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

Plan for Lecture 2:

Reading: Continue reading Chapter 1 in GGGPP; Electrons in one-dimensional periodic potentials

1. **Review of Bloch's Theorem**
2. **Kronig-Penny model potential from the viewpoint of scattering or tunneling**

PHY 752 Solid State Physics

MWF 11 AM-11:50 PM	OPL 103	http://www.wfu.edu/~natalie/f15phy752/

Instructor: Natalie Holzwarth	Phone:758-5510	Office:300 OPL	e-mail:natalie@wfu.edu

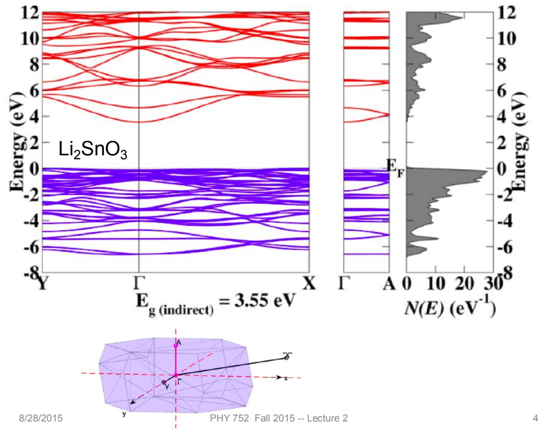
Course schedule

(Preliminary schedule -- subject to frequent adjustment.)

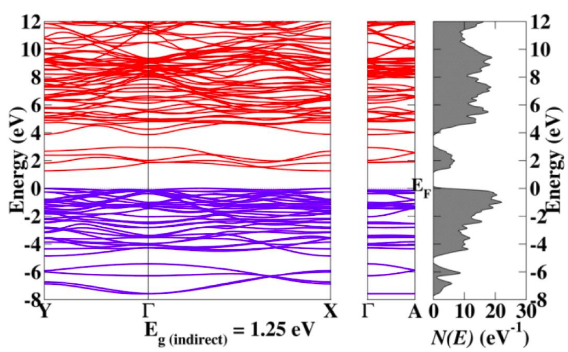
	Date	F&W Reading	Topic	Assignment
1	Wed, 8/26/2015	Chap. 1	Electrons in a periodic one-dimensional potential	#1
2	Fri, 8/28/2015	Chap. 1	Electrons in a periodic one-dimensional potential	#2
3	Mon, 8/31/2015	Chap. 1		
4	Wed, 9/02/2015			
5	Fri, 9/04/2015			
6	Mon, 9/07/2015			
7	Wed, 9/09/2015			
8	Fri, 9/11/2015			
9	Mon, 9/14/2015			
10	Wed, 9/16/2015			

1 Electrons in One-Dimensional Periodic Potentials

Chapter Outline head



Li$_2$SnS$_3$



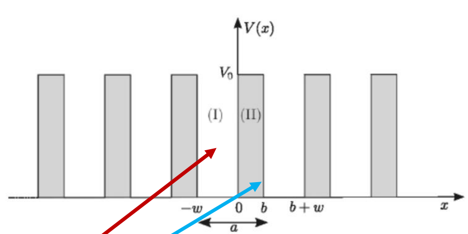


Figure 1.3 One-dimensional potential formed by a periodic array of quantum wells.

$$\begin{cases} \psi_I(x) = Ae^{iqx} + Be^{-iqx} & -w < x < 0 \quad q(E) = \sqrt{2mE/\hbar^2}, \\ \psi_{II}(x) = Ce^{\beta x} + De^{-\beta x} & 0 < x < b \quad \beta(E) = \sqrt{2m(V_0 - E)/\hbar^2}, \end{cases} \tag{1.16}$$

Bloch theorem: $\psi_k(x + t_n) = e^{ikt_n}\psi_k(x)$

Eigenvalue solutions to Kronig-Penny model

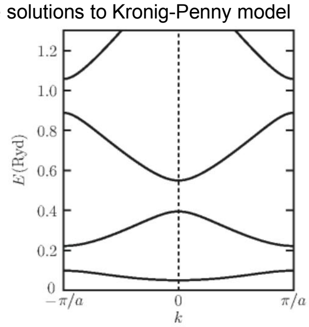


Figure 1.5 Energy bands of lowest energy in the Kronig-Penney model for $P = 3\pi/2$. The energy E (in Rydberg) is plotted as a function of k in the first Brillouin zone; the value of the lattice parameter considered is $a = 10\,a_B$ (a_B Bohr radius).

