

FUNDAMENTALS OF NANOELECTRONICS

B. Quantum Transport

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. Matrix Equation with Basis

1.8. Graphene

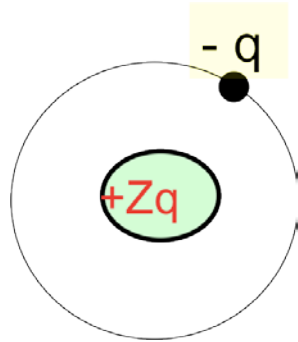
1.9. Valleys

1.10. Summing up ..

1.2a Wave Equation

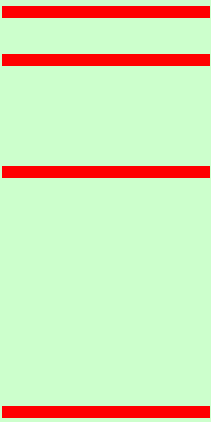
$$E_n = -\frac{Z^2}{n^2} \frac{q^2}{8\pi\epsilon_0 a_0} \quad n \frac{h}{m v} = 2\pi r$$

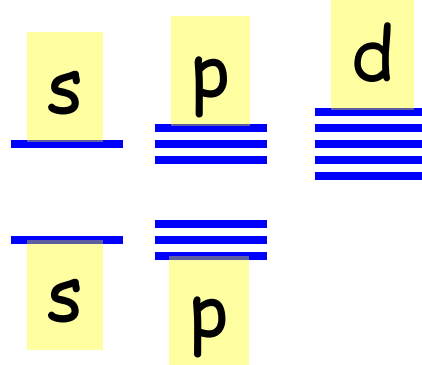
$$a_0 = \frac{4\pi\epsilon_0 \hbar^2}{m q^2}$$



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

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


 $n = 4$
 $n = 3$
 $n = 2$
 $n = 1$



Waves when confined
show resonant
energies / frequencies

1.2b Wave Equation

$$E \psi(\vec{r}) = \left(-\frac{\hbar^2}{2m} \nabla^2 + U_0 \right) \psi(\vec{r})$$

$$\begin{aligned} \psi(\vec{r}) &= e^{+ik_x x} e^{+ik_y y} e^{+ik_z z} \psi_0 \\ &= e^{+i\vec{k} \odot \vec{r}} \psi_0 \end{aligned}$$

$$E(\vec{k}) = \frac{\hbar^2}{2m} (k_x^2 + k_y^2 + k_z^2) + U_0$$

Dispersion relation

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

$$\vec{k} \odot \vec{r} = k_x x + k_y y + k_z z$$

$$\vec{k} = k_x \hat{x} + k_y \hat{y} + k_z \hat{z}$$

$$E \cancel{\psi(\vec{r})} = \left(\frac{\hbar^2}{2m} (k_x^2 + k_y^2 + k_z^2) + U_0 \right) \cancel{\psi(\vec{r})}$$

$$\frac{\partial}{\partial x} \rightarrow ik_x \rightarrow \frac{\partial^2}{\partial x^2} \rightarrow (ik_x)^2 = -k_x^2$$

$$\vec{r} = x \hat{x} + y \hat{y} + z \hat{z}$$

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

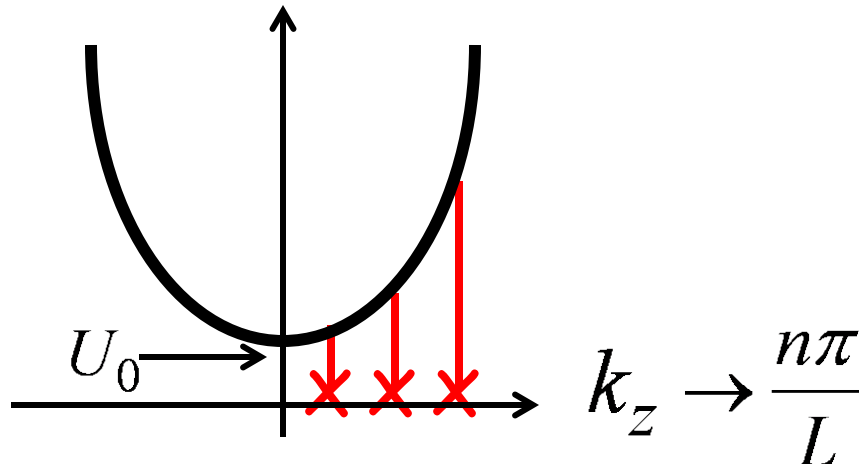
$$E\psi(\vec{r}) = \left(-\frac{\hbar^2}{2m} \nabla^2 + U_0 \right) \psi(\vec{r})$$

