

Arvind Borde / PHY 19, Week 11: Hydrogen Again

§11.1 The Schrödinger Equation in 3d

In three-dimensions, the \mathcal{S} eq. is

where

$$\nabla^2 \equiv \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$$

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Here, too, if we assume that

$$\Psi(x, y, z, t) = \psi(x, y, z)\phi(t)$$

then we get

$$-\frac{\hbar^2}{2m}\nabla^2\psi + U(x, y, z)\psi = E\psi$$

$$i\hbar\frac{\partial\phi}{\partial t} = E\phi$$

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§11.2 Spherical Symmetry

A convenient coordinate to use here is the usual radial coordinate r , given by

$$r^2 = x^2 + y^2 + z^2$$

(1) Find $\partial r/\partial x$.

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(2) If $f = f(r)$ is a function of r , what is $\partial f/\partial x$?

$$\frac{\partial f(r)}{\partial x} =$$

Assuming that ψ is a function of r alone,

$$\frac{\partial\psi}{\partial x} = \frac{x}{r} \frac{d\psi}{dr}$$

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(3) Find $\partial^2\psi/\partial x^2$.

$$\frac{\partial^2\psi}{\partial x^2} =$$

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(4) Find $\nabla^2\psi = \frac{\partial^2\psi}{\partial x^2} + \frac{\partial^2\psi}{\partial y^2} + \frac{\partial^2\psi}{\partial z^2}$.

$$\nabla^2\psi =$$

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ADDITIONAL NOTES

Let $f' \equiv df/dr$.

(5) What's $(r\psi)'$?

(6) What's $(r\psi)''$?

(7) Recognize this?

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Let $\hat{\psi}(r) = r\psi(r)$.

(8) Write the 3-d time-ind. S eq.

$$-\frac{\hbar^2}{2m}\nabla^2\psi(r) + U(x, y, z)\psi(r) = E\psi(r)$$

in terms of $\hat{\psi}(r)$. (Hint: Multiply the above by r .)

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§11.3 The Hydrogen Atom

Since the proton is around a thousand times as massive as the electron (similar to the sun-Jupiter system), we'll consider this as a problem of an electron moving in an electrostatic potential created by a fixed proton.

The potential is only a function of the distance between the electron and the proton.

All this is true for any spherically symmetric case.

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For the Hydrogen atom,

$$U(r) =$$

The equation for $\hat{\psi}$ becomes

Let's try $\hat{\psi}(r) = re^{-\alpha r}$.

(9) Find $\hat{\psi}'(r)$.

$$\hat{\psi}'(r) =$$

(10) Find $\hat{\psi}''(r)$.

$$\hat{\psi}''(r) =$$

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ADDITIONAL NOTES

(11) Plug this into the \mathcal{S} eq.

For this to be a respectable solution, it must work for all r .

(12) What's a good r to try?

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(13) So, what's α ?

(14) Does this look familiar? _____

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α^{-1} is the first Bohr radius.

The associated E is the ground state Bohr energy.

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§11.4 Remarks on Helium

We model this, again, as a fixed nucleus with two electrons buzzing around it.

The potential energy is

$$-k \frac{2e^2}{r_1} - k \frac{2e^2}{r_2} + k \frac{e^2}{r_{12}}$$

(15) Can you interpret these terms? _____

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The problem can be treated exactly if we ignore the electron-electron interaction.

It can be treated approximately, with that term.

The analysis gives energy levels that agree with observation.

This may also be done with more complicated atoms.

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ADDITIONAL NOTES
