Rae & Napolitano Worked Example 10.4

In[102]:=
```
Remove["Global`*"]
$Assumptions = {a > 0, m > 0, ω > 0, ℏ > 0, x0 > 0};
```

Calculate the expectation of the Hamiltonian with the trial wave function. (We took the second derivative of the wave function by hand.)

In[104]:=
```
avgH = Simplify[
   (1 / a) Integrate[
     Cos[Pi x / (2 a)] ×
      (ℏ^2 / (2 m) (Pi / (2 a))^2 + m ω^2 x^2 / 2) ×
      Cos[Pi x / (2 a)],
     {x, -a, a}]]
```

Out[104]= $$\frac{a^2 m \left(-6+\pi^2\right) \omega^2}{6 \pi^2}+\frac{\pi^2 \hbar^2}{8 a^2 m}$$

Take the derivative with respect to a, set it to zero, and solve. Not being fancy, I knew ahead of time that the fourth solution is the positive solution, so I'm just picking out that one.

In[105]:=
```
avgHderv = D[avgH, a]
```

Out[105]= $$\frac{a m \left(-6+\pi^2\right) \omega^2}{3 \pi^2}-\frac{\pi^2 \hbar^2}{4 a^3 m}$$

In[106]:=
```
aMin = a /. Solve[avgHderv == 0, a][[4]]
```

Out[106]= $$\frac{\pi \left(\frac{3}{-24+4 \pi^2}\right)^{1/4} \sqrt{\hbar}}{\sqrt{m} \sqrt{\omega}}$$

In[107]:=
```
N[aMin]
```

Out[107]= $$\frac{2.08448 \sqrt{\hbar}}{\sqrt{m} \sqrt{\omega}}$$

This value agrees with the textbook. Now evaluate the ground state eigenvalue approximation.

In[108]:=
```
avgH /. a → aMin
```

Out[108]= $$\frac{1}{8} \sqrt{\frac{1}{3} \left(-24+4 \pi^2\right)} \omega \hbar+\frac{\left(-6+\pi^2\right) \omega \hbar}{2 \sqrt{3 \left(-24+4 \pi^2\right)}}$$

In[109]:=
```
N[%]
```

Out[109]= $0.567862\, \omega \hbar$

Now get the true ground state wave function, and see how close we are to orthogonality

In[110]:=
```
x0 = Sqrt[ℏ / (m ω)];
expFact = Exp[- x^2 / (2 x0^2)];
normSq = Integrate[expFact^2, {x, -∞, ∞}];
u0 = expFact / Sqrt[normSq]
```

Out[113]=
$$\frac{e^{-\frac{m x^2 \omega}{2 \hbar}}}{\pi^{1/4} \sqrt{\frac{\hbar}{\sqrt{m \omega \hbar}}}}$$

In[114]:=
```
v = (1 / Sqrt[a]) Cos[Pi x / (2 a)];
Integrate[v^2, {x, -a, a}] == 1
```

Out[115]= True

In[116]:=
```
Integrate[u0^2, {x, -∞, ∞}] == 1
```

Out[116]= True

In[117]:=
```
N[Integrate[v u0 /. a → aMin, {x, -aMin, aMin}]]
```

Out[117]= 0.994263 + 0. i

In[118]:=
```
ArcCos[Re[%]]
```

Out[118]= 0.107167

In[119]:=
```
180 × % / Pi
```

Out[119]= 6.14023