FUNDAMENTALS OF NANOELECTRONICS

B. Quantum Transport

1. Schrodinger Equation →

2. Contact-ing Schrodinger

3. Advanced Examples

4. Spin Transport

1.1. Introduction

1.2. Wave Equation

1.3. Differential to Matrix Equation

1.4. Dispersion Relation

1.5. Counting States

1.6. Beyond 1-D

1.7. Lattice with a Basis

1.8. Graphene

1.9. Valleys

1.10. Summing up ..

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May 2015

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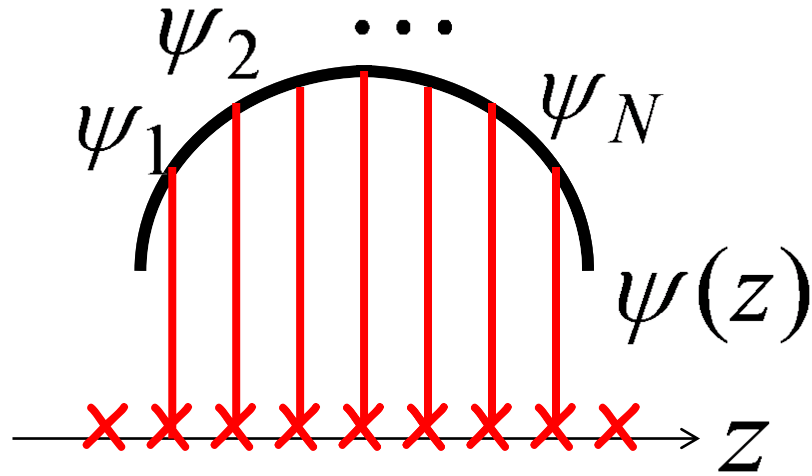
1.3a Differential to Matrix

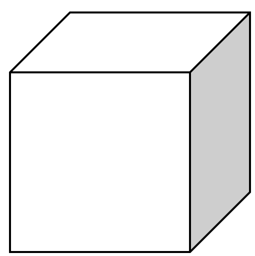
N x N

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

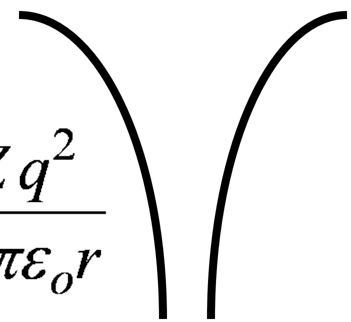


$$E\psi(\vec{r}) = \left(-\frac{\hbar^2}{2m}\nabla^2 + U(\vec{r})\right)\psi(\vec{r})$$

$$100^3 = 10^6\;!!$$



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



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1.3b Differential to Matrix

$$E\begin{bmatrix}1 & s\\ s & 1\end{bmatrix}\begin{Bmatrix}\psi_1\\ \psi_2\end{Bmatrix} = \begin{bmatrix}\varepsilon & t\\ t & \varepsilon\end{bmatrix}\begin{Bmatrix}\psi_1\\ \psi_2\end{Bmatrix}$$

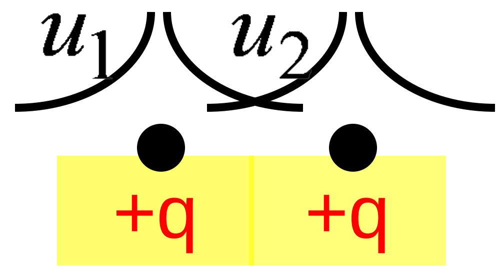
$$E\begin{Bmatrix}\psi_1\\ \psi_2\end{Bmatrix} = \begin{bmatrix}1 & s\\ s & 1\end{bmatrix}^{-1}\begin{bmatrix}\varepsilon & t\\ t & \varepsilon\end{bmatrix}\begin{Bmatrix}\psi_1\\ \psi_2\end{Bmatrix}$$

$$E\begin{Bmatrix}\psi_1\\ \psi_2\end{Bmatrix} = \frac{1}{1-s^2}\begin{bmatrix}\varepsilon - ts & t-\varepsilon s\\ t-\varepsilon s & \varepsilon - ts\end{bmatrix}\begin{Bmatrix}\psi_1\\ \psi_2\end{Bmatrix}$$

$$\frac{\varepsilon - t}{1-s} \quad and \quad \frac{\varepsilon + t}{1+s}$$

$$E[S]\{\psi\} = [H]\{\psi\}$$

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



Hydrogen Molecule

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

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

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

N = number of "basis functions"

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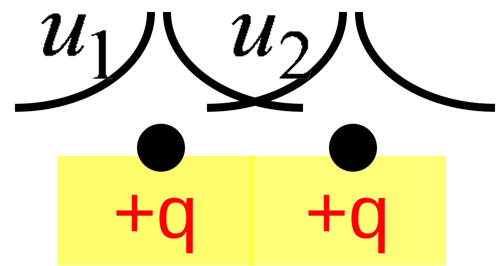
1.3c Differential to Matrix

$$E\begin{bmatrix}1 & s\\ s & 1\end{bmatrix}\begin{Bmatrix}\psi_1\\ \psi_2\end{Bmatrix} = \begin{bmatrix}\varepsilon & t\\ t & \varepsilon\end{bmatrix}\begin{Bmatrix}\psi_1\\ \psi_2\end{Bmatrix}$$

