Solution of the Quantum Harmonic Oscillator

For a spring-mass system, we know that the angular frequency is related to the spring constant and the mass of the system by:

$$\omega = \sqrt{\frac{k}{m}}$$

where K is the spring constant and m is the mass. We also know classically how to get the potential energy of a spring from the Hooke's law force:

$$F = kx \Rightarrow w = \oint kxdx = \int kxdx = \frac{1}{2}kx^2$$

Thus the potential energy of a compressed spring is given by:

$$V(x) = \frac{1}{2}kx^2$$

We'll take this as the form of the quantum potential that is used in the TISWE:

$$-\frac{\hbar^2}{2m}\nabla^2\Psi + V(r)\Psi = E\Psi \; .$$

Let's write this in its 1-D form:

$$-\frac{\hbar^2}{2m}\frac{\partial^2\Psi}{\partial x^2} + V(x)\Psi = E\Psi$$

With the "spring" potential above, we then have:

$$-\frac{\hbar^2}{2m}\frac{\partial^2\Psi}{\partial x^2} + \frac{1}{2}kx^2\Psi = E\Psi$$

Let's write this in a more agreeable form:

$$-\frac{\hbar^2}{2m}\frac{\partial^2\Psi}{\partial x^2} + \frac{1}{2}kx^2\Psi = E\Psi \Rightarrow \frac{\partial^2\Psi}{\partial x^2} = \left(\frac{mK}{\hbar^2}x^2 - \frac{2mE}{\hbar^2}\right)\Psi$$

We'll want to define some variables:

$$\alpha^2 = \frac{mk}{\hbar^2} \text{ and } \beta = \frac{2mE}{\hbar^2}$$

We could also write:

$$\frac{\partial^2\Psi}{\partial x^2} = \left(\alpha^2x^2 - \beta\right)\Psi$$

$$\frac{\partial^2\Psi}{\partial x^2} = \left(\alpha^2 x^2 - \beta\right)\Psi$$

Let's make a variable transformation:

$y \equiv \alpha x$

Then:

$$\frac{\partial}{\partial y} = \frac{1}{\alpha}\frac{\partial}{\partial x} \Rightarrow \frac{\partial}{\partial x} = \alpha\frac{\partial}{\partial y} \Rightarrow \frac{\partial^2}{\partial x^2} = \alpha^2\frac{\partial^2}{\partial y^2}$$

In this form, the equation becomes:

$$\alpha^2\frac{\partial^2\Psi}{\partial y^2} = \left(y^2 - \beta\right)\Psi \Rightarrow \frac{\partial^2\Psi}{\partial y^2} = \left[\left(\frac{y}{\alpha}\right)^2 - \frac{\beta}{\alpha^2}\right]\Psi$$

But $\frac{\beta}{\alpha^2} = \frac{\frac{2mE}{\hbar^2}}{\frac{mk}{\hbar^2}} = \frac{2E}{k} \equiv \gamma$

Thus, the 1DTISWE for the harmonic oscillator looks like:

$$\frac{\partial^2\Psi}{\partial y^2} = \left[\left(\frac{y}{\alpha}\right)^2 - \gamma\right]\Psi$$

This is the differential equation we'll need to solve for the wave function and the energies. Two things that you know from the beginning, however, are these things:
(1) The lowest energy is not going to be zero and
(2) The energy levels are going to be quantized.

Both of these follow from the fact that we have essentially infinite boundaries at some large x ... right?

The solutions to this differential equation are going to be given by the Hermite Polynomials times a bell-shaped gaussian curve. You can find out more about Hermite polynomials at:

http://mathworld.wolfram.com/HermitePolynomial.html

$$\Psi_n(y) = A_n H_n(y) e^{-\frac{y^2}{2}}$$

Please note an error on page 205, equation 6.57 in your text.

Let's show explicitly that this satisfies the 1DTISWE:

$$\frac{\partial\Psi}{\partial y} = A\left[H' e^{-\frac{y^2}{2}} - yHe^{-\frac{y^2}{2}}\right] = A\left[H' - yH\right]e^{-\frac{y^2}{2}}$$

$$\frac{\partial^2\Psi}{\partial y^2} = A\left[H'' - H - yH'\right]e^{-\frac{y^2}{2}} - yA\left[H' - yH\right]e^{-\frac{y^2}{2}} = A\left[H'' - 2yH' + H(y^2 - 1)\right]e^{-\frac{y^2}{2}}$$

Now, we'll use the following property of the Hermite Polynomials:

$$H_n'(x) = 2nH_{n-1}(x) \ :$$

$$\frac{\partial^2\Psi}{\partial y^2} = A\left[4n(n-1)H_{n-2} - 4ynH_{n-1} + (y^2-1)H\right]e^{-\frac{y^2}{2}}$$