$$\psi(\vec{r}) = e^{+i\vec{k}\cdot\vec{r}} \psi_0$$

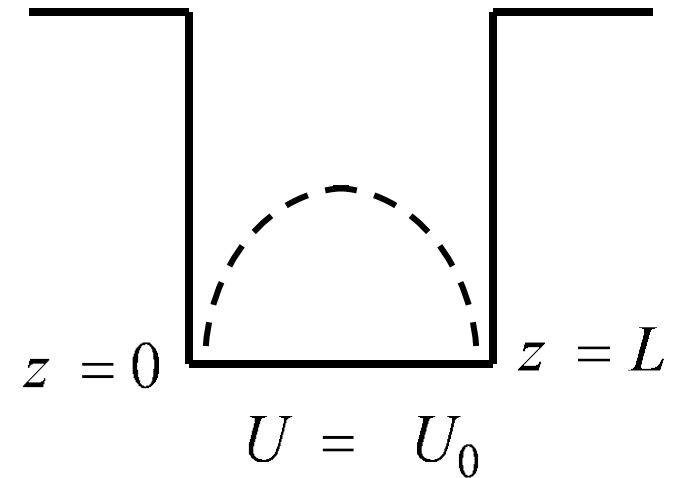
$$E(\vec{k}) = \frac{\hbar^2}{2m} (k_x^2 + k_y^2 + k_z^2) + U_0$$

Dispersion relation

$$1-D: \quad E = \frac{\hbar^2 k_z^2}{2m} + U_0$$



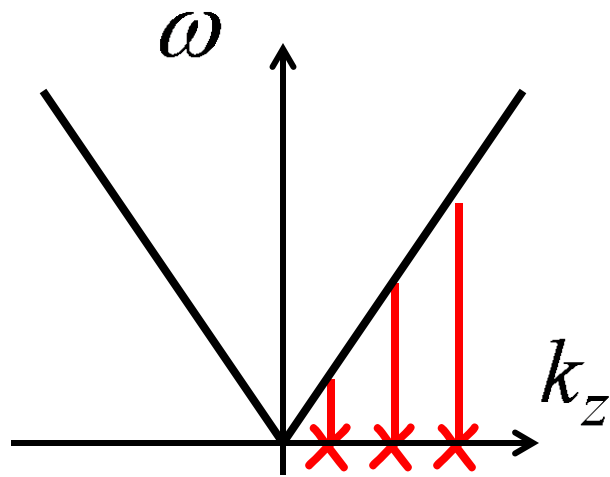
1.2c Wave Equation



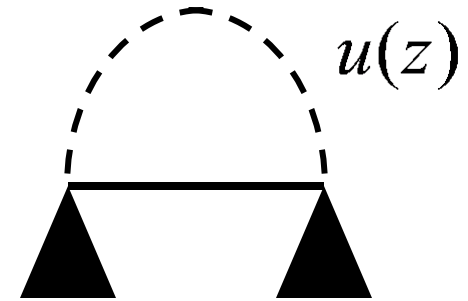
$$\begin{aligned} \psi(z) &= A e^{+ik_z z} + B e^{-ik_z z} \\ &= A \left(e^{+ik_z z} - e^{-ik_z z} \right) \\ &\sim \sin k_z z \end{aligned}$$

