Engel 9.13

Problem. Calculate the mean value of the radius <*r*> at which you would find the electron in a hydrogen atom in the 210 state.

Answer. The 210 (*2p*) wave function is given on Engel p. 164. The mean value of *r* is the expectation value of *r*.

Integration must be performed with respect to all three spherical polar coordinates, but the radial integral will contain an extra factor of *r* because we are trying to establish the expectation value of this quantity.

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Clear[ψ210, N210, R210, Θ210, a0]
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$$N210 = \frac{1}{4\sqrt{2\pi}}\left(\frac{1}{a0}\right)^{3/2}$$

$$R210 = \left(\frac{r}{a0}\right) e^{-r/(2\,a0)}$$

$$Θ210 = \text{Cos}[\theta]$$

$$ψ210 = N210\ R210\ Θ210$$

$$\frac{\left(\frac{1}{a0}\right)^{3/2}}{4\sqrt{2\pi}}$$

$$\frac{e^{-\frac{r}{2\,a0}}\, r}{a0}$$

$$\text{Cos}[\theta]$$

$$\frac{\left(\frac{1}{a0}\right)^{5/2} e^{-\frac{r}{2\,a0}}\, r\,\text{Cos}[\theta]}{4\sqrt{2\pi}}$$

The wave function is independent of ϕ, so we will do this integration first

$$\phi int = \int_0^{2\pi} d\phi$$

$$2\pi$$

The wave function contains a θ-dependent term, and we must remember to use sin θ dθ as the index of integration

$$\theta int = \int_0^{\pi} Θ210^2\, \text{Sin}[\theta]\, d\theta$$

$$\frac{2}{3}$$

The integration with respect to *r* must also include an extra factor of *r* because this is the operator whose expectation value we want to determine, and r^2 *dr* as the index of integration

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Clear[Rint]
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$$\text{Rint} = \int_0^\infty \text{R210}^2(r)\,(r^2)\,dr$$

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Rint = Simplify[Rint, a0 > 0]
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$$\frac{1}{a0^2}\,\text{If}\left[\text{Re}[a0] > 0,\ 120\,a0^6,\ \text{Integrate}\left[e^{-\frac{r}{a0}}\,r^5,\ \{r, 0, \infty\},\ \text{Assumptions} \to \text{Re}[a0] \le 0\right]\right]$$

$$120\,a0^4$$

a_0 is the Bohr radius and is a positive real quantity, so this fact can be used to obtain the necessary integral. Now we combine the normalization constant and the three integrals ...

$$\text{N210}^2\ \phi\text{int}\ \theta\text{int}\ \text{Rint}$$

$$5\,a0$$

The mean radius of the electron is 5 Bohr radii, about 2.5 angstroms, for this energy state.