\sqrt{n(n-1)}\,\langle n|n-2\rangle = 0\\ \langle n|\,\hat{N}\hat{a}^{\dagger^2}\,|n\rangle &= \sqrt{(n+1)(n+2)}\,\langle n|\,\hat{N}\,|n+2\rangle = (n+2)\sqrt{(n+1)(n+2)}\,\langle n|n+2\rangle = 0\\ \langle n|\,\hat{a}^2\hat{N}\,|a\rangle &= n\,\langle n|\,\hat{a}^2\,|n\rangle = n\sqrt{n(n-1)}\,\langle n|n-2\rangle = 0\\ \langle n|\,\hat{a}^{\dagger^2}\hat{N}\,|a\rangle &= n\,\langle n|\,\hat{a}^{\dagger^2}\,|n\rangle = n\sqrt{(n+1)(n+2)}\,\langle n|n+2\rangle = 0\end{aligned}$$

Part e

$$\langle n|\,\hat{H}\,|n\rangle = \hbar\omega\left(\frac{1}{2}\,\langle n|n\rangle + \langle n|\,\hat{N}\,|n\rangle + \frac{\kappa}{4}\,\langle n|\,(\hat{a}+\hat{a}^\dagger)^4\,|n\rangle\right)$$

note that

$$\begin{aligned}\langle n|n\rangle &= 1\\ \langle n|\,\hat{N}\,|n\rangle &= n\,\langle n|n\rangle = n\\ \langle n|\,(\hat{a}+\hat{a}^\dagger)\,|n\rangle &= \langle n|\,\hat{a}^4 + \hat{a}^{\dagger^4} + 2(\hat{a}^2+\hat{a}^{\dagger^2}) + 2\left[\hat{N}(\hat{a}^2+\hat{a}^{\dagger^2}) + (\hat{a}^2+\hat{a}^{\dagger^2})\hat{N}\right] + 3 + 6\hat{N} + 6\hat{N}^2\,|n\rangle\end{aligned}$$

and we have that the above reduces to

$$\langle n|\,(\hat{a}+\hat{a}^\dagger)\,|n\rangle = 3\,\langle n|n\rangle + 6\,\langle n|\,\hat{N}\,|n\rangle + 6\,\langle n|\,\hat{N}^2\,|n\rangle = 3 + 6n + 6n^2$$

and hence

$$\langle n|\,\hat{H}\,|n\rangle = \hbar\omega\left(\frac{1}{2}+n\right) + \frac{\kappa\hbar\omega}{4}\left(2+6n+6n^2\right)$$