

**PHYSICS 4455 — QUANTUM MECHANICS**  
**Problem Set 9 — due 11/17/2005, in class.**

**A few more items about harmonic oscillators.**

1. Many of you wondered in class how the raising and lowering operator formalism connects back to the explicit wave functions in coordinate space. Here, we will see how this connection is established.

An important step in the operator algebra involved the (well-founded) assumption that there had to be a ground state,  $|0\rangle$ , with ground state energy  $\epsilon_o = 1/2$  in dimensionless form. When the lowering operator  $\hat{a}$  acts on this state, the result is 0: Start from the equation

$$\hat{a}|0\rangle = 0 \tag{1}$$

- (i) Express  $\hat{a}$  in terms of the operators  $\hat{x}$  and  $\hat{p}$  and write Eq. (1) in the position representation, as a differential equation for the ground state wave function  $\varphi_o(x)$ . Solve this differential equation and normalize its solution properly.

With the definitions

$$\hat{a} = \sqrt{\frac{m\omega}{2\hbar}} \hat{x} + i\sqrt{\frac{1}{2m\omega\hbar}} \hat{p}$$

$$\hat{a}^+ = \sqrt{\frac{m\omega}{2\hbar}} \hat{x} - i\sqrt{\frac{1}{2m\omega\hbar}} \hat{p}$$

and the identification  $\hat{p} = -i\hbar d/dx$ , the differential equation becomes

$$0 = \left[ \sqrt{\frac{m\omega}{2\hbar}} x + i\sqrt{\frac{1}{2m\omega\hbar}} \left( -i\hbar \frac{d}{dx} \right) \right] \varphi_o(x) \Leftrightarrow \frac{d}{dx} \varphi_o(x) = -\frac{m\omega}{\hbar} x \varphi_o(x)$$

This can be solved by writing

$$\frac{d\varphi_o}{\varphi_o} = -\frac{m\omega}{\hbar} x dx \Rightarrow \ln \varphi_o(x) = -\frac{m\omega}{2\hbar} x^2 + const$$

which results in

$$\varphi_o(x) = C \exp\left(-\frac{m\omega}{2\hbar} x^2\right)$$

where  $C$  is a normalization constant. We can find it with the help of the usual Gaussian integral,

$$\int_{-\infty}^{+\infty} dx e^{-\alpha x^2} = \sqrt{\pi/\alpha}$$

$$1 = \int_{-\infty}^{+\infty} dx \varphi_o^*(x) \varphi_o(x) = C^2 \int_{-\infty}^{+\infty} dx \exp\left(-\frac{m\omega}{\hbar} x^2\right) = C^2 \sqrt{\frac{\pi\hbar}{m\omega}}$$

$$\Rightarrow C = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4}$$

- (ii) Next, we generate the first excited state,  $\varphi_1(x)$ , from the ground state by using the raising operator property

$$|1\rangle = \hat{a}^+|0\rangle \tag{2}$$

Write  $\hat{a}^+$  in terms of the operators  $\hat{x}$  and  $\hat{p}$  and write Eq. (2) in the position representation. Find the explicit form of  $\varphi_1(x)$ . Is it already normalized?

We just read off the definition of  $\hat{a}^+$  from above, whence Eq. (2) translates into

$$\begin{aligned}
 \varphi_1(x) &= \left[ \sqrt{\frac{m\omega}{2\hbar}} x - i \sqrt{\frac{1}{2m\omega\hbar}} (-i\hbar \frac{d}{dx}) \right] \varphi_0(x) \\
 &= \left[ \sqrt{\frac{m\omega}{2\hbar}} x - \hbar \sqrt{\frac{1}{2m\omega\hbar}} \frac{d}{dx} \right] \varphi_0(x) \\
 &= \sqrt{\frac{m\omega}{2\hbar}} x \varphi_0(x) - \sqrt{\frac{\hbar}{2m\omega}} \left( -\frac{m\omega}{\hbar} x \right) \varphi_0(x) \\
 &= 2 \sqrt{\frac{m\omega}{2\hbar}} x \varphi_0(x) \\
 &= \left( \frac{m\omega}{\pi\hbar} \right)^{1/4} 2 \sqrt{\frac{m\omega}{2\hbar}} x \exp\left(-\frac{m\omega}{2\hbar} x^2\right)
 \end{aligned}$$