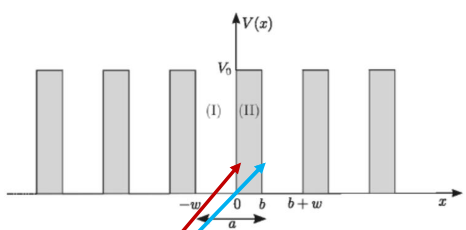


Figure 1.3 One-dimensional potential formed by a periodic array of quantum wells.

$$\psi_I(0) = \psi_{II}(0), \quad \left(\frac{d\psi_I}{dx}\right)_{x=0} = \left(\frac{d\psi_{II}}{dx}\right)_{x=0},$$

$$\psi_{II}(b) = e^{ika}\psi_I(-w), \quad \left(\frac{d\psi_{II}}{dx}\right)_{x=b} = e^{ika}\left(\frac{d\psi_I}{dx}\right)_{x=-w}.$$

From wavefunction matching conditions:

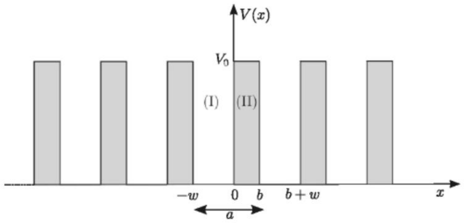
$$\begin{cases} A + B = C + D \\ Aiq - Biq = C\beta - D\beta \\ Ce^{\beta b} + De^{-\beta b} = e^{ika}[Ae^{-iqw} + Be^{+iqw}] \\ C\beta e^{\beta b} - D\beta e^{-\beta b} = e^{ika}[Aiqe^{-iqw} - Biqe^{+iqw}]. \end{cases}$$

Condition for non-trivial solution:

$$\begin{Vmatrix} 1 & 1 & -1 & -1 \\ iq & -iq & -\beta & \beta \\ -e^{ika-iqw} & -e^{ika+iqw} & e^{\beta b} & e^{-\beta b} \\ -iqe^{ika-iqw} & iqe^{ika+iqw} & \beta e^{\beta b} & -\beta e^{-\beta b} \end{Vmatrix} = 0.$$

Simplified result:

$$\boxed{\frac{\beta^2 - q^2}{2q\beta}\sinh\beta b\sin qw + \cosh\beta b\cos qw = \cos ka}.$$



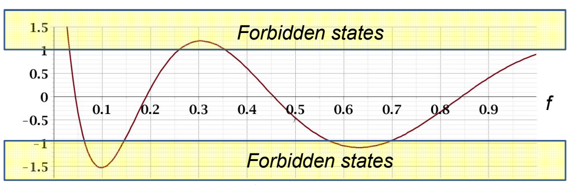
Details for $V_0 = \frac{\hbar^2}{2m}\frac{(2\pi)^2\,49}{16w^2}$; $w = \frac{16}{17}a$; $f = \frac{E}{V_0}$

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

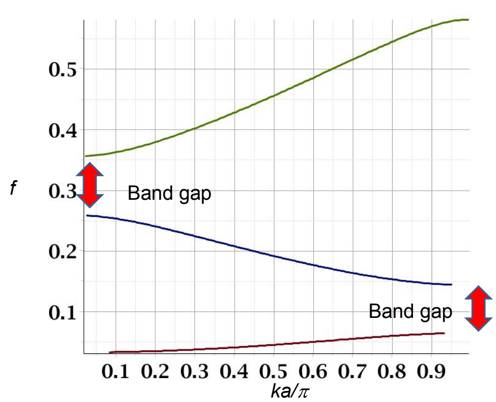
$$\tan\Delta(f) = \frac{1-2f}{2\sqrt{f(1-f)}} \tanh\left(0.687\sqrt{1-f}\right)$$

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

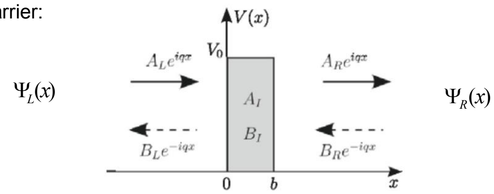
$$\tan\Delta(f) = \frac{1-2f}{2\sqrt{f(1-f)}} \tanh\left(0.687\sqrt{1-f}\right)$$



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



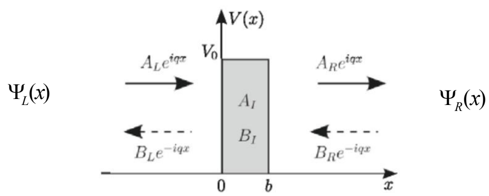
Treatment of same problem in terms of transmission and reflection from a periodic barrier. First consider a single barrier:



$$\begin{cases} \psi_L(x) = A_L e^{iqx} + B_L e^{-iqx} & x \le x_L \\ \psi_R(x) = A_R e^{iqx} + B_R e^{-iqx} & x \ge x_R \end{cases} \qquad q(E) = \sqrt{2mE/\hbar^2} \quad E > 0.$$

Matrix for determining coefficients:

$$\begin{pmatrix} A_R \\ B_R \end{pmatrix} = M(E) \begin{pmatrix} A_L \\ B_L \end{pmatrix} = \begin{bmatrix} m_{11}(E) & m_{12}(E) \\ m_{21}(E) & m_{22}(E) \end{bmatrix} \begin{pmatrix} A_L \\ B_L \end{pmatrix}$$



$$\begin{cases} \psi_L(x) = A_L e^{iqx} + B_L e^{-iqx} & x < 0, \\ \psi_I(x) = A_I e^{\beta x} + B_I e^{-\beta x} & 0 < x < b, \\ \psi_R(x) = A_R e^{iqx} + B_R e^{-iqx} & x > b, \end{cases}$$

where $q^2(E) = 2mE/\hbar^2$ and $\beta^2(E) = 2m(V_0 - E)/\hbar^2$.

