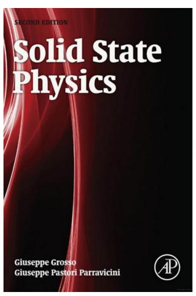
PHY 752 Solid State Physics
11-11:50 AM MWF Olin 103

Plan for Lecture 1:

Reading: Chapter 1 in GGGPP; Electronic Structure

1. **Bloch's Theorem**
2. **Eigenstates of a simple model potential**

Text book



Available from zsr; may also be purchased from Barnes and Noble, etc.

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Solid state physics
by Grosso, Giuseppe.
Published 2014
Other Authors: '; "...Pastori Parravicini, Giuseppe ...."
Call Number: QC176 .G76 2014 WEB

Location: Website
Electronic book DDA.
EBOOK

1 Electrons in One-Dimensional Periodic Potentials

Chapter Outline head

1.1 The Bloch Theorem for One-Dimensional Periodicity

Consider an electron in a one-dimensional potential energy $V(x)$ and the corresponding Schrödinger equation

$$-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} + V(x)\psi(x) = E\psi(x). \qquad (1.1)$$

A potential $V(x)$, of period a, satisfies the relation

$V(x) = V(x+ma)$, for integer m.

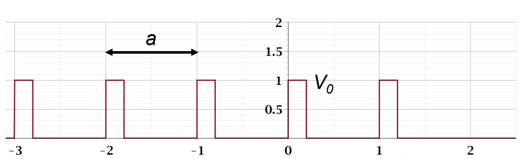
$$\boxed{\psi_k(x) = e^{ikx}u_k(x)} \quad \text{with} \quad \boxed{u_k(x+a) = u_k(x)}. \qquad (1.7)$$

This expresses the Bloch theorem: *any physically acceptable solution of the Schrödinger equation in a periodic potential takes the form of a traveling plane wave modulated on the microscopic scale by an appropriate function with the lattice periodicity.*

The Bloch theorem, summarized by Eq. (1.7), can also be written in the equivalent form

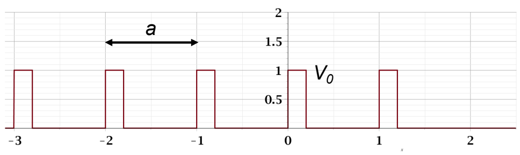
$$\boxed{\psi_k(x+t_n) = e^{ikt_n}\psi_k(x)}. \qquad (1.8)$$

Consider an electron moving in a one-dimensional model potential (Kronig and Penney, *Proc. Roy. Soc. (London)* **130,** 499 (1931)



Schroedinger equation for electron:

$$\left(-\frac{\hbar^2\nabla^2}{2m} + V(x)\right)\Psi(x) = E\Psi(x)$$

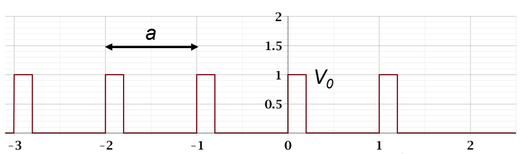


Effects of periodicity: $V(x) = V(x+na)$

$$\left(-\frac{\hbar^2\nabla^2}{2m} + V(x)\right)\Psi(x) = E\Psi(x)$$

$$\left(-\frac{\hbar^2\nabla^2}{2m} + V(x+na)\right)\Psi(x+na) = E\Psi(x+na)$$

$$\left(-\frac{\hbar^2\nabla^2}{2m} + V(x)\right)\Psi(x+na) = E\Psi(x+na)$$



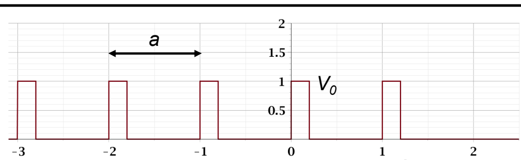
Since $\Psi(x+na)$ and $\Psi(x)$ are solutions of the same eigenvalue problem: $\Psi(x+na) = K\Psi(x)$

Assume $K = e^{i\theta} = e^{ikna}$

Bloch theorem: $\Psi_k(x+na) = e^{ikna}\Psi_k(x)$

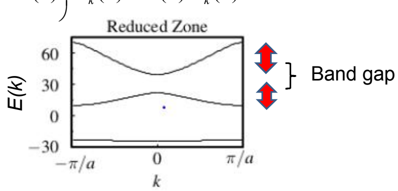
$\Psi_k(x) = e^{ikx}u(x)$

where $u_k(x+na) = u_k(x)$



Eigenstates:

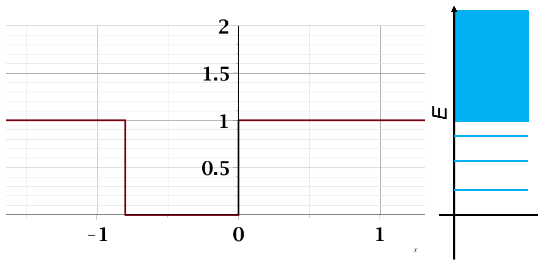
$$\left(-\frac{\hbar^2\nabla^2}{2m} + V(x)\right)\Psi_k(x) = E(k)\Psi_k(x)$$

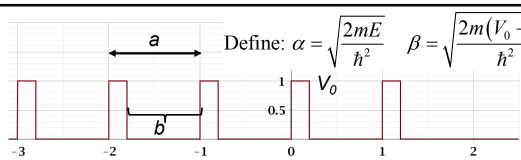


What causes band gaps in the electronic structure?

