CEM 991 **Fall 2023**

Assignment No. 8 (25 pts.) **Due Date: December 8, 2023 (Friday)**

1. (10 pts.) Use the generating function for the Hermite polynomials to evaluate
   (a) [5 pts.] $\langle u_n|\hat{x}^3|u_n\rangle$.
   (b) [5 pts.] $\langle u_n|\hat{x}^4|u_n\rangle$.

   Auxiliary formula: $\int_{-\infty}^{+\infty} x^{2n}e^{-ax^2}dx = \frac{(2n)!}{2^{2n}n!}\sqrt{\frac{\pi}{a^{2n+1}}}$, $a > 0$, $n = 0, 1, 2, \ldots$.

2. (7 pts.) Let $|n\rangle$ be a short-hand, Dirac-style, notation for the n-th eigenstate u_n of the one-dimensional quantum-mechanical harmonic oscillator ($n = 0, 1, \ldots$). Let ω be the angular frequency of the corresponding classical harmonic oscillator and m be its mass. Use the language of second quantization or occupation number representation, i.e., the formulas

$$\hat{x} = \left(\frac{\hbar}{2\omega m}\right)^{\frac{1}{2}} (a + a^\dagger),$$

$$\hat{p} = -i\left(\frac{\hbar\omega m}{2}\right)^{\frac{1}{2}} (a - a^\dagger),$$

$$a|n\rangle = n^{\frac{1}{2}}|n-1\rangle,$$

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

$$N|n\rangle = n|n\rangle,$$

   where $\hat{x}$, $\hat{p}$, a, and $a^\dagger$ are the coordinate, momentum, annihilation, and creation operators, respectively, and $N = a^\dagger a$ is the number operator, to calculate the expectation values of the kinetic and potential energy operators, $\hat{T} = \frac{\hat{p}^2}{2m}$ and $\hat{V} = \frac{1}{2}K\hat{x}^2$, respectively, where $K = m\omega^2$ is the force constant, in the n-th eigenstate $|n\rangle$. Compare the results with the total energy $E_n = \hbar\omega(n + \frac{1}{2})$.

3. (8 pts.) Let us designate the eigenstates of the one-dimensional harmonic oscillator, u_n, as $|n\rangle$, $n = 0, 1, \ldots$. The only non-zero matrix elements of the coordinate and momentum operators, $\hat{x}$ and $\hat{p}$, respectively, in an energy representation defined by the eigenstates $|n\rangle$ are

$$\langle n|\hat{x}|n+1\rangle = (n+1)^{1/2}\left(\frac{\hbar}{2m\omega}\right)^{1/2}, \tag{1}$$

$$\langle n|\hat{x}|n-1\rangle = n^{1/2}\left(\frac{\hbar}{2m\omega}\right)^{1/2}, \tag{2}$$

$$\langle n|\hat{p}|n+1\rangle = -i(n+1)^{1/2}\left(\frac{\hbar m\omega}{2}\right)^{1/2}, \tag{3}$$

$$\langle n|\hat{p}|n-1\rangle = i n^{1/2}\left(\frac{\hbar m\omega}{2}\right)^{1/2}, \tag{4}$$

where m and ω designate the mass and the angular frequency of the classical harmonic oscillator. Use Eqs. (1)–(4) and the resolution of identity involving the eigenstates $|n\rangle$ to calculate matrix elements $\langle 0|\hat{H}|0\rangle$ and $\langle 1|\hat{H}|1\rangle$, where $\hat{H} = \frac{\hat{p}^2}{2m} + \frac{m\omega^2\hat{x}^2}{2}$ is the Hamiltonian of the harmonic oscillator. What should the values of $\langle 0|\hat{H}|0\rangle$ and $\langle 1|\hat{H}|1\rangle$ be? Comment on your findings.

SOLUTIONS

1. (a)

$$\langle u_n | \hat{x}^3 | u_n \rangle =$$

$$= \int_{-\infty}^{\infty} u_n(x)^* x^3 u_n(x)\, dx$$

$$\overset{\xi=\alpha x}{=} \frac{N_n^2}{\alpha^4} \int_{-\infty}^{\infty} H_n(\xi)^2 e^{-\xi^2} \xi^3 \, d\xi$$

$$= \frac{N_n^2}{\alpha^4} I_{nn} \text{, where, in general,}$$

we define I_{nm} as follows:

