PH253 Lecture 17: Hydrogen atom ground state

P. LeClair

Department of Physics & Astronomy The University of Alabama

Spring 2020



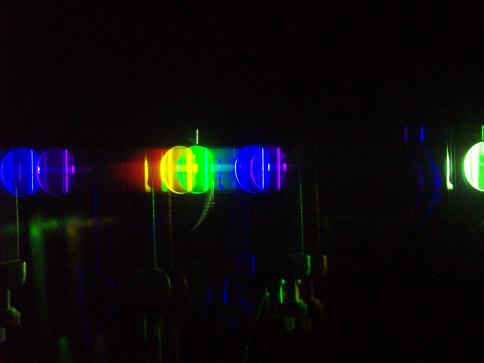
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• Know how to find probability a particle is within some region.



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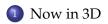
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- HW2: Compton effect, photoelectric effect. All problems similar.

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- HW2: Know how to use the uncertainty principle, particularly for microscope resolution.



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Outline





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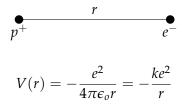


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- First: presume p^+ fixed ($m_p \sim 1800m_e$). Easy to correct later.



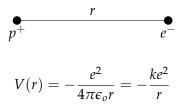
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$$-\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} + V\psi = 0 \quad \text{-or-} \quad \frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} + \left(\frac{e^2}{4\pi\epsilon_0 r} - E\right)\psi = 0$$
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- Just like we did to separate time-dependent Schrödinger ...

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$$\frac{\partial^2 \psi}{\partial x^2} = \frac{\partial^2 \psi}{\partial r^2} \left(\frac{\partial r}{\partial x}\right)^2 + \frac{\partial \psi}{\partial r} \frac{\partial^2 r}{\partial x^2}$$



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• Can do the same for *y* and *z*



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- Can do the same for *y* and *z*
- Just need terms like $\partial r / \partial x$ and $\partial^2 r / \partial x^2$



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$$\frac{\partial r}{\partial x} = \frac{x}{\sqrt{x^2 + y^2 + z^2}} = \frac{x}{r} \qquad \qquad \frac{\partial^2 r}{\partial x^2} = \frac{1}{r} - \frac{x^2}{r^3}$$



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$$\nabla^2 \psi = \frac{\partial^2 \psi}{\partial r^2} \left(\frac{x^2 + y^2 + z^2}{r^2} \right) + \frac{\partial \psi}{\partial r} \left(\frac{3}{r} - \frac{x^2 + y^2 + z^2}{r^3} \right)$$

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$$\frac{\hbar^2}{2m} \left(\frac{\partial^2 \psi}{\partial r^2} + \frac{2}{r} \frac{\partial \psi}{\partial r} \right) + \left(E + \frac{e^2}{4\pi\epsilon_o r} \right) \psi = 0$$



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- Like damped harmonic oscillator, but sign change ...

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- 2nd order equation, 2 arbitrary constants

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- Try Ae^{-cr} fits all conditions



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• Try $\psi(r) = e^{-cr}$ – can fix overall constant *A* with normalization later



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$$\frac{\partial \psi}{\partial r} = -ce^{-cr} = -c\psi$$
$$\frac{\partial^2 \psi}{\partial r^2} = c^2 e^{-cr} = c^2 \psi$$

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• Can already see exponentials will turn our diff. eq. into algebra ...

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$$\frac{\hbar^2}{2m} \left[c^2 e^{-cr} + \frac{2}{r} \left(-ce^{-cr} \right) \right] + \left(E + \frac{e^2}{4\pi\epsilon_o r} \right) e^{-cr} = 0$$

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- Valid for *all r*? Then *r*, 1/*r*, constant terms equate *separately*



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$$E = -\frac{\hbar^2 c^2}{2m} \quad \text{-or-} \quad E = -\frac{me^4}{2 (4\pi\epsilon_o)^2 \hbar^2} = E_{n=1,\text{Bohr}}$$

So what



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• Energy is negative, bound state. Atom is stable!



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- Normalize, $\langle r \rangle$, and so on



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- With $\psi(r)$ properly normalized, we can get P(r) and move on.
- $P(x) dx \rightarrow P(r, \theta, \varphi) dV$ now
- This is the hydrogen 1*s* state. What about 2, and *p*, *d*, *f*?



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$$P(r) = |\psi(r)|^2 4\pi r^2 = \left| \frac{1}{\sqrt{\pi a_o^3}} e^{-r/a_o} \right|^2 4\pi r^2 = \frac{4r^2}{a_o^3} e^{-2r/a_o}$$

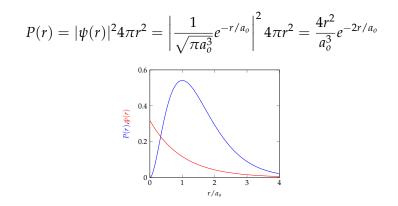
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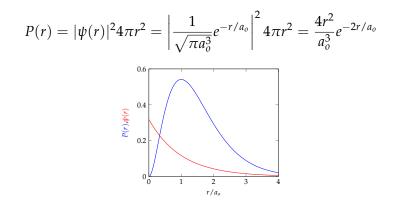


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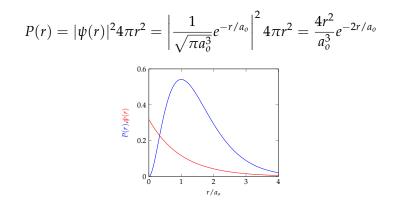
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- This happens at $r = a_0$, semi-classical orbit radius from Bohr



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- Again: in spite of *distribution*, measurement yields 1 *e*⁻ at one spot

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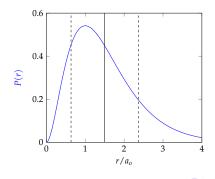


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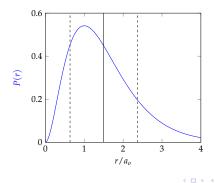
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- Pretty spread out! No "orbit" indeed; uncertainty in position.







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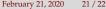
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• Once again: $\int_0^\infty x^n e^{-ax} dx = n!/a^{n+1} \dots$ I told you this would keep showing up

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- I.e., closer than Bohr radius, impossible in Bohr model

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- Need fewer assumptions, better mechanics, more math



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