Quantum harmonic oscillator - EJZ March 2007

Calculate first two p^2 expectation values

In[1]:=
```
Clear[A0, A1];
A0 = Sqrt[Sqrt[m w/(π h)]];
a = m w/(2 h);
A1 = Sqrt[Sqrt[4 m w/(π h)]]
```

In[5]:=
```
Clear[Y0, Y1];
Y0[x_] := A0 Exp[-a x^2];
Y1[x_] := A1 * Sqrt[2 a] * x * Exp[-a x^2]
```

In[8]:=
```
Y0[x]
```

Out[8]= $\frac{e^{-\frac{m w x^2}{2 h}} \left(\frac{m w}{h}\right)^{1/4}}{\pi^{1/4}}$

$< p_0^2 > = -hbar^2 \frac{d^2}{x^2}$

In[9]:=
```
Clear [dY0, ddY0, dY1, ddY1];
dY0[x_] := Simplify[D[Y0[x], x]];
ddY0[x_] := Simplify[D[dY0[x], x]];
dY1[x_] := Simplify[D[Y1[x], x]];
ddY1[x_] := Simplify[D[dY1[x], x]];
```

In[14]:=
```
dY0[x]
```

Out[14]= $-\frac{e^{-\frac{m w x^2}{2 h}} \left(\frac{m w}{h}\right)^{5/4} x}{\pi^{1/4}}$

```
ddY1[x]
```

$\frac{\sqrt{2}\, e^{-\frac{m w x^2}{2 h}} \left(\frac{m w}{h}\right)^{7/4} x \left(-3 h + m w x^2\right)}{h\, \pi^{1/4}}$

In[15]:=
```
Clear[argp0, argp1];
argp0[x_] := Simplify[-h^2 Y0[x] ddY0[x]];
argp1[x_] := Simplify[-h^2 Y1[x] ddY1[x]];
```

In[18]:=
```
argp0[x]
```

Out[18]= $\frac{e^{-\frac{m w x^2}{h}} h \left(\frac{m w}{h}\right)^{3/2} \left(h - m w x^2\right)}{\sqrt{\pi}}$


```
argp1[x]
```

$-\frac{2 e^{-\frac{m w x^2}{h}} h \left(\frac{m w}{h}\right)^{5/2} x^2 \left(-3 h + m w x^2\right)}{\sqrt{\pi}}$

Integrate each of these arguments over all space to find $< p^2 >$

■ Break p0 integral into parts to solve: $< p_0^2 > = \frac{h m w}{2}$

■ construct p0 argument

In[19]:=
```
argp0[x]
```

Out[19]= $\frac{e^{-\frac{m w x^2}{h}} h \left(\frac{m w}{h}\right)^{3/2} \left(h - m w x^2\right)}{\sqrt{\pi}}$

```
Clear[c, i1, i2, int];
c = h (m w/h)^(3/2)/Sqrt[π];
i1[x_] := e^(-m w x^2/h) (h); i2[x_] := e^(-m w x^2/h) (-m w x^2);
int[x_] := c (i1[x] + i2[x])
```

```
int[x]
```

$\frac{h \left(\frac{m w}{h}\right)^{3/2} \left(e^{-\frac{m w x^2}{h}} h - e^{-\frac{m w x^2}{h}} m w x^2\right)}{\sqrt{\pi}}$

In[25]:=
```
Simplify[int[x] - argp0[x]]
```

Out[25]= 0

■ integrate first p0 argument

In[26]:=
```
Clear[s1];
s1 = Integrate[i1[x], {x, -∞, ∞}]
```

Out[27]= $h \,\text{If}\left[\text{Re}\left[\frac{m w}{h}\right] > 0, \frac{\sqrt{\pi}}{\sqrt{\frac{m w}{h}}}, \int_{-\infty}^{\infty} e^{-\frac{m w x^2}{h}} \, dx\right]$

In[28]:=
```
s1 = Simplify[h Sqrt[π]/Sqrt[m w/h]]
```

■ integrate second p0 argument

```
In[29]:= Clear[s2];
         Integrate[i2[x], {x, -∞, ∞}]
```

Out[30]= $-m\,w\,\mathrm{If}\left[\mathrm{Re}\left[\frac{m\,w}{h}\right]>0,\ \frac{\sqrt{\pi}}{2\left(\frac{m\,w}{h}\right)^{3/2}},\ \int_{-\infty}^{\infty}e^{-\frac{m\,w\,x^2}{h}}\,x^2\,dx\right]$