$$I_{nm} = \int_{-\infty}^{\infty} H_n(\xi) H_m(\xi) e^{-\xi^2} \xi^3 d\xi .$$

Consider,

$$\int_{-\infty}^{\infty} S(\xi,s) S(\xi,t) e^{-\xi^2} \xi^3 d\xi =$$

$$= \sum_{n,m} \frac{s^n t^m}{n!\, m!} I_{nm} .$$

$$\int_{-\infty}^{\infty} S(\xi,s)\, S(\xi,t)\, e^{-\xi^2} \xi^3 d\xi =$$

$$= \int_{-\infty}^{\infty} e^{-s^2+2s\xi} e^{-t^2+2t\xi} e^{-\xi^2} \xi^3 d\xi$$

$$= e^{2st} \int_{-\infty}^{\infty} e^{-(\xi-s-t)^2} \xi^3 d\xi$$

$$\overset{\xi-s-t=z}{\underset{d\xi=dz}{=\!=}} e^{2st} \int_{-\infty}^{\infty} e^{-z^2} (z+s+t)^3 dz$$

$$= e^{2st} \left\{ \int_{-\infty}^{\infty} e^{-z^2} z^3 dz + 3(s+t) \int_{-\infty}^{\infty} e^{-z^2} z^2 dz \right.$$

$$+ 3(s+t)^2 \int_{-\infty}^{\infty} e^{-z^2} z\, dz \quad +$$

$$+ (s+t)^3 \int_{-\infty}^{\infty} e^{-z^2} dz \Big\}$$

$$= e^{2st} \Big\{ 3(s+t)\frac{1}{2}\sqrt{\pi} + (s+t)^3 \sqrt{\pi} \Big\},$$

where we used

$$\int_{-\infty}^{\infty} e^{-z^2} z^3 dz = \int_{-\infty}^{\infty} e^{-z^2} z \, dz = 0,$$

and

$$\int_{-\infty}^{\infty} e^{-z^2} z^2 dz = \frac{1}{2}\sqrt{\pi},$$

$$\int_{-\infty}^{\infty} e^{-z^2} dz = \sqrt{\pi}.$$

We have,

$$\int_{-\infty}^{\infty} S(\xi,s) S(\xi,t) e^{-\xi^2} \xi^3 d\xi =$$

$$= \sqrt{\pi}\, e^{2st} \Big\{ \frac{3}{2}(s+t) + (s+t)^3 \Big\} =$$

$$= \sum_{n,m} \frac{s^n t^m}{n!m!} I_{nm}.$$

Notice that the power series expansion of

$$\sqrt{\pi}\, e^{2st}\left\{\frac{3}{2}(s+t) + (s+t)^3\right\}$$

does not contain $s^n t^n$ terms (it contains $s^{n+1}t^n$, $s^n t^{n+1}$, $s^{n+3}t^n$, $s^n t^{n+3}$ terms).

Thus, $I_{nn} = 0$, so that

$$\langle u_n | \hat{x}^3 | u_n \rangle = 0 .$$

We could obtain this result without any calculation. Do you know why? If you do not, please contact me.

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(b) $\langle u_n | \hat{x}^4 | u_n \rangle =$

$$= \int_{-\infty}^{\infty} u_n(x)\, x^4 u_n(x)\, dx$$

$$= \frac{N_n^2}{\alpha^5} \int_{-\infty}^{\infty} H_n(\xi)^2 e^{-\xi^2} \xi^4 \, d\xi$$

$$= \frac{N_n^2}{\alpha^5} I_{nn}\text{, where, in general,}$$

$$I_{nm} = \int_{-\infty}^{\infty} H_n(\xi) H_m(\xi) e^{-\xi^2} \xi^4 \, d\xi .$$

Consider

$$\int_{-\infty}^{\infty} S(\xi, s)\, S(\xi, t)\, e^{-\xi^2} \xi^4 \, d\xi$$

$$= \sum_{n,m} \frac{s^n t^m}{n!\, m!} I_{nm} .$$

We obtain,

$$\int_{-\infty}^{\infty} S(\xi,s)\, S(\xi,t)\, e^{-\xi^2} \xi^4 d\xi =$$

$$= \int_{-\infty}^{\infty} e^{-s^2+2s\xi} e^{-t^2+2t\xi} e^{-\xi^2} \xi^4 d\xi$$

$$= e^{2st} \int_{-\infty}^{\infty} e^{-(\xi-s-t)^2} \xi^4 d\xi$$

$$\overset{\xi-s-t=z}{\underset{d\xi=dz}{=\!=}} \quad e^{2st} \int_{-\infty}^{\infty} e^{-z^2} (z+s+t)^4 dz$$

$$= e^{2st} \Big\{ \int_{-\infty}^{\infty} e^{-z^2} z^4 dz + 4(s+t) \int_{-\infty}^{\infty} e^{-z^2} z^3 dz$$