The recursion relation for Hermite polynomials is:

$$H_n = 2yH_{n-1} - 2(n-1)H_{n-2} \Rightarrow 4n(n-1)H_{n-2} = 4nyH_{n-1} - 2nH_n$$

Thus:

$$\frac{\partial^2\Psi}{\partial y^2} = A\left[4nyH_{n-1} - 2nH_n - 4ynH_{n-1} + (y^2-1)H_n\right]e^{-\frac{y^2}{2}}$$

$$\frac{\partial^2\Psi}{\partial y^2} = A\left(y^2 - 1 - 2n\right)H_n e^{-\frac{y^2}{2}}$$

If this is a solution of the SWE, then it must satisfy:

$$\frac{\partial^2\Psi}{\partial y^2} = \left[\left(\frac{y}{\alpha}\right)^2 - \gamma\right]\Psi \Rightarrow A\left(y^2-1-2n\right)H_n e^{-\frac{y^2}{2}} = A\left[\left(\frac{y}{\alpha}\right)^2 - \gamma\right]H_n e^{-\frac{y^2}{2}}$$

Clearly then, we require:

$$\left(y^2 - 1 - 2n\right) = \left[\left(\frac{y}{\alpha}\right)^2 - \gamma\right]$$

Also, now, equally clear is the fact that we must have

$$\alpha = 1$$

This give us:

$$\gamma = 2n + 1 = \frac{2E}{k} \Rightarrow E_n = \frac{k}{2}\left(2n+1\right) = k(n + \tfrac{1}{2})$$

$$\alpha = 1 = \frac{m\omega}{\hbar} \Rightarrow \omega = \frac{\hbar}{m}$$

Since $\alpha = 1 \Rightarrow \frac{mk}{\hbar^2} = 1 \Rightarrow k = \frac{\hbar^2}{m} = \frac{\hbar}{m}\hbar = \hbar\omega$

Where ω is the classical frequency of oscillation: $\omega = \sqrt{\frac{k}{m}}$.

Thus, the energy levels are given by:

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

Let's look at several of the resulting energies:

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

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

$$E_2 = \tfrac{5}{2}\hbar\omega$$

...

Notice that the energies are ***equally spaced***. This is probably the only potential that produces equally spaced energies. You can also see, that the ***lowest energy is not zero***. Let's now calculate some general properties associated with the solutions.

Normalization:

To normalize the wavefunctions, we require:

$$\int_{-\infty}^{+\infty} \Psi_n^*(x)\Psi_n(x)dx = 1$$

It'll be more useful to write this in terms of y as:

$$\frac{1}{\alpha}\int_{-\infty}^{+\infty} \Psi_n^*(y)\Psi_n(y)dy = 1$$

Thus:

$$\Psi_n(y) = A_n H_n(y) e^{-\frac{y^2}{2}}$$

$$\frac{A_n^2}{\alpha}\int_{-\infty}^{+\infty} H_n^2 e^{-y^2} dy = 1$$

(The Hermite Polynomials are real if the argument is real)

From the reference site for Hermite Polynomials, you'll find:

$$\int_{-\infty}^{+\infty} H_m(y)H_n(y)e^{-y^2} = \delta_{mn} 2^n n! \sqrt{\pi}$$

$$\text{where } \delta_{mn} = \begin{bmatrix} 0 \text{ if } m \neq n \\ 1 \text{ if } m = n \end{bmatrix}$$

Thus, we have as the normalization condition:

$$\frac{A_n^2}{\alpha}\left[2^n n! \sqrt{\pi}\right] = 1 \Rightarrow A_n = \sqrt{\frac{\alpha}{\left[2^n n! \sqrt{\pi}\right]}}$$

Of course, our solutions have $\alpha = 1$. Thus,

$$A_n = \sqrt{\frac{1}{\left[2^n n! \sqrt{\pi}\right]}}$$

Calculation of uncertainties:

<x>

$$< x >= \int_{-\infty}^{+\infty} \Psi_n^* x \Psi_n dx = \frac{1}{\alpha^2} \int_{-\infty}^{+\infty} \Psi_n^* y \Psi_n dy$$

We can directly integrate this result:

$$< x >= \frac{A_n^2}{\alpha^2} \int_{-\infty}^{+\infty} y H_n^2 e^{-y^2} dy =$$

$$\frac{A_n^2}{\alpha^2} \int_{-\infty}^{+\infty} \frac{1}{2} H_n H_{n+1} e^{-y^2} dy + \frac{A_n^2}{\alpha^2} \int_{-\infty}^{+\infty} n H_n H_{n-1} e^{-y^2} dy = 0$$

where I have used the recursion relation and also the integral result.

