FUNDAMENTALS OF NANOELECTRONICS

B. Quantum Transport

Schrodinger Equation →

2. Contact-ing Schrodinger

3. Advanced Examples

4. Spin Transport

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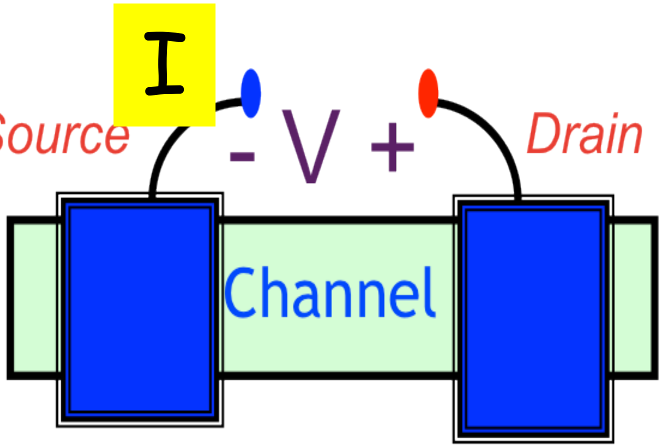
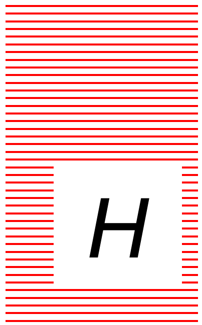
http://nanohub.org/groups/lnebook



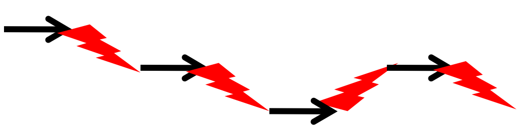
$$E\psi = H\psi$$

Schrodinger + = NEGF

Quantum Transport



Semiclassical Transport



Entropy driven *Force driven*

Newton + =

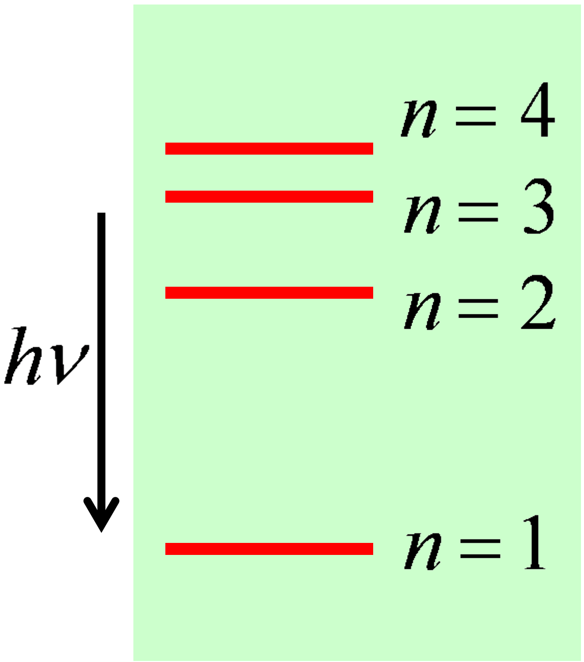
1.1b Introduction

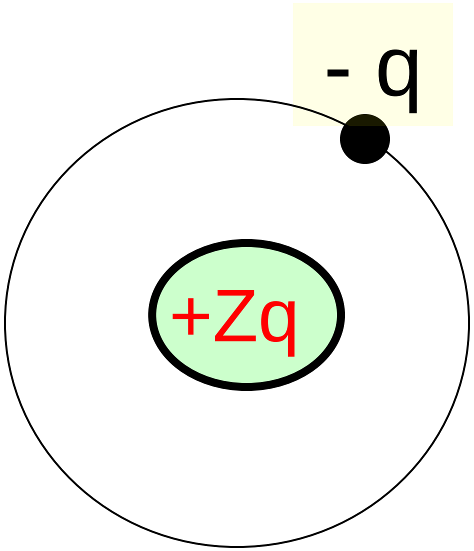
$$E = -\frac{Zq^2}{4\pi\varepsilon_0 r} + \frac{mv^2}{2} = -\frac{Zq^2}{8\pi\varepsilon_0 r}$$

$$\boxed{E_n = -\frac{Zq^2}{8\pi\varepsilon_0 r_n} = -\frac{Z^2}{n^2}\,\frac{q^2}{8\pi\varepsilon_0 a_0}}$$

