

Fundamentals of Nanoelectronics

ECE495 - Session 11, Sept 18, 2009

Charging Energy

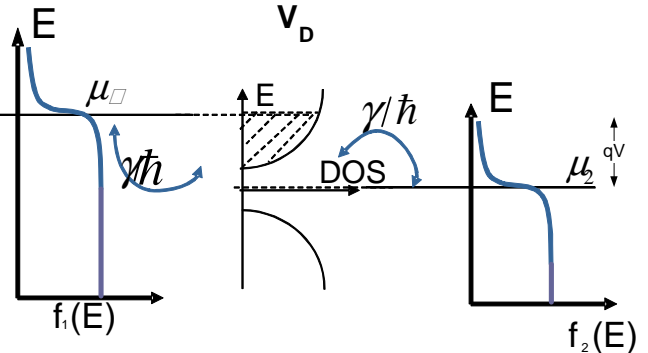
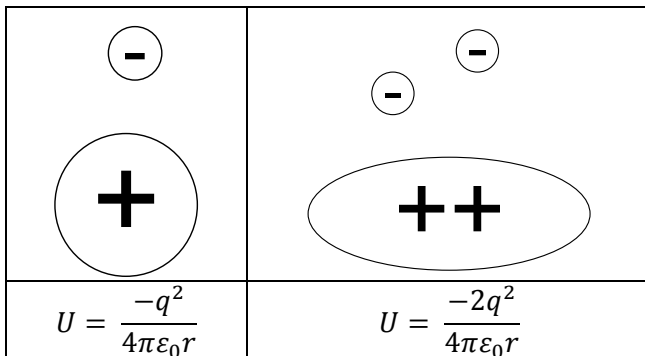
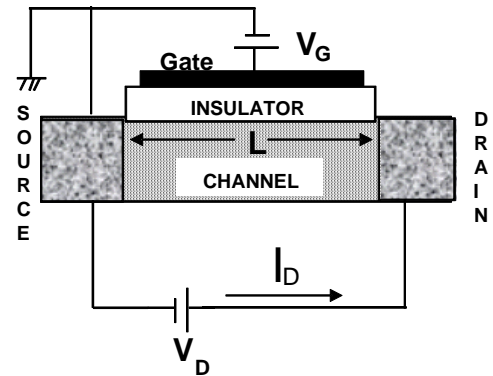
Ref: Chapters 3.1

Professor Supriyo Datta

Class notes taken by: Mehdi Salmani

$$E\Psi = -\frac{\hbar^2}{2m}\nabla^2\Psi + U_N(\vec{r})\Psi$$

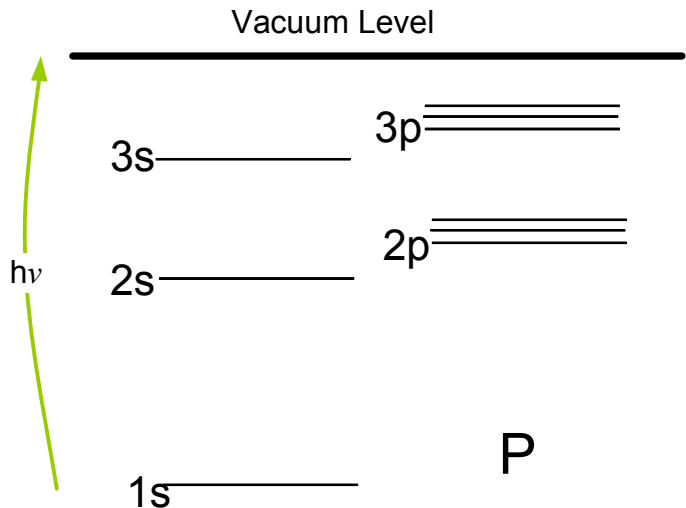
If we use the above equation for Helium, we will not get correct answer.