Thus: $< x >= 0$

Let's now calculate $<x^2>$:

$$< x^2 >= \int_{-\infty}^{+\infty} \Psi_n^* x^2 \Psi_n dx = \frac{1}{\alpha^3} \int_{-\infty}^{+\infty} \Psi_n^* y^2 \Psi_n dy$$

We'll basically do the same thing above twice:

$$< x^2 >= \frac{A_n^2}{\alpha^3} \int_{-\infty}^{+\infty} \left(y H_n\right)^2 e^{-y^2} dy = \frac{A_n^2}{\alpha^3} \int_{-\infty}^{+\infty} \left(\frac{1}{2} H_{n+1} - n H_{n-1}\right)^2 e^{-y^2} dy$$

$$< x^2 >= \frac{A_n^2}{\alpha^3} \int_{-\infty}^{+\infty} \left(\frac{1}{4} H_{n+1}^2 + n^2 H_{n-1}^2\right) e^{-y^2} dy$$

(the cross terms integrate to zero).

Thus,

$$< x^2 >= \frac{A_n^2}{\alpha^3} \left[\frac{1}{4} 2^{n+1} (n+1)! \sqrt{\pi} + n^2 2^{n-1} (n-1)! \sqrt{\pi}\right]$$

We know also that:

$$A_n^2 = \frac{1}{\left[2^n n! \sqrt{\pi}\right]}$$

so:

$$< x^2 >= \frac{1}{\alpha^3} \frac{\frac{1}{4} 2^{n+1} (n+1)! \sqrt{\pi} + n^2 2^{n-1} (n-1)! \sqrt{\pi}}{\left[2^n n! \sqrt{\pi}\right]} = \frac{1}{\alpha^3} \left[\frac{\frac{1}{4} 2 (n+1) + n^2 \frac{1}{2} \frac{1}{n}}{1}\right] = \frac{1}{\alpha^3} \left[\frac{n+1}{2} + \frac{n}{2}\right] = \frac{1}{2\alpha^3} \left(2n+1\right)$$

Of course, our solutions have $\alpha = 1$. Thus,

$$< x^2 >= \left(n + \frac{1}{2}\right)$$

We can now calculate the uncertainty in position:

$$\Delta x \equiv \sqrt{< x^2 > - < x >^2} = \sqrt{(n + \frac{1}{2})}$$

<p>:

Remember: $\hat{p} = -i\hbar \frac{\partial}{\partial x}$

$$< p > = -i\hbar \int_{-\infty}^{+\infty} \Psi^* \frac{\partial}{\partial x}\Psi dx = -i\hbar \int_{-\infty}^{+\infty} \Psi^* \frac{\partial}{\partial y}\Psi dy$$

Of course, this has got to equal zero (<p> needs to be real).
Let's show this. We had:

$$\frac{\partial \Psi}{\partial y} = A\left[H' - yH\right]e^{-\frac{y^2}{2}}$$

but

$$H_n' = 2nH_{n-1}$$

so

$$\frac{\partial \Psi}{\partial y} = A_n\left[2nH_{n-1} - yH_n\right]e^{-\frac{y^2}{2}}$$

Thus:

$$< p > = -i\hbar A_n^2 \int_{-\infty}^{+\infty} H_n\left[2nH_{n-1} - yH_n\right]e^{-y^2}dy = -i\hbar A_n^2 \int_{-\infty}^{+\infty} yH_n^2 e^{-y^2}dy$$

We can evaluate this with the recursion relation:

$$H_n = 2yH_{n-1} - 2(n-1)H_{n-2} \Rightarrow yH_n = \frac{1}{2}H_{n+1} + nH_{n-1}$$

Thus,

$$< p > = -i\hbar A_n^2 \int_{-\infty}^{+\infty} H_n\left[\frac{1}{2}H_{n+1} + nH_{n-1}\right]e^{-y^2}dy = 0$$

$$A_n = \sqrt{\frac{1}{\left[2^n n!\sqrt{\pi}\right]}}$$

<p^2>:

$$\hat{p}^2 = \hat{p} \bullet \hat{p} = \left(-i\hbar \frac{\partial}{\partial x}\right) \bullet \left(-i\hbar \frac{\partial}{\partial x}\right) = -\hbar^2 \frac{\partial^2}{\partial x^2}$$

and so:

$$< p^2 >= \int_{-\infty}^{+\infty} \Psi^* \hat{p}^2 \Psi dx = -\hbar^2 \int_{-\infty}^{+\infty} \Psi^* \frac{\partial^2 \Psi}{\partial x^2} dx = -\hbar^2 \int_{-\infty}^{+\infty} \Psi^* \alpha^2 \frac{\partial^2 \Psi}{\partial y^2} \frac{1}{\alpha} dy$$

$$< p^2 >= -\alpha\hbar^2 \int_{-\infty}^{+\infty} \Psi^* \frac{\partial^2 \Psi}{\partial y^2} dy$$

