

Fundamentals of Nanoelectronics

Prof. Supriyo Datta
ECE 453
Purdue University

09.10.2004

Lecture 7: Hydrogen Atom

Ref. Chapter 2.1

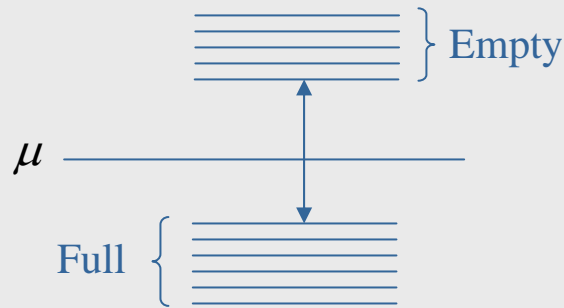


Network for Computational Nanotechnology

nanoHUB NCN
online simulations and more

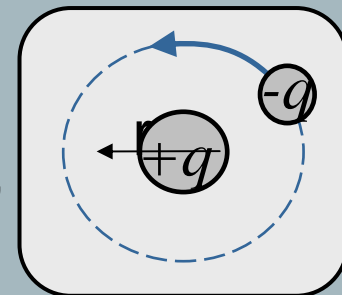
Energy Levels Hydrogen Atom

00:02



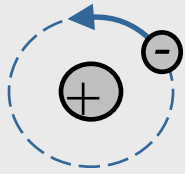
- As we've been discussing, any material that forms the channel in a transistor can be visualized in terms of its energy levels. Current flow is introduction of an electron top one side of the channel and its going out from the other side. Any time an electron enters the channel, it has to go into an empty level. Taking out an electron involves and electron getting out of a filled level.
- Given a set of energy levels or Density of States (DOS), we've talked about the I-V characteristics of a device. What we want to understand now is how to model such energy levels / DOS.

- To achieve this, scientists started with the simplest material possible, namely the Hydrogen atom.



- A natural way to think about this atom is that the positive charge attracts the negative charge and the electron (negative charge) will circle around the proton kind of like rotation of earth around sun.

H atom Energy Levels (Early Understanding)



Electron rotates on a circle of radius r with velocity v . The radius and the velocity can be related to each other by equating the electrostatic and the centripetal forces.

- Equate electrostatic and centripetal forces: $\frac{Zq^2}{4\pi\epsilon_0 r^2} = \frac{mv^2}{r}$
- Thus, velocity can be computed in terms of other quantities from the above.
- Total system energy is given as: $E = \text{Potential} + \text{Kinetic}$. Incorporating the above results we can get an expression for the energy.

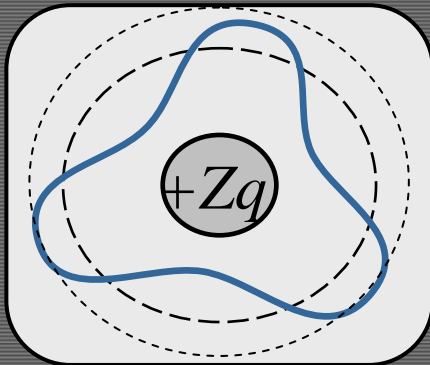
$$E = \frac{-Zq^2}{4\pi\epsilon_0 r} + \frac{1}{2}mv^2 = \frac{-Zq^2}{4\pi\epsilon_0 r} + \frac{1}{2}m\left(\frac{Zq^2}{4\pi\epsilon_0 mr}\right) = \frac{-Zq^2}{8\pi\epsilon_0 r}$$

- But this is wrong! There are two main problems:
 - One: energy is not discrete (r is continuous)! The experiments showed that the energy is actually discrete. Electron slides down in energy and emits a photon. The fact is that the frequency of this light is discrete indicating the discreteness of energy levels.
 - Two: the electron is under continual centripetal acceleration and so must radiate electromagnetic waves, eventually collapsing into the nucleus.

H atom Energy Levels (Correct view point)

11:57

- To explain the discreteness of the energy levels, Bohr postulated a second relation for the velocity of electron and the radius of the circle it rotates: $2\pi r = nh / mv$ (n: integer)
- This relation was successful in explaining the experiments. To explain this:
 - de Broglie suggested that we endow the electron with wave like properties. The wavelength of the electron, λ , should then be: $\lambda = h / (mv)$. (v is the velocity of electron). Since it is a wave an integer number of wavelengths must fit in the circle's circumference.