For electronic energy levels we also have to include the potential due to the other electron which is a **repulsive** potential. So we need to add something to U_N . But we do not know that potential unless we know the electron's wave function. The electron wavefunction has to be found from Schrödinger equation which requires the electron potential to be solved. Then Schrodinger equation will change

to
$$E\Psi = \left(-\frac{\hbar^2}{2m}\nabla^2 + U_N(\vec{r}) + U_e\right)\Psi$$

- First ionization
- Second ionization
- Third ionization



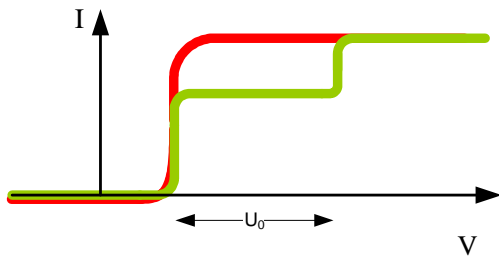
To solve the new Schrödinger equation we need to use **Self Consistent Field (SCF)**. method One starts with a reasonable guess for U_e . Then solves the Schrödinger equation and finds the wavefunctions which in turn gives the electron density:

$$n(\vec{r}) = \Psi^* \Psi$$

From electron density one finds the corresponding potential and compares it with the initial guess and modifies the guess to match the calculated result better. This process goes on till the answer converges. That is to say the guessed value and the calculated value are very close to each other.

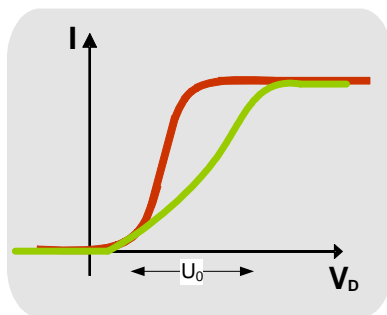
SCF is not exact solution but it is a good approximate.

The broken curve shows the effect of electron-electron interaction.

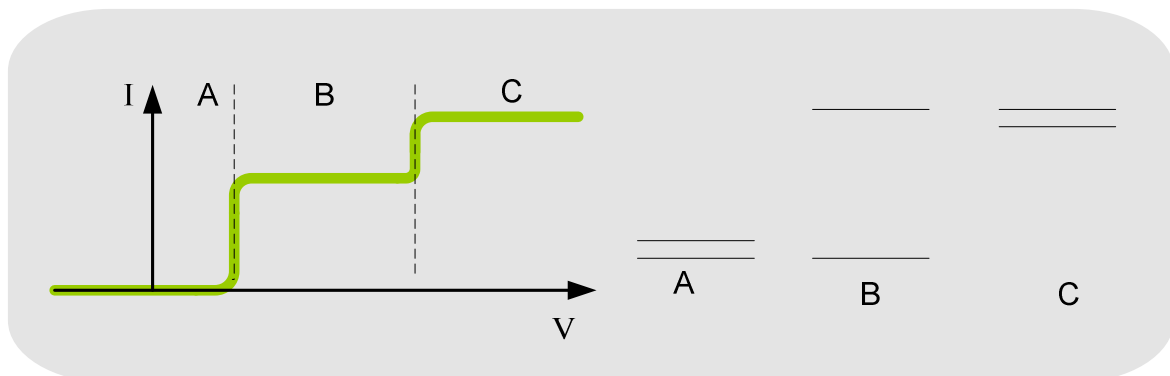


$$2 \frac{q}{\hbar} \frac{\gamma_1 \gamma_2}{\gamma_1 + \gamma_2} \xrightarrow{\text{if}} \gamma_1 = \gamma_2 \xrightarrow{\text{yields}} 2 \frac{q}{\hbar} \frac{\gamma_1}{2} = \frac{q \gamma_1}{\hbar}$$

When we use SCF we will achieve I-V characteristics like below:



$$U = U_L + U_0 \Delta N$$



SIC Self Interaction Correction: Each electron does not feel anything from itself only from others. That is the reason why only one level floats up and not both them. This is part that makes hard to add it up to Schrödinger equation and solve it.