# PH253 Lecture 17: Hydrogen atom ground state 

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


## Outline

(1) Now in 3D

## How do we use Schrödinger's equation in 3D?

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\stackrel{p^{+}}{e^{-}} \\
V(r)=-\frac{e^{2}}{4 \pi \epsilon_{o} r}=-\frac{k e^{2}}{r} \\
-\frac{\hbar^{2}}{2 m} \frac{\partial^{2} \psi}{\partial x^{2}}+V \psi=0 \quad \text {-or- } \frac{\hbar^{2}}{2 m} \frac{\partial^{2} \psi}{\partial x^{2}}+\left(\frac{e^{2}}{4 \pi \epsilon_{o} r}-E\right) \psi=0
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- Rectangular coordinate system, radial potential = pain


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- Second: presume $\Psi(r, \theta, \varphi)=f(\theta, \varphi) \psi(r)$ - separable


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- Just like we did to separate time-dependent Schrödinger ...


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- Try $A e^{-c r}$ - fits all conditions


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


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


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\frac{\hbar^{2} c^{2}}{2 m}+\frac{\hbar^{2}}{2 m} \frac{2}{r}(-c)+\left(E+\frac{e^{2}}{4 \pi \epsilon_{o} r}\right)=0
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- Normalize, $\langle r\rangle$, and so on


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- Again: in spite of distribution, measurement yields $1 e^{-}$at one spot


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- Next? Need $\theta, \varphi$ dependence for other orbitals ( $p, d, f$ orbitals)


## Probability of finding within a region?

- Specifically, probability $e^{-}$is in $\left[0, a_{0}\right]$ ?
- I.e., closer than Bohr radius, impossible in Bohr model

$$
P\left(r \text { in }\left[0, a_{0}\right]\right)=\frac{4}{a_{0}^{3}} \int_{0}^{a_{0}} r^{2} e^{-2 r / a_{0}} d r=\frac{1}{2} \int_{0}^{2} u^{2} e^{-u} d u \approx \frac{1}{3}
$$

- Numerical evaluation is straightforward and well-tabulated
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- Also excited $s$ states. Need a better approach, but a good start!


## Probability of finding within a region?

- Specifically, probability $e^{-}$is in $\left[0, a_{0}\right]$ ?
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$$
P\left(r \text { in }\left[0, a_{0}\right]\right)=\frac{4}{a_{0}^{3}} \int_{0}^{a_{o}} r^{2} e^{-2 r / a_{o}} d r=\frac{1}{2} \int_{0}^{2} u^{2} e^{-u} d u \approx \frac{1}{3}
$$

- Numerical evaluation is straightforward and well-tabulated
- Next? Need $\theta, \varphi$ dependence for other orbitals ( $p, d, f$ orbitals)
- Also excited s states. Need a better approach, but a good start!
- Need fewer assumptions, better mechanics, more math

