TZDII Problem 8.43

What is the probability that a 1s electron in hydrogen will be found outside the Bohr radius?

Write out the wave function for a 1s electron:

In[1]:=
```
R1s[r_] := 1/Sqrt[π * a_B^3] * Exp[-r/a_B]
```

```
R1s[r]
R1s[r]^2
```

Out[2]=
$$\frac{e^{-\frac{r}{a_B}}}{\sqrt{\pi}\ \sqrt{a_B^3}}$$

Out[3]=
$$\frac{e^{-\frac{2r}{a_B}}}{\pi\, a_B^3}$$

Write out the wave function for a 1s electron:

In[6]:=
```
ProbDens1s[r_] := 4 * π * r^2 * R1s[r]^2
ProbDens1s[r]
```

Out[7]=
$$\frac{4\, e^{-\frac{2r}{a_B}}\, r^2}{a_B^3}$$

To find the probability of finding it outside a_B, integrate from a_B to infinity:

In[8]:=
```
Integrate[ProbDens1s[r], {r, a_B, ∞}]
```

Out[8]=
$$\frac{5}{e^2} \quad \text{if} \quad \text{Re}[a_B] > 0$$

So the probability is (5/e)^2, or

In[9]:=
```
N[5 / e^2]
```

Out[9]=
```
0.676676
```

This means that the electron has a 68% chance of being outside the Bohr orbit and a 32% chance of being inside it … yeah, there's a long tail on the wave function, so this makes sense. Plotting the probability density shows that the area under the cure outside of a_B is greater than that within a_B.

In[10]:=
```
a_B = 1;
```

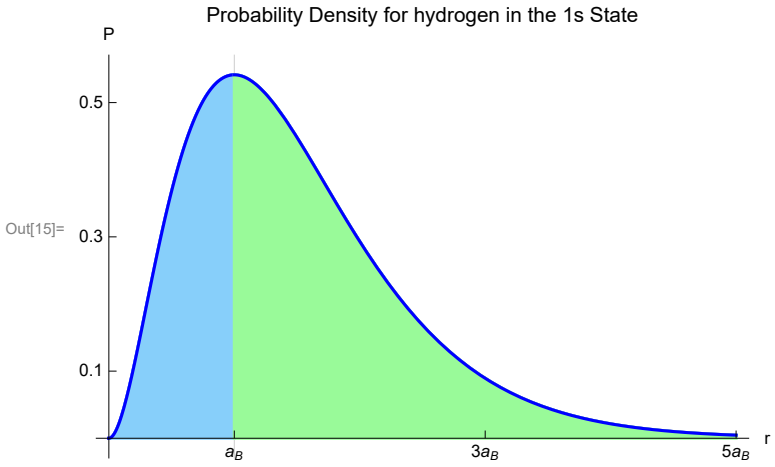
In[11]:=
```
Pall = Plot[ProbDens1s[r], {r, 0, 5} , PlotStyle → {Blue}, GridLines → {{1}, None},
   Ticks → {{{1, "a_B" }, {3, "3a_B" }, {5, "5a_B" }}, {0.1, 0.3, 0.5}}, AxesLabel → {"r", "P"}];
```

In[13]:=
```
Pinside = Plot[ProbDens1s[r], {r, 0, 1} , PlotRange → {Automatic, 0.6},
   PlotStyle → {Blue}, Filling → 0, FillingStyle → RGBColor[0.53, 0.81, 0.98]];
```

In[14]:=
```
Poutside = Plot[ProbDens1s[r], {r, 1, 5} , PlotRange → {Automatic, 0.6},
   PlotStyle → {Blue}, Filling → 0, FillingStyle → RGBColor[0.60, 0.98, 0.60]];
```

In[15]:=
```
Show[Pall, Pinside, Poutside,
 PlotLabel → "Probability Density for hydrogen in the 1s State" ]
```

Out[15]=



In[16]:=
```
Export["TZDII_Pr08-43.pdf", SelectedNotebook[]]
```

Out[•]=
```
TZDII_Pr08-43.pdf
```