- First Principles
- Semi - empirical



Hydrogen Molecule

$$E\begin{Bmatrix}\psi_1\\ \psi_2\end{Bmatrix} = \frac{1}{1-s^2}\begin{bmatrix}\varepsilon - ts & t-\varepsilon s\\ t-\varepsilon s & \varepsilon - ts\end{bmatrix}\begin{Bmatrix}\psi_1\\ \psi_2\end{Bmatrix}$$

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

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

$$\frac{\varepsilon - t}{1-s} \qquad \frac{\varepsilon + t}{1+s}$$

$$E[S]\{\psi\} = [H]\{\psi\}$$

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

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

N = number of "basis functions"

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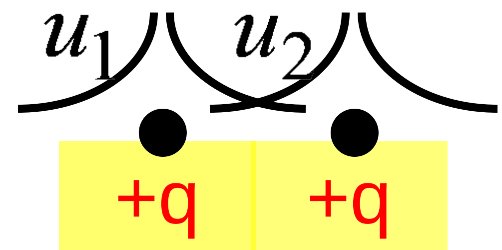
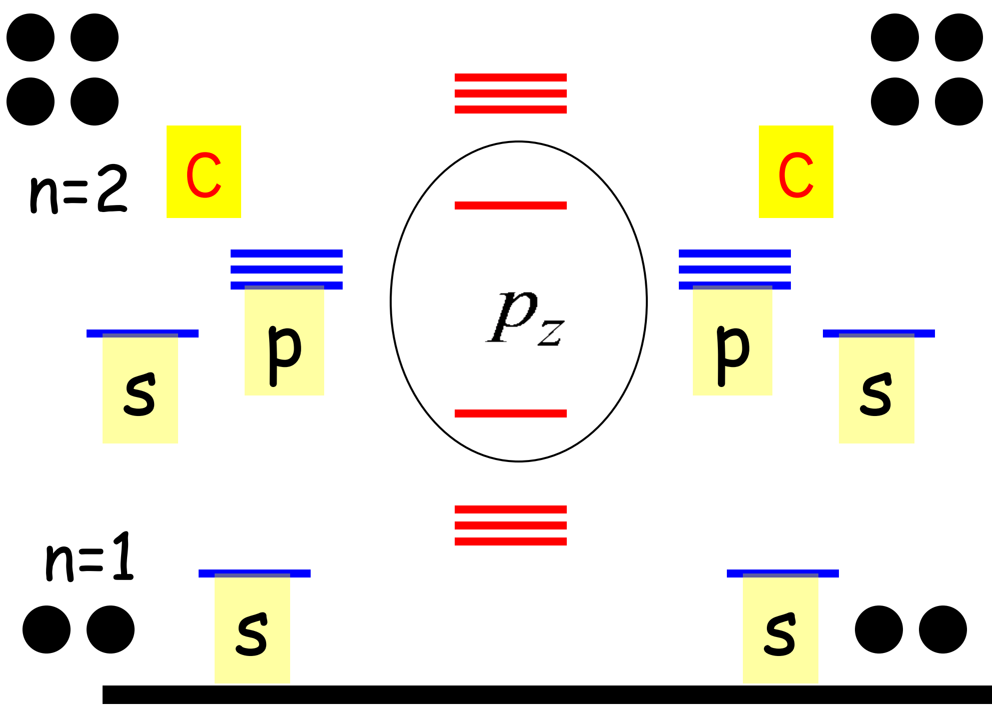
1.3d Differential to Matrix

$$E\begin{Bmatrix}\psi_1\\ \psi_2\end{Bmatrix} = \frac{1}{1-s^2}\begin{bmatrix}\varepsilon - ts & t-\varepsilon s\\ t-\varepsilon s & \varepsilon - ts\end{bmatrix}\begin{Bmatrix}\psi_1\\ \psi_2\end{Bmatrix}$$

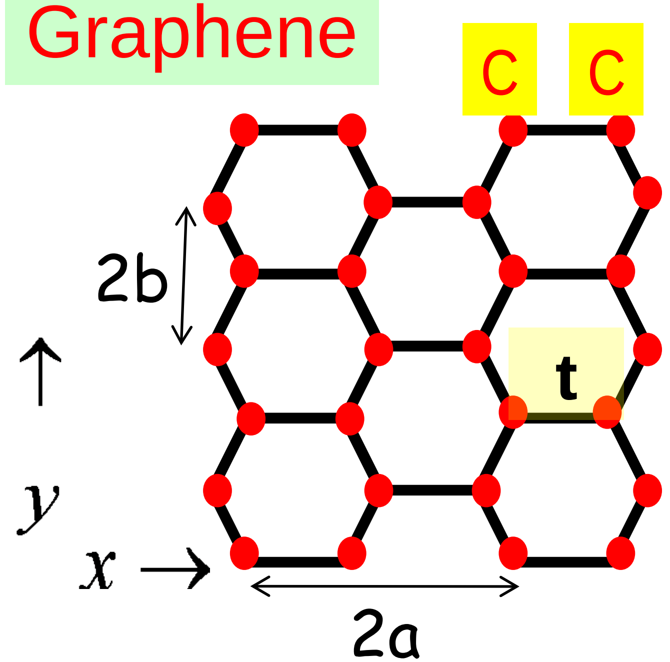
$$\frac{\varepsilon - t}{1-s} \qquad \frac{\varepsilon + t}{1+s}$$

Hydrogen Molecule





Graphene



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Coming up next ..

Bandstructure

Eigenvalues of a Periodic Matrix