We know what the derivative is. It is given by:

$$\frac{\partial^2 \Psi}{\partial y^2} = \left[\left(\frac{y}{\alpha}\right)^2 - \gamma\right] \Psi$$

(hmmm ... recognize this from somewhere? :))

so,

$$< p^2 >= -\alpha\hbar^2 \int_{-\infty}^{+\infty} \Psi^* \left[\left(\frac{y}{\alpha}\right)^2 - \gamma\right] \Psi dy$$

or

$$< p^2 >= -\alpha\hbar^2 A_n^2 \int_{-\infty}^{+\infty} \left[\left(\frac{y}{\alpha}\right)^2 - \gamma\right] H_n^2 e^{-y^2} dy$$

So,

$$< p^2 >= -\frac{1}{\alpha}\hbar^2 A_n^2 \int_{-\infty}^{+\infty} y^2 H_n^2 e^{-y^2} dy + \alpha\hbar^2 A_n^2 \int_{-\infty}^{+\infty} \gamma H_n^2 e^{-y^2} dy$$

We'll use the recursion relation again:

$$H_n = 2yH_{n-1} - 2(n-1)H_{n-2} \Rightarrow yH_n = \frac{1}{2}H_{n+1} + nH_{n-1}$$

$$< p^2 >= -\frac{1}{\alpha}\hbar^2 A_n^2 \int_{-\infty}^{+\infty} \left[\frac{1}{2}H_{n+1} + nH_{n-1}\right]^2 e^{-y^2} dy + \alpha\hbar^2 A_n^2 \int_{-\infty}^{+\infty} \gamma H_n^2 e^{-y^2} dy$$

and the normalization condition:

$$\int_{-\infty}^{+\infty} H_m(y) H_n(y) e^{-y^2} = \delta_{mn} 2^n n! \sqrt{\pi}$$

$$< p^2 >= -\frac{1}{\alpha}\hbar^2 A_n^2 \int_{-\infty}^{+\infty} \left[\frac{1}{4}H_{n+1}^2 + n^2 H_{n-1}^2\right] e^{-y^2} dy + \gamma\alpha\hbar^2 A_n^2 2^n n! \sqrt{\pi}$$

$$< p^2 >= -\frac{1}{\alpha}\hbar^2 A_n^2 \left[\frac{1}{4} 2^{n+1}(n+1)! \sqrt{\pi} + n^2 2^{n-1}(n-1)! \sqrt{\pi}\right] + \gamma\alpha\hbar^2 A_n^2 2^n n! \sqrt{\pi}$$

But, we found

$$A_n^2 = \frac{1}{\left[2^n n! \sqrt{\pi}\right]}$$

Thus:

$$< p^2 >= -\frac{1}{\alpha}\hbar^2 \left[\frac{1}{4} 2(n+1) + n^2 \frac{1}{2(n)}\right] + \gamma\alpha\hbar^2$$

$$< p^2 >= -\frac{1}{2\alpha}\hbar^2 \left[2n+1\right] + (2n+1)\alpha\hbar^2 = (2n+1)\hbar^2 \left(1 - \frac{1}{2}\right) = \hbar^2 (n + \frac{1}{2})$$

We thus have $\Delta p = \hbar\sqrt{n + \frac{1}{2}}$

We can now calculate:

$$\Delta p \Delta x = \hbar\sqrt{n+\tfrac{1}{2}}\sqrt{n+\tfrac{1}{2}} = \hbar\left(n+\tfrac{1}{2}\right) = \tfrac{\hbar}{2}(1+2n)$$

Notice, that in accord with the Heisenburg uncertainty principle, $\Delta x \Delta p \geq \frac{\hbar}{2}$ for all n.