$$+ 6(s+t)^2 \int_{-\infty}^{\infty} e^{-z^2} z^2 dz + 4(s+t)^3 \int_{-\infty}^{\infty} e^{-z^2} z\, dz$$

$$+ (s+t)^4 \int_{-\infty}^{\infty} e^{-z^2} dz \Big\}.$$

Now, $\displaystyle\int_{-\infty}^{\infty} e^{-z^2} z^4 dz = \frac{3}{4}\sqrt{\pi}$,

$$\int_{-\infty}^{\infty} e^{-z^2} z^3 dz = \int_{-\infty}^{\infty} e^{-z^2} z\, dz = 0,$$

$$\int_{-\infty}^{\infty} e^{-z^2} z^2 \, dz = \frac{1}{2}\sqrt{\pi},$$

$$\int_{-\infty}^{\infty} e^{-z^2} \, dz = \sqrt{\pi}.$$

Thus,

$$\int_{-\infty}^{\infty} S(\xi, s)\, S(\xi, t)\, e^{-\xi^2} \xi^4 \, d\xi =$$

$$= \sqrt{\pi}\, e^{2st} \left\{ \frac{3}{4} + 3(s+t)^2 + (s+t)^4 \right\}$$

$$= \sqrt{\pi}\, e^{2st} \left\{ \frac{3}{4} + 3s^2 + 3t^2 + 6st \right.$$

$$\left. + \; s^4 + 4s^3 t + 6s^2 t^2 + 4st^3 + t^4 \right\} =$$

$$= \sqrt{\pi} \left\{ \sum_n \frac{3 \cdot 2^n s^n t^n}{4\, n!} + \sum_n \frac{3 \cdot 2^n s^{n+2} t^n}{n!} + \right.$$

$$+ \sum_n \frac{3\cdot 2^n s^n t^{n+2}}{n!} + \sum_n \frac{6\cdot 2^n s^{n+1} t^{n+1}}{n!}$$

$$+ \sum_n \frac{2^n s^{n+4} t^n}{n!} + \sum_n \frac{4\cdot 2^n s^{n+3} t^{n+1}}{n!}$$

$$+ \sum_n \frac{6\cdot 2^n s^{n+2} t^{n+2}}{n!} + \sum_n \frac{4\cdot 2^n s^{n+1} t^{n+3}}{n!}$$

$$+ \sum_n \frac{2^n s^n t^{n+4}}{n!} \Bigg\} =$$

$$= \sum_{n,m} \frac{s^n t^m}{n!\, m!} I_{nm} .$$

At $s^n t^n$, we have:

$$\frac{I_{nn}}{(n!)^2} = \sqrt{\pi} \left\{ \frac{3\cdot 2^n}{4n!} + \frac{6\cdot 2^{n-1}}{(n-1)!} + \right.$$

$$\left. + \frac{6\cdot 2^{n-2}}{(n-2)!} \right\} ,$$ so that

$$I_{nn} = \frac{1}{4} 2^n n! \sqrt{\pi} \left\{ 3 + 12n + 6n(n-1) \right\}$$

$$= \frac{1}{4} 2^n n! \sqrt{\pi} \left[3 + 12n + 6n^2 - 6n \right]$$

$$= \frac{1}{4} 2^n n! \sqrt{\pi} \left[3 + 6n + 6n^2 \right]$$

$$= \frac{3}{4} 2^n n! \sqrt{\pi} \left[1 + 2n + 2n^2 \right].$$

$$\langle u_n | \hat{x}^4 | u_n \rangle = \frac{N_n^2}{\alpha^5} I_{nn} =$$

$$= \frac{\alpha}{\cancel{2^n n! \sqrt{\pi}}} \cdot \frac{1}{\alpha^5} \cdot \frac{3}{4} \cancel{2^n n! \sqrt{\pi}} \times$$

$$\times \left(1 + 2n + 2n^2\right) = \frac{3}{4\alpha^4} \left(1 + 2n + 2n^2\right).$$

$$\rightarrow \langle u_n | \hat{x}^4 | u_n \rangle = \frac{3}{4\alpha^4} \left(1 + 2n + 2n^2\right).$$

2. Let us calculate the expectation value of the kinetic energy operator $\hat{T} = \frac{\hat{p}^2}{2m}$,

$$\langle \hat{T} \rangle_n = \langle n | \hat{T} | n \rangle = \frac{1}{2m} \langle n | \hat{p}^2 | n \rangle.$$

We have

$$\hat{p} = -i \left(\frac{\hbar \omega m}{2} \right)^{\frac{1}{2}} (a - a^\dagger).$$

