

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

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 ($n = 0, 1, \dots$). 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

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

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

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

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

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

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 $|n\rangle$, $n = 0, 1, \dots$. 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

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

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

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

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

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)

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

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

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

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

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,

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

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

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

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

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

$$\begin{matrix} \xi - s - t = z \\ \underline{\underline{d\xi = dz}} \end{matrix} e^{2st} \int_{-\infty}^{\infty} e^{-z^2} (z + s + t)^3 dz$$

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

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

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

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,

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

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

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

Notice that the power series expansion of

$$\sqrt{15} e^{2st} \left\{ \frac{3}{2}(s+t) + (s+t)^3 \right\}$$

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,

$$I_{nn} = 0, \text{ so that}$$

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

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

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Pibb Picuch

$$(b) \quad \langle u_n | x^4 | u_n \rangle =$$

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

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

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

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

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,

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

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

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

$$\begin{aligned} \xi-s-t &= z \\ \underline{d\xi} &= dz \end{aligned} \quad e^{2st} \int_{-\infty}^{\infty} e^{-z^2} (z+s+t)^4 dz$$

$$\begin{aligned} = e^{2st} & \left\{ \int_{-\infty}^{\infty} e^{-z^2} z^4 dz + 4(s+t) \int_{-\infty}^{\infty} e^{-z^2} z^3 dz \right. \\ & + 6(s+t)^2 \int_{-\infty}^{\infty} e^{-z^2} z^2 dz + 4(s+t)^3 \int_{-\infty}^{\infty} e^{-z^2} z dz \\ & \left. + (s+t)^4 \int_{-\infty}^{\infty} e^{-z^2} dz \right\} \end{aligned}$$

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

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

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

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

Thus,

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

~~$$\int_{-\infty}^{\infty} e^{-\xi^2} \xi^4 d\xi = \frac{3}{4} \sqrt{\pi} + 3(s+t)^2 + (s+t)^4$$~~

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

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

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

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

$$\begin{aligned}
 & + \sum_n \frac{3 \cdot 2^n s^n t^{n+2}}{n!} + \sum_n \frac{6 \cdot 2^n s^{n+1} t^{n+1}}{n!} \\
 & + \sum_n \frac{2^n s^{n+4} t^n}{n!} + \sum_n \frac{4 \cdot 2^n s^{n+3} t^{n+1}}{n!} \\
 & + \sum_n \frac{6 \cdot 2^n s^{n+2} t^{n+2}}{n!} + \sum_n \frac{4 \cdot 2^n s^{n+1} t^{n+3}}{n!} \\
 & + \sum_n \frac{2^n s^n t^{n+4}}{n!} \} =
 \end{aligned}$$

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

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

$$\begin{aligned}
 \frac{I_{nn}}{(n!)^2} &= \sqrt{n} \left\{ \frac{3 \cdot 2^n}{4n!} + \frac{6 \cdot 2^{n-1}}{(n-1)!} + \right. \\
 & \left. + \frac{6 \cdot 2^{n-2}}{(n-2)!} \right\}, \text{ so that}
 \end{aligned}$$

$$\begin{aligned}
 I_{nn} &= \frac{1}{4} 2^n n! \sqrt{\pi} \{ 3 + 12n + 6n(n-1) \} \\
 &= \frac{1}{4} 2^n n! \sqrt{\pi} [3 + \underbrace{12n} + \underbrace{6n^2 - 6n}] \\
 &= \frac{1}{4} 2^n n! \sqrt{\pi} [3 + 6n + 6n^2] \\
 &= \frac{3}{4} 2^n n! \sqrt{\pi} [1 + 2n + 2n^2] .
 \end{aligned}$$

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

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

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

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

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,

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

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

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

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

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

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

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

We know that the number operator

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

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

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

This means that

$$\begin{aligned}\langle \hat{T} \rangle_n &= \frac{1}{4} \hbar \omega \langle n | 2N+1 | n \rangle \\ &= \frac{1}{4} \hbar \omega (2n+1) \\ &= \frac{1}{2} \hbar \omega \left(n + \frac{1}{2}\right) = \frac{1}{2} E_n,\end{aligned}$$

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,

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

where we used the fact that

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

We can write,

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

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

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

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

We need to know

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

and

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

We obtain,

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

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

$$\begin{aligned} \langle 0 | \hat{x}^2 | 0 \rangle &= \sum_{n=0}^{\infty} \langle 0 | \hat{x} | n \rangle \langle n | \hat{x} | 0 \rangle \\ &= \langle 0 | \hat{x} | 1 \rangle \langle 1 | \hat{x} | 0 \rangle = \left(\frac{\hbar}{2m\omega} \right)^{\frac{1}{2}} \left(\frac{\hbar}{2m\omega} \right)^{\frac{1}{2}} \\ &= \frac{\hbar}{2m\omega}, \end{aligned}$$

$$\begin{aligned} \langle 1 | \hat{p}^2 | 1 \rangle &= \sum_{n=0}^{\infty} \langle 1 | \hat{p} | n \rangle \langle n | \hat{p} | 1 \rangle \\ &= \langle 1 | \hat{p} | 0 \rangle \langle 0 | \hat{p} | 1 \rangle + \langle 1 | \hat{p} | 2 \rangle \langle 2 | \hat{p} | 1 \rangle \\ &= +i \left(\frac{\hbar m \omega}{2} \right)^{\frac{1}{2}} (-i) \left(\frac{\hbar m \omega}{2} \right)^{\frac{1}{2}} \\ &\quad + (-i) 2^{\frac{1}{2}} \left(\frac{\hbar m \omega}{2} \right)^{\frac{1}{2}} i 2^{\frac{1}{2}} \left(\frac{\hbar m \omega}{2} \right)^{\frac{1}{2}} \end{aligned}$$

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

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

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

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

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

Thus,

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

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

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

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.

Prof. J. J. J.