$$n\frac{h}{mv} = 2\pi r$$

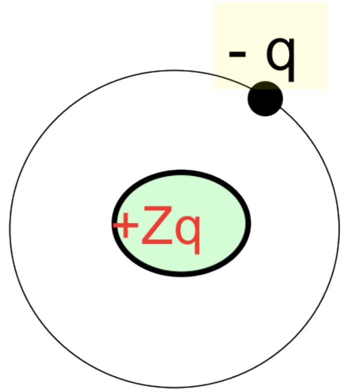
$$r_n = \underbrace{\frac{4\pi\varepsilon_0 \hbar^2}{m q^2}}_{\equiv\, a_0} \times \frac{n^2}{Z}$$





$$v = \sqrt{\frac{Zq^2}{4\pi\varepsilon_0 mr}} \leftarrow \frac{Zq^2}{4\pi\varepsilon_0 r^2} = \frac{mv^2}{r}$$

$$a_0 = \frac{4\pi\varepsilon_0 \hbar^2}{m q^2}$$

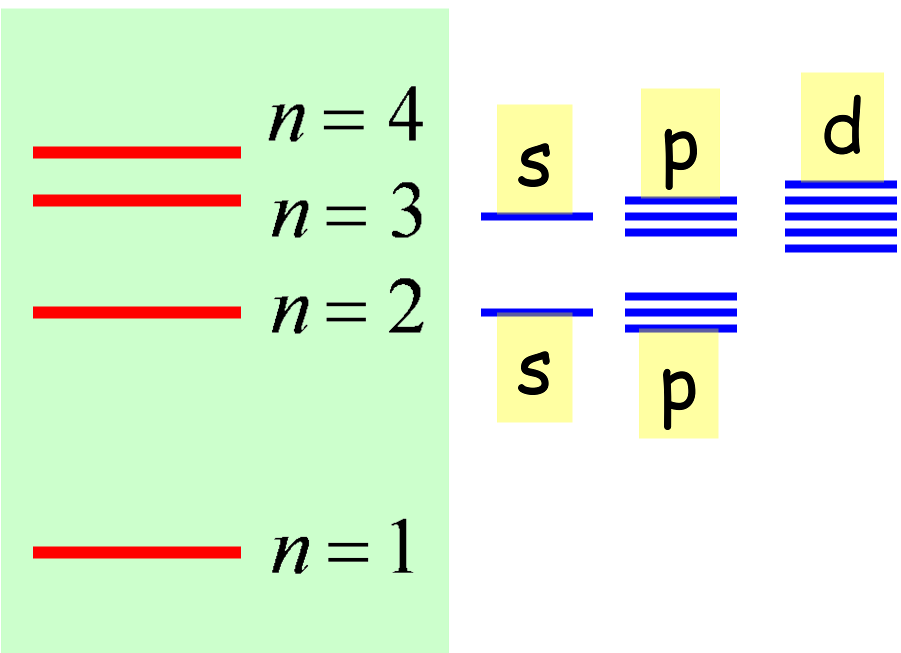


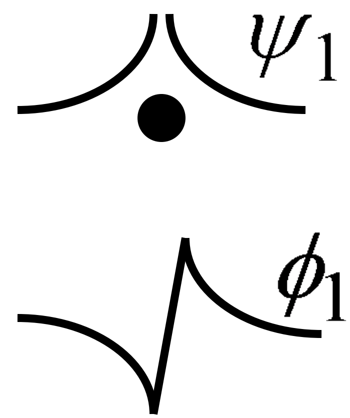
$$n \frac{h}{mv} = 2\pi r$$

$$E_n = -\frac{Z^2}{n^2}\frac{q^2}{8\pi\varepsilon_0 a_0}$$

$$E\psi(\vec{r}) = \left(-\frac{\hbar^2}{2m}\nabla^2 + U(\vec{r})\right)\psi(\vec{r})$$