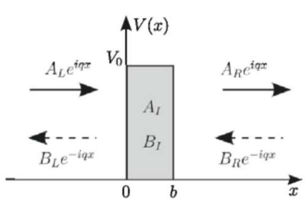
Matching conditions for wavefunction coefficients:

$$\begin{pmatrix} A_I \\ B_I \end{pmatrix} = \frac{1}{2\beta} \begin{bmatrix} iq+\beta & -iq+\beta \\ -iq+\beta & iq+\beta \end{bmatrix} \begin{pmatrix} A_L \\ B_L \end{pmatrix}. \qquad \begin{pmatrix} A_R \\ B_R \end{pmatrix} = \frac{1}{2iq} \begin{bmatrix} (iq+\beta)e^{(-iq+\beta)b} & (iq-\beta)e^{(-iq-\beta)b} \\ (iq-\beta)e^{(+iq+\beta)b} & (iq+\beta)e^{(+iq-\beta)b} \end{bmatrix} \begin{pmatrix} A_I \\ B_I \end{pmatrix}$$

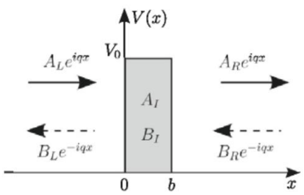
Solving for transfer matrix elements:

$$m_{11} = e^{-iqb}\left[\cosh \beta b + i\frac{q^2-\beta^2}{2q\beta}\sinh \beta b\right] \qquad m_{22} = m_{11}^*$$

$$m_{12} = e^{-iqb}(-i)\frac{q^2+\beta^2}{2q\beta}\sinh \beta b \qquad m_{21} = m_{12}^*$$



$$\begin{pmatrix} A_R \\ B_R \end{pmatrix} = \begin{bmatrix} m_{11}(E) & m_{12}(E) \\ m_{21}(E) & m_{22}(E) \end{bmatrix} \begin{pmatrix} A_L \\ B_L \end{pmatrix}$$



$$\begin{pmatrix} A_R \\ B_R \end{pmatrix} = \begin{bmatrix} m_{11}(E) & m_{12}(E) \\ m_{21}(E) & m_{22}(E) \end{bmatrix} \begin{pmatrix} A_L \\ B_L \end{pmatrix}$$

Transmittance

$$t = \frac{A_R}{A_L} \qquad T = |t|^2 = \left| \frac{1}{m_{22}} \right|^2$$

After some algebra:

$$T(E) = \frac{1}{1 + \dfrac{V_0^2}{4E(V_0 - E)} \sinh^2 \sqrt{\dfrac{2m(V_0 - E)b^2}{\hbar^2}}} \quad 0 \le E \le V_0.$$

$$T(E) = \frac{1}{1 + \dfrac{V_0^2}{4E(E - V_0)} \sin^2 \sqrt{\dfrac{2m(E - V_0)b^2}{\hbar^2}}} \quad E \ge V_0.$$

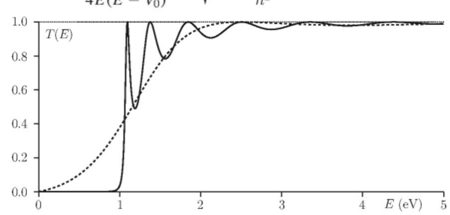
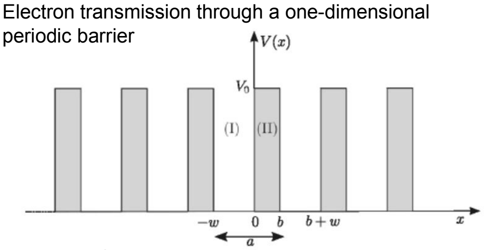


Figure 1.8 Transmission coefficient through a barrier of height $V_0 = 1$ eV and length $b = 5$ Å (dashed line), and through a barrier of height $V_0 = 1$ eV and length $b = 20$ Å (solid line).

Electron transmission through a one-dimensional periodic barrier



Because of Bloch theorem:

$$\psi_R(a) = e^{ika}\psi_L(0) \quad \text{and} \quad \left(\frac{d\psi_R}{dx}\right)_{x=a} = e^{ika}\left(\frac{d\psi_L}{dx}\right)_{x=0}.$$

Bloch theorem & transmission coefficients:

$$\begin{pmatrix} A_R \\ B_R \end{pmatrix} = \begin{pmatrix} m_{11}e^{iqa} & m_{12}e^{iqa} \\ m_{21}e^{-iqa} & m_{22}e^{-iqa} \end{pmatrix} \begin{pmatrix} A_L \\ B_L \end{pmatrix} = e^{ika} \begin{pmatrix} A_L \\ B_L \end{pmatrix}$$

Condition for solution:

$$\boxed{\mathrm{Re}\left[m_{11}e^{iqa}\right] = \cos ka}.$$

$$\cosh \beta b \cos qw - \frac{q^2 - \beta^2}{2q\beta} \sinh \beta b \sin qw = \cos ka.$$