Let's calculate the probability of radiative transfer between two states. This is basically given by the expectation of the dipole moment and thus, this probability is proportional to:

$$\Re \equiv \int_{-\infty}^{+\infty} \Psi_m^* x \Psi_n dx$$

Let's see that this will give us. Basically the important parts of this integral will be:

$$\Re = \tfrac{1}{\alpha^2} A_m A_n \int_{-\infty}^{+\infty} H_m y H_n e^{-y^2} dy$$

We can evaluate this integral via the recursion relation:

$$H_n = 2yH_{n-1} - 2(n-1)H_{n-2} \Rightarrow yH_n = \tfrac{1}{2}H_{n+1} + nH_{n-1}$$

$$\Re_{m,n} = A_m A_n \int_{-\infty}^{+\infty} H_m \left[\tfrac{1}{2}H_{n+1} + nH_{n-1}\right] e^{-y^2} dy$$

We can evaluate this integral with:

$$\int_{-\infty}^{+\infty} H_m(y) H_n(y) e^{-y^2} = \delta_{mn} 2^n n! \sqrt{\pi}$$

$$\Re_{m,n} = A_m A_n \left[\tfrac{1}{2}\delta_{m,n+1} 2^{n+1}(n+1)!\sqrt{\pi} + \delta_{mn-1} 2^{n-1} n! \sqrt{\pi}\right]$$

But, we had:

$$A_n = \sqrt{\frac{1}{\left[2^n n! \sqrt{\pi}\right]}}$$

So,

$$\Re_{m,n} = \sqrt{\frac{1}{2^n 2^m n! m!}} 2^n n! \left[\delta_{m,n+1}(n+1) + \tfrac{1}{2}\delta_{m,n-1}\right]$$

$$\Re_{m,n} = \sqrt{\frac{2^n n!}{2^m m!}} \left[\delta_{m,n+1}(n+1) + \tfrac{1}{2}\delta_{m,n-1}\right]$$

The only two states that produce this dipole radiation are m=n+1 and m=n-1

If m=n+1, then:

$$\Re_{n+1,n} = \sqrt{\frac{n+1}{2}}$$

If m=n-1, then:

$$\Re_{n-1,n} = \sqrt{\frac{n}{2}}$$

There are other modes of radiation which are possible ... you'd work out these probabilities as being proportional to x^p where p is an integer.

Sometimes you'll see things written in a matrix format. Let's see what this might look like here ...

$$\overleftrightarrow{\mathfrak{R}} = \sqrt{\tfrac{1}{2}}\begin{bmatrix} m\downarrow/n\rightarrow & 0 & 1 & 2 & 3 & 4 & 5 & 6 \\ 0 & 0 & \sqrt{1} & 0 & 0 & 0 & 0 & 0 \\ 1 & \sqrt{1} & 0 & \sqrt{2} & 0 & 0 & 0 & 0 \\ 2 & 0 & \sqrt{2} & 0 & \sqrt{3} & 0 & 0 & 0 \\ 3 & 0 & 0 & \sqrt{3} & 0 & \sqrt{4} & 0 & 0 \\ 4 & 0 & 0 & 0 & \sqrt{4} & 0 & \sqrt{5} & 0 \\ 5 & 0 & 0 & 0 & 0 & \sqrt{5} & 0 & \sqrt{6} \\ 6 & 0 & 0 & 0 & 0 & 0 & \sqrt{6} & 0 \end{bmatrix}$$

This shows for the first 7 states relative probabilities of transitions between two states via dipole radiation. You probably want to check for yourself that I've represented this correctly. Notice that under dipole radiation, the transition n->m is as likely as the transition m<-n. This point made me very happy when I finished this matrix because it tends to confirm symmetry but there really ought to not be a promise that this will always happen for any type or radiation. Also, transitions forbidden under dipole radiation may be permitted under higher modes of radiation (note the zeros in the matrix above).

While we're doing such a treatment of the harmonic oscillator, we ought to look at the expectation values of the kinetic energy. This is given by:

$$\langle KE\rangle = \left\langle \frac{p^2}{2m}\right\rangle = \frac{1}{2m}\left\langle p^2\right\rangle = \frac{\hbar^2\left(n+\frac{1}{2}\right)}{2m} = \frac{\hbar}{2m\omega}\left[\hbar\omega\left(n+\tfrac{1}{2}\right)\right] = \frac{\hbar}{2m\omega}E_n = \tfrac{1}{2}E_n$$

That's very good ... the expected kinetic energy is 1/2 of the total energy.
Let's see what the expected potential energy is (as if you can't already imagine) ...

$$\langle V\rangle = \tfrac{1}{2}k\left\langle x^2\right\rangle = \tfrac{1}{2}k\left(n+\tfrac{1}{2}\right) = \tfrac{1}{2}k\frac{E_n}{\hbar\omega} = \tfrac{1}{2}\frac{k}{\hbar\omega}E_n = \tfrac{1}{2}E_n$$

Yes, that's right ... on the average, the energy comes 1/2 from the kinetic energy and 1/2 from the potential energy. There's a theorem or two out there involving this that we won't cover right now.