Why was Bor right?
Estimated radius for an electron in an s orbital
article amsmath
We want to evaluate the following integral:

$$\int_0^{2a_0} r^2 e^{-\frac{2r}{a_0}}\, dr$$

$$x = \frac{2r}{a_0} \quad \Rightarrow \quad r = \frac{a_0 x}{2}, \quad dr = \frac{a_0}{2} dx$$

$r = 0$, $x = 0$, and when $r = 2a_0$, $x = 4$.

$$\begin{aligned}\int_0^{2a_0} r^2 e^{-\frac{2r}{a_0}} dr &= \int_0^4 \left(\frac{a_0 x}{2}\right)^2 e^{-x} \cdot \frac{a_0}{2} dx \\ &= \int_0^4 \frac{a_0^3 x^2}{4} e^{-x} \cdot \frac{1}{2} dx \\ &= \frac{a_0^3}{8} \int_0^4 x^2 e^{-x} dx\end{aligned}$$

$\int_0^4 x^2 e^{-x} dx$

$$\int x^2 e^{-x} dx = -x^2 e^{-x} + 2 \int x e^{-x} dx$$

$$\int x e^{-x} dx = -x e^{-x} - e^{-x} + C$$

So:

$$\int x^2 e^{-x} dx = -x^2 e^{-x} - 2x e^{-x} - 2e^{-x} + C = -e^{-x}(x^2 + 2x + 2) + C$$

$$\begin{aligned}\int_0^4 x^2 e^{-x} dx &= \left[-e^{-x}(x^2 + 2x + 2)\right]_0^4 \\ &= -e^{-4}(16 + 8 + 2) + e^0(0 + 0 + 2) \\ &= -26e^{-4} + 2 = 2 - 26e^{-4}\end{aligned}$$

$$\begin{aligned}\int_0^{2a_0} r^2 e^{-\frac{2r}{a_0}} dr &= \frac{a_0^3}{8}(2 - 26e^{-4}) \\ &= \frac{a_0^3}{4}(1 - 13e^{-4})\end{aligned}$$

If you solve it, it will give you a percentage. Let's replace the missing number.

$$P(r \le a_0) = \int_0^{a_0} 4\pi r^2 |\psi_{1s}(r)|^2 \, dr = \int_0^{a_0} \frac{4r^2}{a_0^3} e^{-2r/a_0} \, dr$$

$$x = \frac{2r}{a_0} \quad \Rightarrow \quad r = \frac{a_0 x}{2}, \quad dr = \frac{a_0}{2} dx$$

$r = 0$, then $x = 0$; and when $r = a_0$, then $x = 2$. We also have:

$$r^2 = \left(\frac{a_0 x}{2}\right)^2 = \frac{a_0^2 x^2}{4}, \quad e^{-2r/a_0} = e^{-x}$$

$$P(r \le a_0) = \int_0^{a_0} \frac{4r^2}{a_0^3} e^{-2r/a_0} \, dr = \frac{4}{a_0^3} \cdot \int_0^{a_0} r^2 e^{-2r/a_0} \, dr$$

$$= \frac{4}{a_0^3} \cdot \int_0^{a_0} \frac{a_0^2 x^2}{4} \cdot e^{-x} \cdot \frac{a_0}{2} dx = \frac{4}{a_0^3} \cdot \frac{a_0^3}{8} \cdot \int_0^2 x^2 e^{-x} dx = \frac{1}{2} \int_0^2 x^2 e^{-x} dx$$

$$\int x^2 e^{-x} \, dx = -e^{-x}(x^2 + 2x + 2) + C$$

$$\int_0^2 x^2 e^{-x} \, dx = [-e^{-x}(x^2+2x+2)]_0^2 = -e^{-2}(4+4+2) + e^0(0+0+2) = -10e^{-2} + 2$$

$$P(r \le a_0) = \frac{1}{2}(2 - 10e^{-2}) = 1 - 5e^{-2}$$

$$e^{-2} \approx 0.1353 \Rightarrow 1 - 5e^{-2} \approx 1 - 0.6767 = 0.3233$$

$$P(r \le a_0) = 1 - 5e^{-2} \approx 0.3233 \quad \text{or } 32.33\%$$

The most likely is near a distance of Bohr.