$$-\frac{Zq^2}{4\pi\varepsilon_o r}$$





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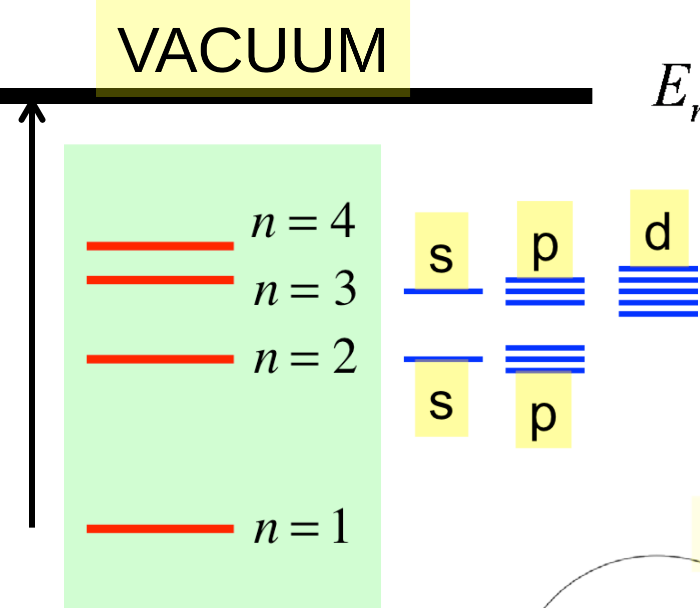
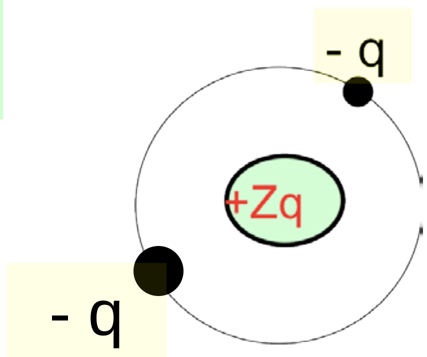
1.1d Introduction

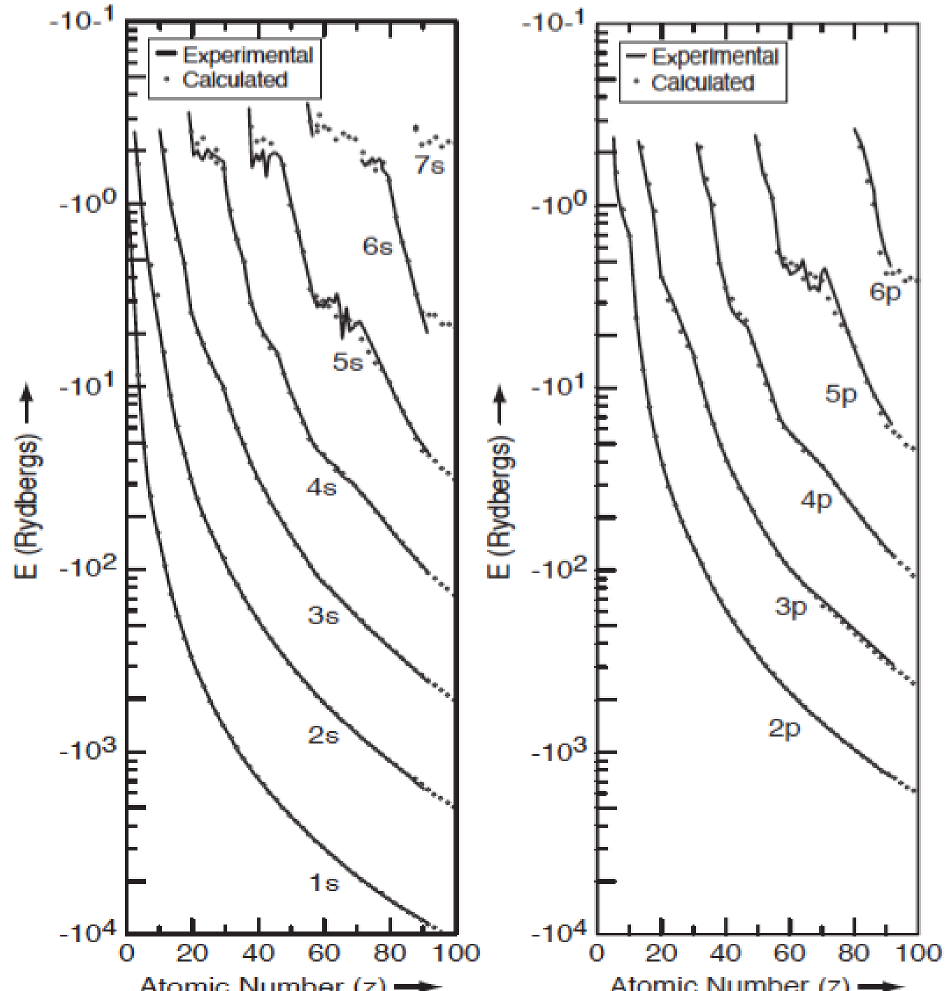


$$E_n = -\frac{Z^2}{n^2}\,\frac{q^2}{8\pi\varepsilon_0 a_0}$$

13.6 eV



Herman & Skillman (1963)