In[31]:= $s2 = \mathrm{Simplify}\left[\frac{-m\,w\,\sqrt{\pi}}{2\left(\frac{m\,w}{h}\right)^{3/2}}\right]$

■ Combine into $< p_0^2 >$

```
In[34]:= Clear[sum];
         sum = Simplify[s1 + s2]
```

Out[35]= $\frac{h\sqrt{\pi}}{2\sqrt{\frac{m\,w}{h}}}$

```
In[33]:= c
In[36]:= Simplify[c * sum]
```

Out[36]= $\frac{h\,m\,w}{2}$

■ Break p1 integral into parts to solve: $< p_1^2 > = \frac{3\,h\,m\,w}{2}$

```
argp1[x]
```

$-\frac{2\,e^{-\frac{m\,w\,x^2}{h}}\,h\left(\frac{m\,w}{h}\right)^{5/2}x^2\left(-3\,h+m\,w\,x^2\right)}{\sqrt{\pi}}$

■ construct p1 argument

```
Clear[c, i1, i2, int];
```

$c = -\frac{2\,h\left(\frac{m\,w}{h}\right)^{5/2}}{\sqrt{\pi}};$

$i1[x\_] := e^{-\frac{m\,w\,x^2}{h}}\,x^2\,(-3\,h);\quad i2[x\_] := e^{-\frac{m\,w\,x^2}{h}}\,x^2\,(m\,w\,x^2);$

```
int[x_] := c (i1[x] + i2[x]);
int[x]
```

$-\frac{2\,h\left(\frac{m\,w}{h}\right)^{5/2}\left(-3\,e^{-\frac{m\,w\,x^2}{h}}\,h\,x^2+e^{-\frac{m\,w\,x^2}{h}}\,m\,w\,x^4\right)}{\sqrt{\pi}}$


```
Simplify[int[x] - argp1[x]]
```

0

■ integrate first p1 argument

```
Clear[s1];
s1 = Integrate[i1[x], {x, -∞, ∞}]
```

$-3\,h\,\mathrm{If}\left[\mathrm{Re}\left[\frac{m\,w}{h}\right]>0,\ \frac{\sqrt{\pi}}{2\left(\frac{m\,w}{h}\right)^{3/2}},\ \int_{-\infty}^{\infty}e^{-\frac{m\,w\,x^2}{h}}\,x^2\,dx\right]$

$s1 = \mathrm{Simplify}\left[-3\,h\,\frac{\sqrt{\pi}}{2\left(\frac{m\,w}{h}\right)^{3/2}}\right]$

■ integrate second p0 argument

```
Clear[s2];
Integrate[i2[x], {x, -∞, ∞}]
```

$m\,w\,\mathrm{If}\left[\mathrm{Re}\left[\frac{m\,w}{h}\right]>0,\ \frac{3\sqrt{\pi}}{4\left(\frac{m\,w}{h}\right)^{5/2}},\ \int_{-\infty}^{\infty}e^{-\frac{m\,w\,x^2}{h}}\,x^4\,dx\right]$

$s2 = \mathrm{Simplify}\left[m\,w\,\frac{3\sqrt{\pi}}{4\left(\frac{m\,w}{h}\right)^{5/2}}\right]$

■ Combine into $< p_1^2 >$

```
Clear[sum];
sum = Simplify[s1 + s2]
```

$-\frac{3\,h\sqrt{\pi}}{4\left(\frac{m\,w}{h}\right)^{3/2}}$

```
c
Simplify[c * sum]
```

$\frac{3\,h\,m\,w}{2}$

Check normalization of the first two wavefunctions

■ Y0

```
Clear[Y0, A0];
Y0[x_] := A0 Exp[(-m w)/(2 h) x^2]
```

```
Y0[x]
```

$A0\, e^{-\frac{m w x^2}{2 h}}$

```
Integrate[Y0[x]^2, {x, -∞, ∞}]
```

$A0^2\, \text{If}\left[\text{Re}\left[\frac{m w}{h}\right] > 0, \frac{\sqrt{\pi}}{\sqrt{\frac{m w}{h}}}, \int_{-\infty}^{\infty} e^{-\frac{m w x^2}{h}}\, dx\right]$