FUNDAMENTALS OF NANOELECTRONICS

B. Quantum Transport

Schrodinger Equation

2. Contact-ing Schrodinger

3. Advanced Examples

4. Spin Transport

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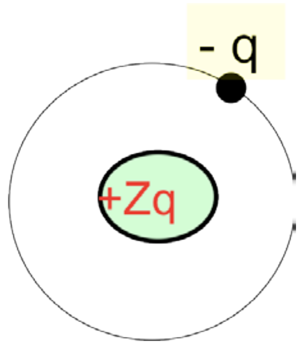
http://nanohub.org/groups/lnebook

1.2a Wave Equation

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

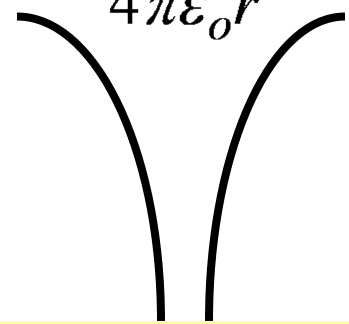
$$n\frac{h}{mv} = 2\pi r$$

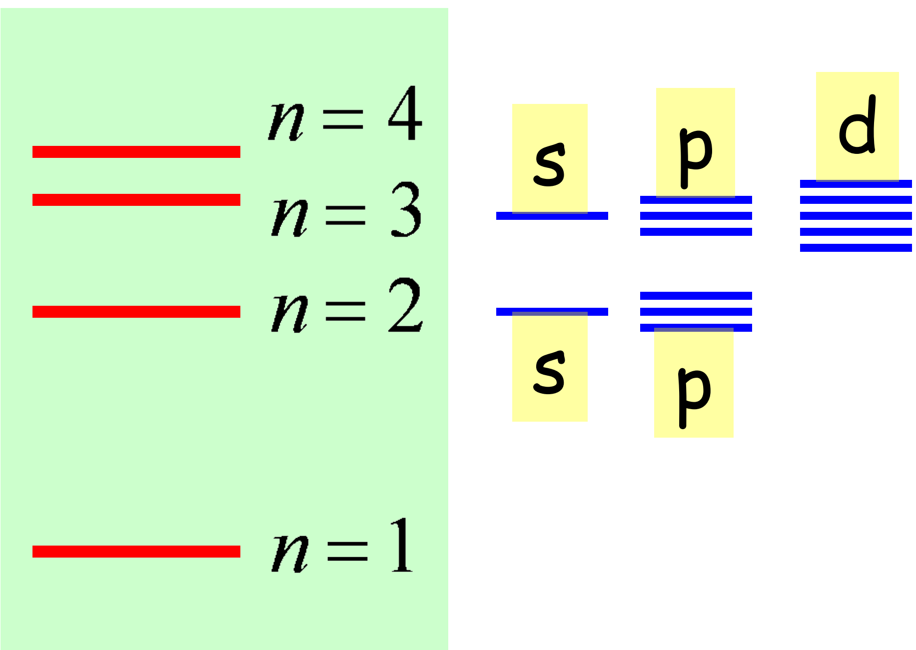
$$a_0 = \frac{4\pi\varepsilon_0\hbar^2}{mq^2}$$



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

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





Waves when confined show resonant energies / frequencies

1.2b Wave Equation

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

$$\psi(\vec{r}) = e^{+ik_x x}\, e^{+ik_y y}\, e^{+ik_z z}\, \psi_0$$

$$= e^{+i\vec{k}\circ\vec{r}}\, \psi_0$$

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

Dispersion relation

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

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

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

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

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

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

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

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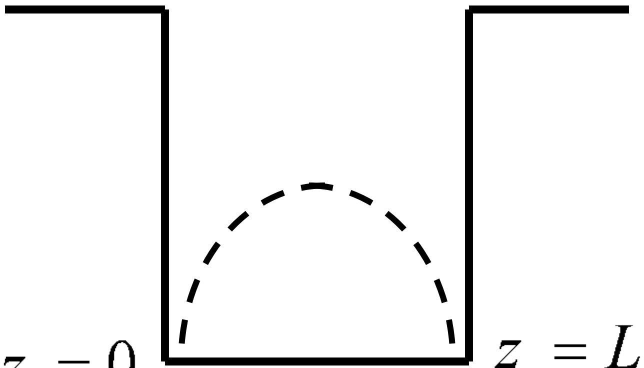
1.2c Wave Equation