Thus,

$$\langle \hat{T} \rangle_n = \frac{1}{2\cancel{m}} (-1) \frac{\hbar \omega \cancel{m}}{2} \times$$

$$\times \langle n | (a - a^\dagger)^2 | n \rangle = -\frac{1}{4} \hbar \omega$$

$$\times \langle n | (a - a^\dagger)^2 | n \rangle.$$

Expanding $(a-a^{\dagger})^2$, we obtain

$$\langle \hat{T} \rangle_n = -\frac{1}{4}\hbar\omega \langle n | a^2 - aa^{\dagger} - a^{\dagger}a + (a^{\dagger})^2 | n \rangle.$$

Since $a^2|n\rangle \sim |n-2\rangle$ and $(a^{\dagger})^2|n\rangle \sim |n+2\rangle$ and since eigenstates $|n\rangle$ are orthonormal, we can write

$$\langle \hat{T} \rangle_n = +\frac{1}{4}\hbar\omega \langle n | aa^{\dagger} + a^{\dagger}a | n \rangle.$$

We know that the number operator

$$\hat{N} = a^{\dagger}a$$

and $[a, a^{\dagger}] = 1$, so that

$$aa^{\dagger} + a^{\dagger}a = a^{\dagger}a + 1 + a^{\dagger}a = N + 1 + N$$
$$= 2N + 1.$$

This means that

$$\langle \hat{T} \rangle_n = \frac{1}{4} \hbar\omega \langle n | 2N+1 | n \rangle$$

$$= \frac{1}{4} \hbar\omega \, (2n+1)$$

$$= \frac{1}{2} \hbar\omega \left(n + \frac{1}{2}\right) = \frac{1}{2} E_n ,$$

where we used the fact that

$$N|n\rangle = n|n\rangle .$$

A very similar calculation can be performed for the expectation value of the potential energy operator

$$\hat{V} = \frac{1}{2} k \hat{x}^2 = \frac{1}{2} m\omega^2 \hat{x}^2 ,$$

$$\langle \hat{V} \rangle_n = \langle n | \hat{V} | n \rangle = \frac{1}{2} m\omega^2 \langle n | \hat{x}^2 | n \rangle .$$

We obtain,

$$\langle \hat{V} \rangle_n = \frac{1}{2} \cancel{m} \cdot \omega^{\cancel{2}} \cdot \frac{\hbar}{2 \cancel{\omega} \cancel{m}} \langle n | (a + a^\dagger)^2 | n \rangle,$$

where we used the fact that

$$\hat{x} = \left(\frac{\hbar}{2\omega m} \right)^{\frac{1}{2}} (a + a^\dagger) .$$

We can write,

$$\langle \hat{V} \rangle_n = \frac{1}{4} \hbar\omega \langle n | (a + a^\dagger)^2 | n \rangle$$

$$= \frac{1}{4} \hbar\omega \langle n | a^2 + a a^\dagger + a^\dagger a + (a^\dagger)^2 | n \rangle$$

$$= \frac{1}{4} \hbar\omega \langle n | a a^\dagger + a^\dagger a | n \rangle,$$

since $a^2 |n\rangle \sim |n-2\rangle$, $(a^\dagger)^2 |n\rangle \sim$
$\sim |n+2\rangle$, and

eigenstates $|n\rangle$ are orthonormal.

As in the case of the kinetic energy calculation,

$aa^\dagger + a^\dagger a = 2N+1$, where

$N = a^\dagger a$. Thus, we can write

$$\langle \hat{V} \rangle_n = \frac{1}{4}\hbar\omega \langle n|2N+1|n\rangle$$

$$= \frac{1}{4}\hbar\omega(2n+1)$$

$$= \frac{1}{2}\hbar\omega\left(n+\frac{1}{2}\right) = \frac{1}{2}E_n,$$

where again we used the fact that $N|n\rangle = n|n\rangle$.