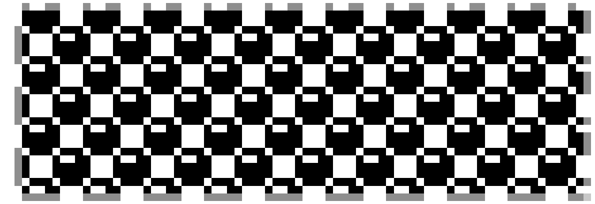
$$E\,\psi(\vec{r}) = \left(-\frac{\hbar^2}{2m}\nabla^2 + U(\vec{r})\right)\psi(\vec{r})$$

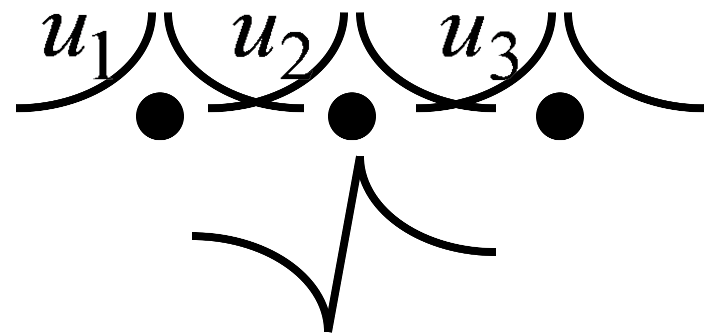
$$-\frac{Zq^2}{4\pi\varepsilon_o r} \qquad +U_{ee}$$

1.1e Introduction

N x N

$$E\,[S]\begin{Bmatrix}\psi_1\\ \psi_2\\ \cdots\\ \cdots\\ \psi_N\end{Bmatrix} = \begin{bmatrix}\cdots & \cdots & \cdots\\ \cdots & H & \cdots\\ \cdots & \cdots & \cdots\end{bmatrix}\begin{Bmatrix}\psi_1\\ \psi_2\\ \cdots\\ \cdots\\ \psi_N\end{Bmatrix}$$





$$H_{mn} = \int dV\, u_m^*(\vec{r})\, H_{op}\, u_n(\vec{r})$$

$$S_{mn} = \int dV\, u_m^*(\vec{r})\, u_n(\vec{r})$$

$$E\,\psi(\vec{r}) = \left(-\frac{\hbar^2}{2m}\nabla^2 + U(\vec{r})\right)\psi(\vec{r})$$

$$-\frac{Z\,q^2}{4\pi\varepsilon_o r} \qquad + U_{ee}$$

$$\psi(\vec{r}) = \sum_{m=1}^{N}\psi_m\, u_m(\vec{r})$$

N = number of “basis functions”

1.1f Introduction

N x N

$$E\,[S]\begin{Bmatrix}\psi_1\\ \psi_2\\ \cdots\\ \cdots\\ \psi_N\end{Bmatrix} = \begin{bmatrix}\cdots & \cdots & \cdots\\ \cdots & H & \cdots\\ \cdots & \cdots & \cdots\end{bmatrix}\begin{Bmatrix}\psi_1\\ \psi_2\\ \cdots\\ \cdots\\ \psi_N\end{Bmatrix}$$

How to write [H]?

- First Principles
- Semi - empirical

$$H_{mn} = \int dV\, u_m^*(\vec{r})\, H_{op}\, u_n(\vec{r})$$

$$S_{mn} = \int dV\, u_m^*(\vec{r})\, u_n(\vec{r})$$

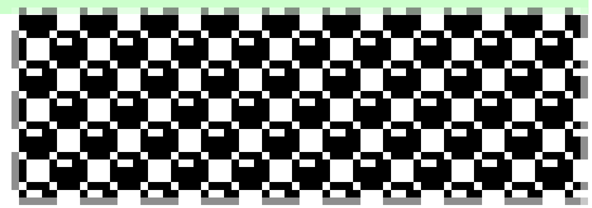
$$E\,\psi(\vec{r}) = \left(-\frac{\hbar^2}{2m}\nabla^2 + U(\vec{r})\right)\psi(\vec{r})$$

$$-\frac{Z q^2}{4\pi\varepsilon_o r}$$

$$+U_{ee}$$

Bandstructure

Eigenvalues of a Periodic Matrix



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Coming up next ..

Bandstructure

Eigenvalues of a Periodic Matrix