Checking the explicit form of  $\varphi_1(x)$  from the lecture notes, we have, with  $H_1(y) = 2y$

$$\begin{aligned}
 \varphi_1(x) &= \left( \frac{m\omega}{4\pi\hbar} \right)^{1/4} H_1\left(\sqrt{\frac{m\omega}{\hbar}} x\right) \exp\left(-\frac{m\omega}{2\hbar} x^2\right) \\
 &= \left( \frac{m\omega}{4\pi\hbar} \right)^{1/4} 2 \sqrt{\frac{m\omega}{\hbar}} x \exp\left(-\frac{m\omega}{2\hbar} x^2\right)
 \end{aligned}$$

which agrees. By construction,  $\varphi_1(x)$  generated in this way is normalized; you can also check this with the help of the integral

$$\int_{-\infty}^{+\infty} dx x^2 e^{-\alpha x^2} = (-1) \frac{d}{d\alpha} \int_{-\infty}^{+\infty} dx e^{-\alpha x^2} = (-1) \frac{d}{d\alpha} \sqrt{\pi/\alpha} = \frac{\sqrt{\pi}}{2} \alpha^{-3/2}$$

(iii) Now, write a general expression for  $\varphi_n(x)$ , by translating the relation

$$|n\rangle = \frac{1}{\sqrt{n!}} (\hat{a}^+)^n |0\rangle$$

into position space. By comparing this general form with the explicit solution for  $\varphi_n(x)$ , show that the Hermite polynomials can be generated recursively from the relation

$$H_n(y) = e^{y^2/2} \left( y - \frac{d}{dy} \right)^n e^{-y^2/2}$$

In position space, the equation for  $|n\rangle$  reads:

$$\begin{aligned}
 \varphi_n(x) &= \frac{1}{\sqrt{n!}} \left[ \sqrt{\frac{m\omega}{2\hbar}} x - i \sqrt{\frac{1}{2m\omega\hbar}} (-i\hbar \frac{d}{dx}) \right]^n \varphi_0(x) \\
 &= \frac{1}{\sqrt{n!}} \left[ \sqrt{\frac{m\omega}{2\hbar}} x - \sqrt{\frac{\hbar}{2m\omega}} \frac{d}{dx} \right]^n \varphi_0(x)
 \end{aligned}$$

Defining

$$y \equiv \sqrt{\frac{m\omega}{\hbar}} x \Rightarrow \sqrt{\frac{\hbar}{m\omega}} \frac{d}{dx} = \frac{d}{dy}$$

we obtain

$$\begin{aligned}
\varphi_n(x) &= \frac{1}{\sqrt{n!}} \left[ \sqrt{\frac{m\omega}{2\hbar}} x - i \sqrt{\frac{1}{2m\omega\hbar}} (-i\hbar \frac{d}{dx}) \right]^n \varphi_0(x) \\
&= \frac{1}{\sqrt{n!}} \frac{1}{2^{n/2}} \left[ y - \frac{d}{dy} \right]^n \left( \frac{m\omega}{\pi\hbar} \right)^{1/4} \exp(-y^2/2) \\
&= \left( \frac{m\omega}{2^{2n}(n!)^2\pi\hbar} \right)^{1/4} \left[ y - \frac{d}{dy} \right]^n \exp(-y^2/2)
\end{aligned}$$

In this dimensionless representation, the left hand side takes the form (from the lectures!)

$$\varphi_n(x) = \left( \frac{m\omega}{2^{2n}(n!)^2\pi\hbar} \right)^{1/4} H_n(y) \exp(-y^2/2)$$

Comparing the two expressions, we have

$$\begin{aligned}
\left( \frac{m\omega}{2^{2n}(n!)^2\pi\hbar} \right)^{1/4} H_n(y) \exp(-y^2/2) &= \left( \frac{m\omega}{2^{2n}(n!)^2\pi\hbar} \right)^{1/4} \left[ y - \frac{d}{dy} \right]^n \exp(-y^2/2) \\
&\Leftrightarrow \\
H_n(y) &= \exp(+y^2/2) \left[ y - \frac{d}{dy} \right]^n \exp(-y^2/2)
\end{aligned}$$

as expected.

2. The raising and lowering operator formalism is also very convenient when it comes to computing expectation values. Here is a simple example to demonstrate its power.

(i) Starting from the explicit form of the wave function  $\varphi_3(x)$ , compute the expectation values

$$\langle 3 | \hat{x} | 3 \rangle = \int_{-\infty}^{+\infty} dx \varphi_3^*(x) x \varphi_3(x)$$

and

$$\langle 3 | \hat{x}^2 | 3 \rangle = \int_{-\infty}^{+\infty} dx \varphi_3^*(x) x^2 \varphi_3(x)$$

by evaluating the integrals on the right hand side explicitly.