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

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

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

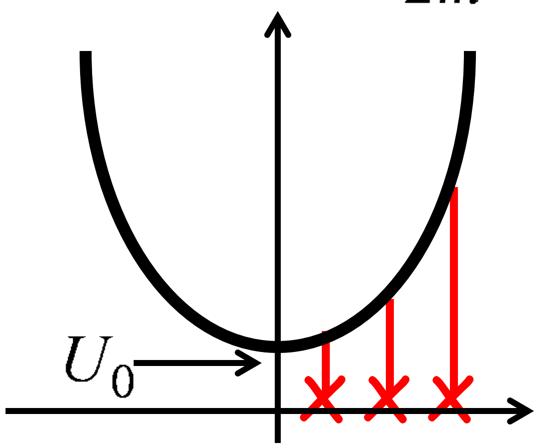
Dispersion relation



$z = 0$ $\quad$ $z = L$

$$U = U_0$$

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



$$k_z \rightarrow \frac{n\pi}{L}$$

$$\psi(z) = A\,e^{+ik_z z} + B\,e^{-ik_z z}$$

$$= A\left(e^{+ik_z z} - e^{-ik_z z}\right)$$

$$\sim \sin k_z z$$

$$k_z L = n\pi$$

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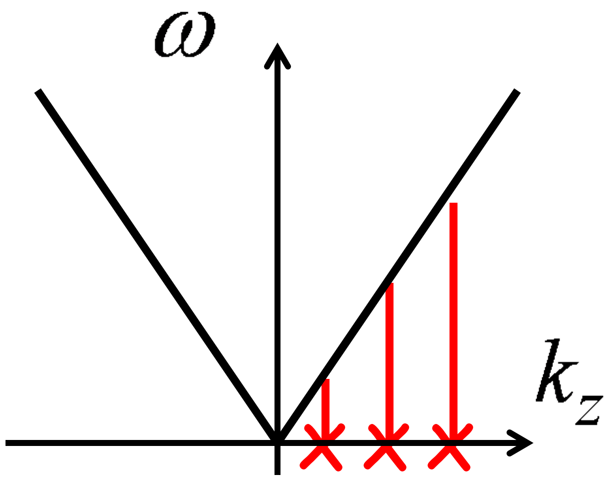
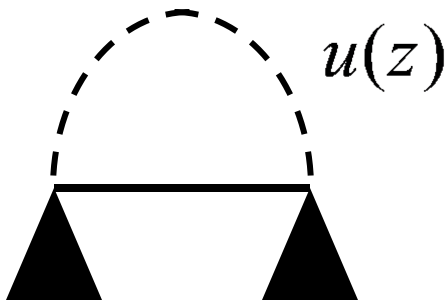
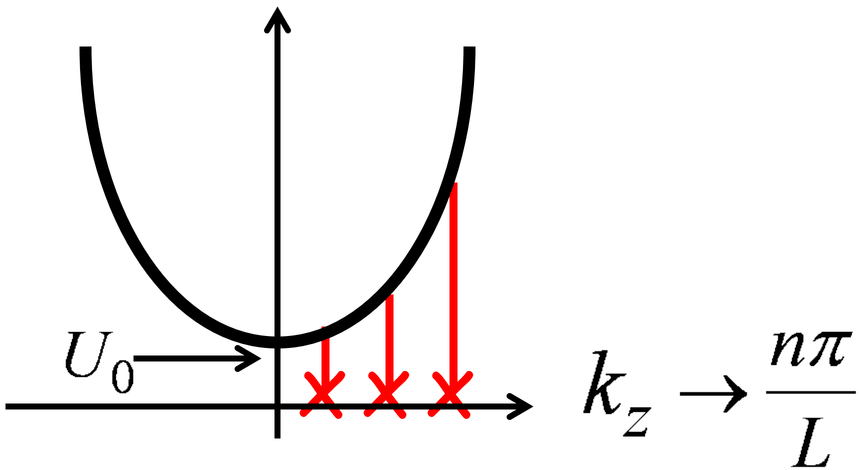
1.2d Wave Equation