$$k_z L = n\pi$$

1.2d Wave Equation

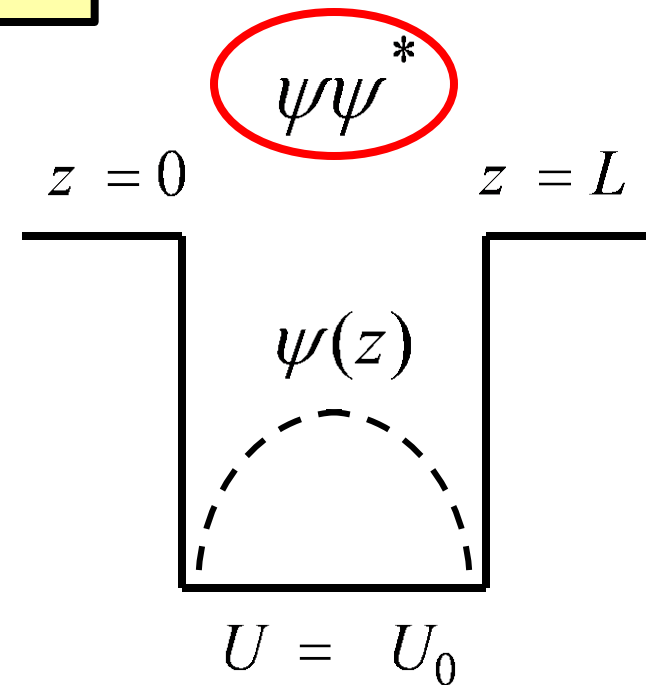


Waves when confined
show resonant
energies / frequencies

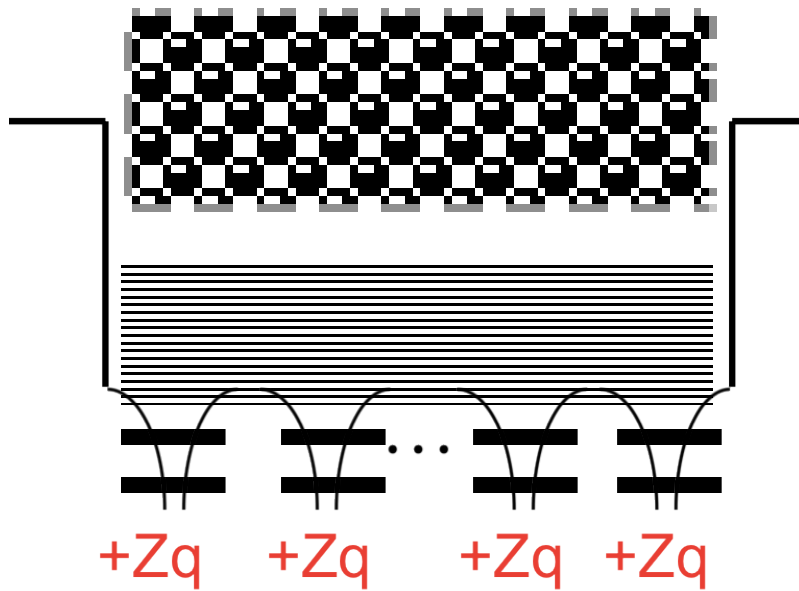


1-D:
$$E = \frac{\hbar^2 k_z^2}{2m} + U_0$$

A graph showing a parabolic potential well. The vertical axis is energy E and the horizontal axis is wave vector k_z . A parabola opens upwards, with its minimum at $E = U_0$ on the k_z axis. Three red vertical arrows point from the k_z axis to the parabola, with red 'x' marks at their bases. Below the k_z axis, the expression $k_z \rightarrow \frac{n\pi}{L}$ is shown.



1.2e Wave Equation



$$E\psi(\vec{r}) = \left(-\frac{\hbar^2}{2m_0} \nabla^2 + U(\vec{r}) \right) \psi(\vec{r})$$

Free electron
mass

Microscopic
potentials

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

Effective
mass

Additional
potentials

Coming up next ..

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



$$E \begin{Bmatrix} \psi_1 \\ \psi_2 \\ \dots \\ \psi_N \end{Bmatrix} = \begin{bmatrix} \dots & \dots & \dots \\ \dots & H & \dots \\ \dots & \dots & \dots \end{bmatrix} \begin{Bmatrix} \psi_1 \\ \psi_2 \\ \dots \\ \psi_N \end{Bmatrix}$$

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1.9. Reciprocal Lattice / Valleys

1.10. Summing up ..