- Accepting these relations, we can derive the right expression for the energy levels of a hydrogen atom. Use:

$$1) \frac{Zq^2}{4\pi\epsilon_0 r^2} = \frac{mv^2}{r}, \quad 2) 2\pi r = nh / mv$$

- To write: $m^2 v^2 = \frac{n^2 \hbar^2}{4\pi^2 r^2} = \frac{Zq^2 m}{4\pi\epsilon_0 r}$
- Finding "r" from above (a_0 : Bohr radius):

$$r_n = \frac{n^2 \epsilon_0 \hbar^2}{Z \pi m q^2} \Rightarrow r_0 \approx 5 \times 10^{-11} m \equiv a_0$$
- We see that the radius is quantized. It is a principal number a_0 time n^2 . But this explains why the energy is quantized:

$$E_n = \frac{-Zq^2}{8\pi\epsilon_0 r_n} = -\frac{Z^2}{n^2} \frac{q^2}{8\pi\epsilon_0 a_0}$$

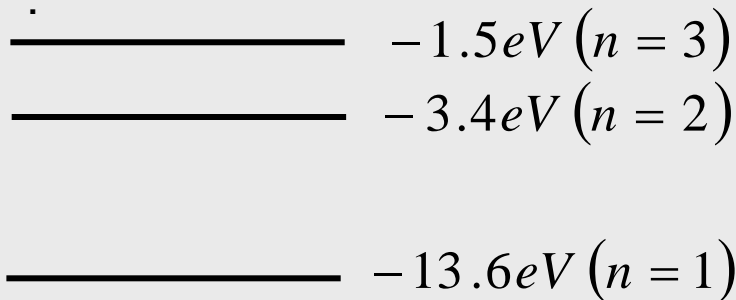
- Summarizing the results...

$$E_n = -\frac{Z^2}{n^2} \left(\frac{q^2}{8\pi\epsilon_0 a_0} \right), \quad \left(a_0 \equiv \frac{\epsilon_0 h^2}{\pi m q^2} \right)$$

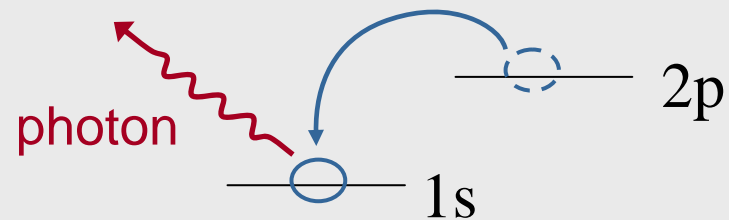
$$E_0 = -\frac{1^2}{1^2} \left(\frac{1.6 \times 10^{-19}}{8 \times 3.14 \times 10^{-12} \times 5.29 \times 10^{-11}} \right) = -13.6 eV$$

- What helped us to get here is the important relation: $2\pi r = nh / mv$
- We can use the expression for energy to write:

Discrete Energy Levels



This process of photon emission produces light with discrete frequencies



- We've seen that with a relatively simple model, one could get all the right answers for the H atom energy levels. In order to do this a big postulate beyond classical mechanics was needed: $2\pi r = nh/mv$
- The evidence for the correctness of the described model was the measurement of the frequency of emitted light, which matched the model's prediction:

$$h\nu = E_0 \left(\frac{1}{n_1^2} - \frac{1}{n_2^2} \right) \quad E_0 = 13.6eV$$

- So people realized that this model was right. The next step was to come up with a theory/equation that could explain this and tell one what to do in a different situation. A general scheme was needed. In 1930's Schrödinger came up with the idea. Even today his equation is the starting point to understand energy levels in materials.

- Schrödinger equation:

$$i\hbar \frac{\partial \Psi}{\partial t} = \frac{-\hbar^2}{2m} \nabla^2 \Psi + U(r)\Psi$$

- U is the potential energy. For H atom this is the potential energy that electron feels due to the positive nucleolus:

$$U = -\frac{q^2}{4\pi\epsilon_0 r}$$

- By solving his equation, Schrödinger showed, one gets solutions of the form:

$$\psi_n(\vec{r}, t) = e^{-iE_n t/\hbar} \phi_n(\vec{r})$$

- Which is called a wavefunction. For each value of n, there is a wavefunction and a corresponding energy. The expression for the energy, exactly matches the one we got earlier today. Since it is impossible to solve the equation analytically for anything beyond Hydrogen atom, we'll learn to solve it numerically.