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]= E^(-m w x^2/(2 h)) (m w/h)^(1/4) / π^(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]= -E^(-m w x^2/(2 h)) (m w/h)^(5/4) x / π^(1/4)

         ddY1[x]

         Sqrt[2] E^(-m w x^2/(2 h)) (m w/h)^(7/4) x (-3 h + m w x^2) / (h π^(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]= E^(-m w x^2/h) h (m w/h)^(3/2) (h - m w x^2) / Sqrt[π]
```

```
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]
```

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

```
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, -∞, ∞}]
```

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

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

■ integrate second p0 argument

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

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

```
In[31]:= s2 = Simplify[ -m w √π / (2 (m w / h)^(3/2)) ]
```

■ Combine into $< p_0^2 >$

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

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

```
In[33]:= c
```

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

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

■ 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 = -2 h (m w / h)^(5/2) / √π;
i1[x_] := e^-(m w x^2 / h) x^2 (-3 h);   i2[x_] := e^-(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, -∞, ∞}]
```

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

```
s1 = Simplify[-3 h Sqrt[π] / (2 (m w / h)^(3/2))]
```

■ integrate second p0 argument

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

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

```
s2 = Simplify[m w 3 Sqrt[π] / (4 (m w / h)^(5/2))]
```

■ 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]
```

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