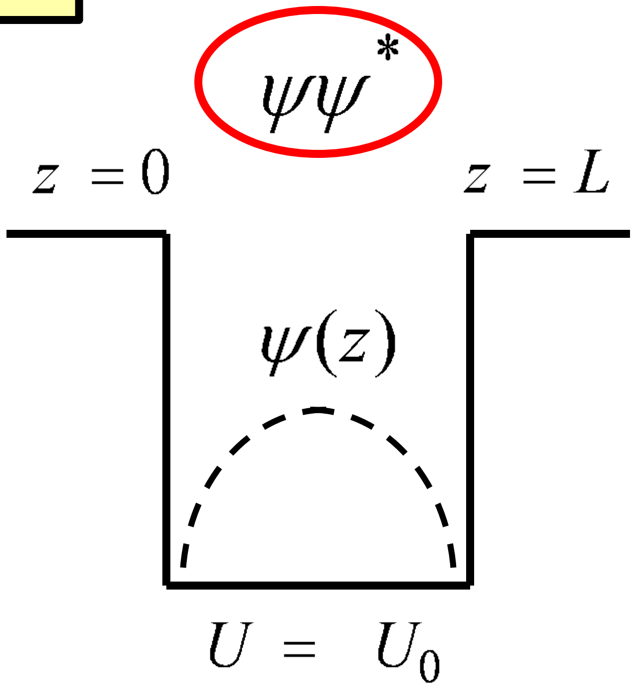


Waves when confined show resonant energies / frequencies



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





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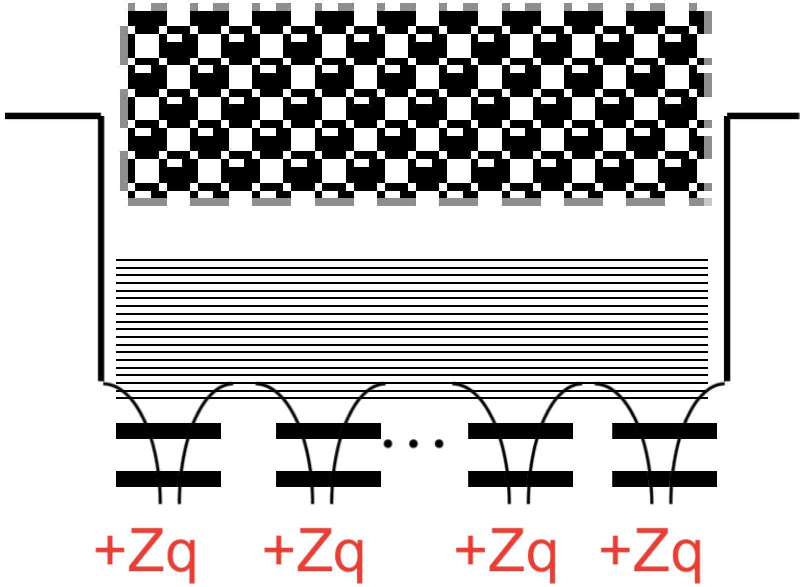
1.2e Wave Equation



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

Effective mass

Additional potentials

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

Free electron mass

Microscopic potentials

Coming up next ..

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

$$\downarrow$$

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