Matrix elements of $\hat{a}$ and $\hat{a}^\dagger$

- We'll now calculate the constants that result when the raising and lowering operators act on states

\[
\hat{a} |E_n\rangle = c_n |E_n\rangle \quad \Rightarrow \quad \langle E_n | \hat{a}^\dagger = c_n^* \\
\langle E_n | \hat{a}^\dagger \hat{a} |E_n\rangle = n \quad \Rightarrow \quad |c_n|^2 = n
\]

We can absorb an overall phase into the eigenstates and make $c_n$ real. Then $c_n = \sqrt{n}$.

- We have then

\[
\hat{a} |E_n\rangle = \sqrt{n} |E_{n-1}\rangle \quad \hat{a}^\dagger |E_{n-1}\rangle = \sqrt{n} |E_n\rangle \quad \text{or} \quad \hat{a}^\dagger |E_n\rangle = \sqrt{n+1} |E_{n+1}\rangle
\]

\[
\langle E_{n-1} | \hat{a} |E_n\rangle = \langle E_n | \hat{a}^\dagger |E_{n-1}\rangle = \sqrt{n} \quad \langle E_{n+1} | \hat{a}^\dagger |E_n\rangle = \sqrt{n+1}
\]

Ground eigenstate wave function

- We will now find the ground state wave function.

\[
\hat{a} |E_0\rangle = |\emptyset\rangle \quad \Rightarrow \quad (\hat{x}'+i\hat{p}') |E_0\rangle = |\emptyset\rangle \quad \Rightarrow \quad \langle x' | (\hat{x}'+i\hat{p}') |E_0\rangle = \langle x | \emptyset \rangle
\]

This gives a simple first order differential equation:

\[
\left( x' + \frac{d}{dx'} \right) u_0(x') = 0
\]

- It’s easy to see that the solution to this equation is:

\[
u_0(x') = A'_0 e^{-x'^2/2}
\]

Using $x' = \sqrt{\frac{m\omega}{\hbar}} x$, we have: $u_0(x) = A_0 e^{-m\omega x^2/2\hbar}$

First executed state

- We now solve for the first excited state $u_1(x)$.

\[
\hat{a}^\dagger |E_0\rangle = |E_1\rangle \quad \Rightarrow \quad (\hat{x}'-i\hat{p}') |E_0\rangle = |E_1\rangle \quad \Rightarrow \quad \langle x' | (\hat{x}'-i\hat{p}') |E_0\rangle = \langle x | E_1 \rangle
\]

This gives the first order differential equation:

\[
\left( x' - \frac{d}{dx'} \right) u_0(x') = u_1(x')
\]
• From the differential equation for $u_0(x')$ above we have that:

$$\frac{d}{dx'} u_0(x') = -x'u_0(x')$$

which gives:

$$u_1(x') = 2x'u_0(x') = A_1' x'e^{-x'^2/2}$$

Using $x' = \sqrt{\frac{m\omega}{\hbar}x}$, we have:

$$u_1(x) = A_1 x e^{-m\omega x^2/2\hbar}$$

• We can now get $u_2(x')$ by solving

$$\left(x' - \frac{d}{dx'}\right) u_1(x') = u_2(x')$$

and continue on getting all of the $u_n(x')$'s. We would find:

$$u_n(x') = H_n(x') e^{-x'^2/2}$$

where $H_n(x')$ is the Hermite polynomial of order $n$. The even $n$ Hermite polynomials have only even power terms in $x'$ and the odd $n$ Hermite polynomials have only odd power terms in $x'$. If you are interested, you can find a listing of the Hermite polynomials on wikipedia or in almost any quantum mechanics text book.

Plots of wave functions and probability distributions

• The plots below show the $n = 0$, $n = 1$, $n = 2$ and $n = 3$ wave functions.

• The plot below shows the probability distribution $u_n^*(x)u_n(x)$ for $n = 50$. The blue curve is the classical expectation. It is the position probability distribution that you would get if you randomly took photographs of a mass on the end of a
spring. For a very high energy states as $n \to \infty$, the position distribution of the quantum harmonic oscillator approaches the classical case.

![Graph showing position distribution](http://demonstrations.wolfram.com/QuantumClassicalCorrespondence/)

### Calculating SHO matrix elements

- Using:
  \[
  \hat{x}' = \frac{1}{\sqrt{2}} (\hat{a}^\dagger + \hat{a}) \quad \text{and} \quad \hat{p}' = \frac{i}{\sqrt{2}} (\hat{a}^\dagger - \hat{a})
  \]

  and the orthonormality of the energy eigenstates, we can evaluate the matrix elements of any powers of $\hat{x}'$ or $\hat{p}'$ between energy eigenstates.

- For example,
  \[
  \langle E_m | \hat{x}' | E_n \rangle = \frac{1}{\sqrt{2}} \langle E_m | (\hat{a}^\dagger + \hat{a}) | E_n \rangle \\
  = \frac{1}{\sqrt{2}} \left( \sqrt{n + 1} \langle E_m | E_{n+1} \rangle + \sqrt{n} \langle E_m | E_{n-1} \rangle \right) \\
  = \sqrt{\frac{n+1}{2}} \delta_{m,n+1} + \sqrt{\frac{n}{2}} \delta_{m,n-1}
  \]