This is reasonably tedious: First, we write down

$$\begin{aligned}
\varphi_3(x) &= \left( \frac{m\omega}{2^6(3!)^2\pi\hbar} \right)^{1/4} H_3\left(\sqrt{\frac{m\omega}{\hbar}} x\right) \exp\left(-\frac{m\omega}{2\hbar} x^2\right) \\
&= \left( \frac{m\omega}{2^6(3!)^2\pi\hbar} \right)^{1/4} \left[ (-12) \left( y - \frac{2}{3} y^3 \right) \right] \exp(-y^2/2)
\end{aligned}$$

where the dimensionless variable  $y$  was defined above. Noting that  $\varphi_3(x)$  is even, it is obvious that

$$\langle 3 | \hat{x} | 3 \rangle = \int_{-\infty}^{+\infty} dx \varphi_3^*(x) x \varphi_3(x) = 0$$

but we have to suffer for the other integral. Transforming the integration variable to  $y$ , we obtain

$$\langle 3 | \hat{x}^2 | 3 \rangle = \int_{-\infty}^{+\infty} dx \varphi_3^*(x) x^2 \varphi_3(x) = \left( \frac{\hbar}{m\omega} \right)^{3/2} \int_{-\infty}^{+\infty} dy \varphi_3^*(y) y^2 \varphi_3(y)$$

The integral that we have to perform is easy, if we remember a few tricks from Gaussian integrals: Using

$$\begin{aligned}
\int_{-\infty}^{+\infty} dx x^{2n} e^{-\alpha x^2} &= (-1)^n \frac{d^n}{d\alpha^n} \int_{-\infty}^{+\infty} dx e^{-\alpha x^2} = (-1)^n \frac{d^n}{d\alpha^n} \sqrt{\frac{\pi}{\alpha}} \\
&= (-1)^n \sqrt{\pi} \left(-\frac{1}{2}\right) \left(-\frac{3}{2}\right) \dots \left(-\frac{2n-1}{2}\right) \alpha^{-(2n+1)/2} \\
&= \frac{(2n-1)!!}{2^n} \sqrt{\pi} \alpha^{-(2n+1)/2}
\end{aligned}$$

So, we have

$$\begin{aligned}
\langle 3|\hat{x}^2|3\rangle &= \left(\frac{\hbar}{m\omega}\right)^{3/2} \left(\frac{m\omega}{2^6(3!)^2\pi\hbar}\right)^{1/2} \int_{-\infty}^{+\infty} dy \left[(-12)\left(y - \frac{2}{3}y^3\right)\right]^2 y^2 e^{-y^2} \\
&= \left(\frac{\hbar}{m\omega}\right)^{3/2} \left(\frac{m\omega}{2^6(3!)^2\pi\hbar}\right)^{1/2} (12)^2 \int_{-\infty}^{+\infty} dy \left(y^4 - \frac{4}{3}y^6 + \frac{4}{9}y^8\right) e^{-y^2} \\
&= \left(\frac{\hbar}{m\omega}\right) \frac{(12)^2}{2^3(3!) \sqrt{\pi}} \sqrt{\pi} \left[\frac{(4-1)!!}{2^2} - \frac{4}{3} \frac{(6-1)!!}{2^3} + \frac{4}{9} \frac{(8-1)!!}{2^4}\right] \\
&= \left(\frac{\hbar}{m\omega}\right) 3 \left[\frac{3}{4} - \frac{2}{3} \frac{5 \times 3}{4} + \frac{1}{9} \frac{7 \times 5 \times 3}{4}\right] \\
&= \frac{7}{2} \left(\frac{\hbar}{m\omega}\right)
\end{aligned}$$

Quite a bit of work, right? Especially if your computer refuses to run Mathematica or Maple, yes??

(ii) Now, compute the same expectation values by expressing  $\hat{x}$  and  $\hat{x}^2$  in terms of  $\hat{a}$  and  $\hat{a}^+$  and exploit the properties of the raising and lowering operators, as well as the orthonormality of the states  $|n\rangle$ . If all goes well, you will arrive at the same answer as under (i), but without doing a single integral!