In summary,

$$\langle \hat{T} \rangle_n = \langle \hat{V} \rangle_n = \frac{1}{2}\hbar\omega\left(n+\frac{1}{2}\right) = \frac{1}{2}E_n.$$

3. $$\hat{H} = \frac{\hat{p}^2}{2m} + \frac{m\omega^2 \hat{x}^2}{2}.$$

We need to know

$$\langle 0|\hat{H}|0\rangle = \frac{1}{2m}\langle 0|\hat{p}^2|0\rangle + \frac{m\omega^2}{2}\langle 0|\hat{x}^2|0\rangle$$

and

$$\langle 1|\hat{H}|1\rangle = \frac{1}{2m}\langle 1|\hat{p}^2|1\rangle + \frac{m\omega^2}{2}\langle 1|\hat{x}^2|1\rangle.$$

We obtain,

$$\langle 0|\hat{p}^2|0\rangle = \sum_{n=0}^{\infty}\langle 0|\hat{p}|n\rangle\langle n|\hat{p}|0\rangle$$

$$= \langle 0|\hat{p}|1\rangle\langle 1|\hat{p}|0\rangle =$$

$$= -i\left(\frac{\hbar m\omega}{2}\right)^{\frac{1}{2}} i\left(\frac{\hbar m\omega}{2}\right)^{\frac{1}{2}} = \frac{\hbar m\omega}{2},$$

$$\langle 0|\hat{x}^2|0\rangle = \sum_{n=0}^{\infty} \langle 0|\hat{x}|n\rangle\langle n|\hat{x}|0\rangle$$

$$= \langle 0|\hat{x}|1\rangle\langle 1|\hat{x}|0\rangle = \left(\frac{\hbar}{2m\omega}\right)^{\frac{1}{2}}\left(\frac{\hbar}{2m\omega}\right)^{\frac{1}{2}}$$

$$= \frac{\hbar}{2m\omega},$$

$$\langle 1|\hat{p}^2|1\rangle = \sum_{n=0}^{\infty} \langle 1|\hat{p}|n\rangle\langle n|\hat{p}|1\rangle$$

$$= \langle 1|\hat{p}|0\rangle\langle 0|\hat{p}|1\rangle + \langle 1|\hat{p}|2\rangle\langle 2|\hat{p}|1\rangle$$

$$= +i\left(\frac{\hbar m\omega}{2}\right)^{\frac{1}{2}}(-i)\left(\frac{\hbar m\omega}{2}\right)^{\frac{1}{2}}$$

$$+ (-i)\ 2^{\frac{1}{2}}\left(\frac{\hbar m\omega}{2}\right)^{\frac{1}{2}} i\ 2^{\frac{1}{2}}\left(\frac{\hbar m\omega}{2}\right)^{\frac{1}{2}}$$

$$= \frac{\hbar m\omega}{2} + \cancel{2}\frac{\hbar m\omega}{\cancel{2}} = \frac{3}{2}\hbar m\omega$$

$$\langle 1|\hat{x}^2|1\rangle = \sum_{n=0}^{\infty} \langle 1|\hat{x}|n\rangle\langle n|\hat{x}|1\rangle$$

$$= \langle 1|\hat{x}|0\rangle\langle 0|\hat{x}|1\rangle + \langle 1|\hat{x}|2\rangle\langle 2|\hat{x}|1\rangle$$

$$= \left(\frac{\hbar}{2m\omega}\right)^{\frac{1}{2}}\left(\frac{\hbar}{2m\omega}\right)^{\frac{1}{2}} + 2^{\frac{1}{2}}\left(\frac{\hbar}{2m\omega}\right)^{\frac{1}{2}} 2^{\frac{1}{2}}\left(\frac{\hbar}{2m\omega}\right)^{\frac{1}{2}}$$

$$= \frac{\hbar}{2m\omega} + \cancel{2}\frac{\hbar}{\cancel{2}m\omega} = \frac{3}{2}\frac{\hbar}{m\omega}$$

Thus,

$$\langle 0|\hat{H}|0\rangle = \frac{1}{2\cancel{m}}\cdot\frac{\hbar\cancel{m}\omega}{2} + \frac{\cancel{m\omega^2}}{2}\frac{\hbar}{2\cancel{m\omega}}$$

$$= \frac{\hbar\omega}{2},$$

$$\langle 1|\hat{H}|1\rangle = \frac{1}{2\cancel{m}}\cdot\frac{3}{2}\hbar\cancel{m}\omega + \frac{\cancel{m}\omega^{\cancel{2}}}{2}\cdot\frac{3}{2}\frac{\hbar}{\cancel{m\omega}}$$

$$= \frac{3}{2}\hbar\omega.$$

The values of $\langle 0|\hat{H}|0\rangle$ and $\langle 1|\hat{H}|1\rangle$ should be

$$E_0 = \frac{1}{2}\hbar\omega$$

and

$$E_1 = \frac{3}{2}\hbar\omega$$

(in general, $E_n = \left(n+\frac{1}{2}\right)\hbar\omega$).

Thus, we managed to show that the values of $\langle 0|\hat{H}|0\rangle$ and $\langle 1|\hat{H}|1\rangle$ resulting from the use of Eqs. (1) - (4) lead to E_0 and E_1, as expected.

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