Consider a single potential well

Spectrum





Define: $\alpha = \sqrt{\frac{2mE}{\hbar^2}}$ $\quad \beta = \sqrt{\frac{2m(V_0 - E)}{\hbar^2}}$

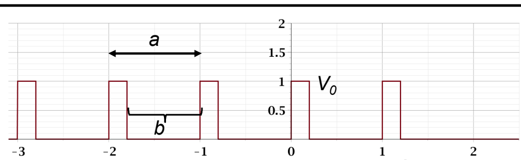
For $0 \le x \le (a-b)$ $\quad \Psi_1(x) = Ae^{\beta x} + Be^{-\beta x}$

For $(a-b) \le x \le a$ $\quad \Psi_2(x) = Ce^{i\alpha x} + De^{-i\alpha x}$

Continuity conditions: $\Psi_1(0) = \Psi_2(0)$ $\quad \frac{d\Psi_1(0)}{dx} = \frac{d\Psi_2(0)}{dx}$

$$\Psi_1(a-b) = \Psi_2(a-b) \qquad \frac{d\Psi_1(a-b)}{dx} = \frac{d\Psi_2(a-b)}{dx}$$

Also note: $\Psi(x+a) = e^{ika}\Psi(x)$

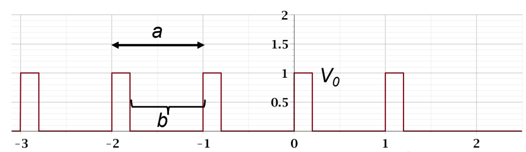


Matching conditions reduce to:

$$\cos(ka) = F(E)\cos\left(\alpha b - \Delta(E)\right)$$

$$F(E) \equiv \left(1 + \frac{V_0^2}{4E\left(E - V_0\right)}\sinh^2\left(\beta(a-b)\right)\right)^{1/2}$$

$$\tan\Delta(E) = \frac{V_0 - 2E}{2\sqrt{E\left(V_0 - E\right)}}\tanh\left(\beta(a-b)\right)$$



Details for $V_0 = \frac{\hbar^2}{2m}\frac{(2\pi)^2\, 49}{16 b^2}; \quad b = \frac{16}{17} a$

Let $\quad f \equiv \frac{E}{V_0}$

$$\cos(ka) = \left(1 + \frac{\sinh^2\left(0.687\sqrt{1-f}\right)}{4f(1-f)}\right)^{1/2} \cos\left(11.7\sqrt{f} - \Delta(f)\right)$$

$$\tan\Delta(f) = \frac{1-2f}{2\sqrt{f(1-f)}}\tanh\left(0.687\sqrt{1-f}\right)$$

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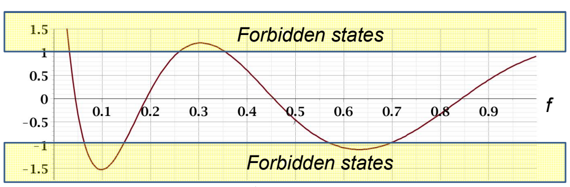
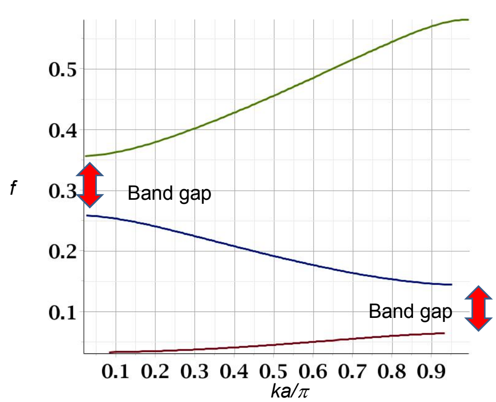
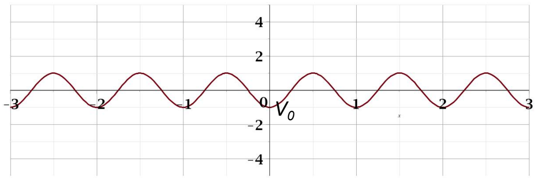


$$X(f) = \left(1 + \frac{\sinh^2\left(0.687\sqrt{1-f}\right)}{4f(1-f)}\right)^{1/2} \cos\left(11.7\sqrt{f} - \Delta(f)\right)$$



Electrons in the presence of a weak periodic potential



$$\mathcal{H} = \mathcal{H}^0 + \mathcal{H}^1$$

$$\mathcal{H}^0 = -\frac{\hbar^2 d^2}{2m dx^2} \qquad \mathcal{H}^1 = V_0 \cos\left(\frac{2\pi x}{a}\right)$$

$$\Psi(x) = \sum_n C_n e^{i\left(k + n\frac{2\pi}{a}\right)x} \qquad -\frac{\pi}{a} \le k \le \frac{\pi}{a}$$

$$E^0_{nk} = \frac{\hbar^2 \left|k + n\frac{2\pi}{a}\right|^2}{2m}$$

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$$\Psi(x) = \sum_n C_n e^{i\left(k + n\frac{2\pi}{a}\right)x} \qquad -\frac{\pi}{a} \le k \le \frac{\pi}{a}$$

$$E^0_{nk} = \frac{\hbar^2 \left|k + n\frac{2\pi}{a}\right|^2}{2m}$$

Note that $E^0_{0\frac{\pi}{a}} = E^0_{1-\frac{\pi}{a}} = \frac{\hbar^2 \pi^2}{2ma^2}$

Degenerate perturbation theory

$$\begin{pmatrix} \frac{\hbar^2\pi^2}{2ma^2} & V_0 \\ V_0 & \frac{\hbar^2\pi^2}{2ma^2} \end{pmatrix} \begin{pmatrix} C_0 \\ C_1 \end{pmatrix} = E^1 \begin{pmatrix} C_0 \\ C_1 \end{pmatrix}$$

$$E^1 = \pm V_0$$