So, here's the easy version: First, we invert the equations for  $\hat{a}$  and  $\hat{a}^+$  to obtain

$$\begin{aligned}
\hat{x} &= \sqrt{\frac{\hbar}{2m\omega}} (\hat{a}^+ + \hat{a}) \\
\hat{p} &= i \sqrt{\frac{m\omega\hbar}{2}} (\hat{a}^+ - \hat{a})
\end{aligned}$$

So,

$$\begin{aligned}
\langle 3|\hat{x}|3\rangle &= \sqrt{\frac{\hbar}{2m\omega}} \langle 3|\hat{a}^+ + \hat{a}|3\rangle = \sqrt{\frac{\hbar}{2m\omega}} \{\langle 3|\hat{a}^+|3\rangle + \langle 3|\hat{a}|3\rangle\} \\
&= \sqrt{\frac{\hbar}{2m\omega}} \{\sqrt{4}\langle 3|4\rangle + \sqrt{3}\langle 3|2\rangle\} \\
&= 0
\end{aligned}$$

since  $\langle n|m\rangle = \delta_{n,m}$ . Next, watching the order of  $\hat{a}$  and  $\hat{a}^+$  very carefully, we have

$$\begin{aligned}
\langle 3|\hat{x}^2|3\rangle &= \frac{\hbar}{2m\omega} \langle 3|(\hat{a}^+ + \hat{a})^2|3\rangle = \frac{\hbar}{2m\omega} \langle 3|(\hat{a}^+\hat{a}^+ + \hat{a}^+\hat{a} + \hat{a}\hat{a}^+ + \hat{a}\hat{a})|3\rangle \\
&= \frac{\hbar}{2m\omega} \{\sqrt{4 \times 5}\langle 3|5\rangle + \sqrt{3 \times 3}\langle 3|3\rangle + \sqrt{4 \times 4}\langle 3|3\rangle + \sqrt{3 \times 2}\langle 3|1\rangle\} \\
&= \frac{\hbar}{2m\omega} \{0 + 3 + 4 + 0\} \\
&= \frac{7}{2} \frac{\hbar}{m\omega}
\end{aligned}$$

which is the same answer, requiring considerably less work!

(iii) *Extra credit.* Exploit the operator formalism to show that the average kinetic energy and the average potential energy are equal to each other, in eigenstate  $|n\rangle$ . That is the so-called “virial theorem”; see Liboff Problem 7.10 for parts of the solution.

After part (ii), this should be straightforward. The average kinetic energy is  $\hat{p}^2/2m$ , and the average potential energy is  $m\omega^2\hat{x}^2/2$ . Translating  $\hat{p}^2$  into  $\hat{a}$ 's and  $\hat{a}^+$ 's, similarly to  $\hat{x}^2$ , it should be clear now that only  $\hat{a}^+\hat{a}$  and  $\hat{a}\hat{a}^+$  can give rise to non-vanishing contributions:

$$\begin{aligned}\langle n|\hat{x}^2|n\rangle &= \frac{\hbar}{2m\omega}\langle n|(\hat{a}^+ + \hat{a})^2|n\rangle = \frac{\hbar}{2m\omega}\langle n|(\hat{a}^+\hat{a}^+ + \hat{a}^+\hat{a} + \hat{a}\hat{a}^+ + \hat{a}\hat{a})|n\rangle \\ &= \frac{\hbar}{2m\omega}\{0 + \sqrt{n}\times n\langle n|n\rangle + \sqrt{(n+1)\times(n+1)}\langle n|n\rangle + 0\} \\ &= \frac{\hbar}{2m\omega}(2n+1) \\ \langle n|\hat{p}^2|n\rangle &= -\frac{m\omega\hbar}{2}\langle n|(\hat{a}^+ - \hat{a})^2|n\rangle = -\frac{m\omega\hbar}{2}\langle n|(\hat{a}^+\hat{a}^+ - \hat{a}^+\hat{a} - \hat{a}\hat{a}^+ + \hat{a}\hat{a})|n\rangle \\ &= -\frac{m\omega\hbar}{2}\{0 - \sqrt{n}\times n\langle n|n\rangle - \sqrt{(n+1)\times(n+1)}\langle n|n\rangle + 0\} \\ &= \frac{m\omega\hbar}{2}(2n+1)\end{aligned}$$

Including the prefactors, we find

$$\begin{aligned}\langle E_{kin}\rangle &= \langle n|\frac{\hat{p}^2}{2m}|n\rangle = \frac{m\omega\hbar}{4m}(2n+1) = \frac{1}{2}\hbar\omega(n + \frac{1}{2}) \\ \langle E_{pot}\rangle &= \langle n|\frac{m\omega^2\hat{x}^2}{2}|n\rangle = \frac{m\omega^2}{2}\frac{\hbar}{2m\omega}(2n+1) = \frac{1}{2}\hbar\omega(n + \frac{1}{2})\end{aligned}$$

Clearly,

$$\langle E\rangle = \langle E_{kin}\rangle + \langle E_{pot}\rangle = \hbar\omega(n + \frac{1}{2})$$

as you should expect for the “average” energy of eigenstate  $|n\rangle$ .

**You should review:**

Liboff, Chapter 7.1 – 7.9, 8.5 and 8.6.