FYS3410 - Vår 2010 (Kondenserte fasers fysikk)

http://www.uio.no/studier/emner/matnat/fys/FYS3410/index-eng.xml

Based on Introduction to Solid State Physics by Kittel

Course content

- Periodic structures, understanding of diffraction experiment and reciprocal lattice
- Crystal binding, elastic strain and waves
- Imperfections in crystals: point defects and diffusion
- Crystal vibrations: phonon heat capacity and thermal conductivity
- Free electron Fermi gas: density of states, Fermi level, and electrical conductivity
- **Electrons in periodic potential: energy bands theory classification of metals, semiconductors and insulators**
- Semiconductors: band gap, effective masses, charge carrier distributions, doping, pn-junctions
- Metals: Fermi surfaces, temperature dependence of electrical conductivity

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FYS3410 lecture schedule and exams: Spring 2010

M/18/1/2010:	Introduction and motivation. Periodicity and lattices	2h
W/20/1/2010:	Index system for crystal planes. Crystal structures	1h
M/25/1/2010:	Reciprocal space, Laue condition and Ewald construction	2h
W/27/1/2010:	Brillouin Zones. Interpretation of a diffraction experiment	1h
M/01/2/2010:	Crystal binding, elastic strain and waves	2h
W/03/2/2010:	Elastic waves in cubic crystals; defects in crystals	1h
M/08/2/2010:	Defects in crystals; case study - vacancies	2h
W/10/2/2010:	Diffusion	1h
M/15/2/2010:	Crystal vibrations and phonons	2h
W/17/2/2010:	Crystal vibrations and phonons	1h
M/22/2/2010:	Lattice heat capacity: Dulong-Petit and Einstein models	2h
W/24/2/2010:	Phonon density of states (DOS) and Debye model	1h
M/01/3/2010:	General result for DOS; role of anharmonic interactions	2h
W/03/3/2010:	Thermal conductivity	1h
M/08/3/2010:	Free electron Fermi gas in 1D and 3D – ground state	2h
W/10/3/2010:	Density of states, effect of temperature – FD distribution	1h
M/15/3/2010:	Heat capacity and thermal conductivity of FEFG	2h
W/17/3/2010:	Repetition	1h
22/3/2010:	Mid-term exam	

M/12/4/2010:	**Drude model and the idea of energy bands**	**2h**
W/14/4/2010:	**Nearly free electron model; Kronig - Penny model**	**2h**
M/19/4/2010:	no lectures	
W/21/4/2010:	Empty lattice approximation; number of orbitals in a band	2h
M/26/4/2010:	Semiconductors, effective mass method, intrinsic carriers	2h
W/28/4/2010:	Impurity states in semiconductors and carrier statistics	2h
M/03/5/2010:	p-n junctions and heterojunctions	2h
W/05/5/2010:	surface structure, surface states, Schottky contacts	2h
M/10/5/2010:	Metals and Fermi surfaces	
W/12/5/2010:	no lectures	
W/19/5/2010:	no lectures	2h
W26/5/2010:	Repetition	2h
27-28/5/2010:	**Final Exam (sensor: Prof. Arne Nylandsted Larsen at the Aarhus University, Denmark, http://person.au.dk/en/anl@phys.au.dk)**	

Lecture 20: Nearly free electron model; Kronig - Penny model

- **Energy bands idea from "bonding" point of view**
- **Free versus nearly free electron model**
- **Periodic potential, Bloch functions and nearly free electron model**
- **Kronig-Penney model**

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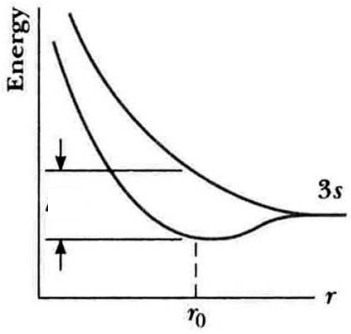
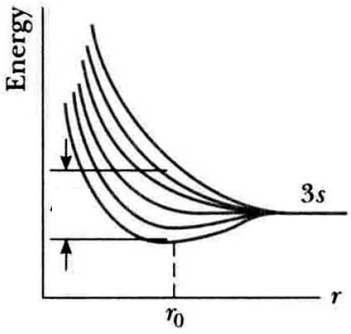
Energy bands idea from "bonding" point of view

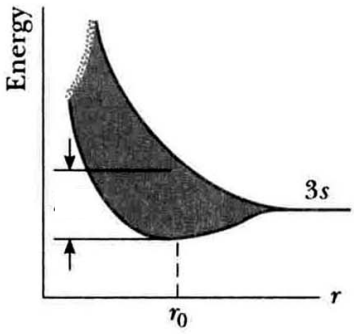
Two atoms



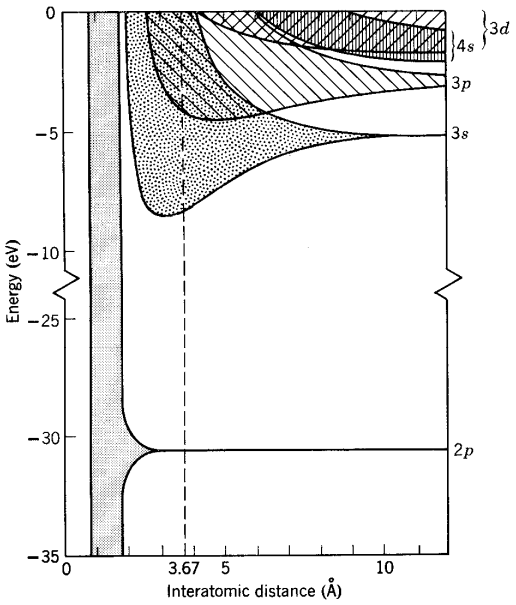
Six atoms



Solid of N atoms



Solid composed of ~N_A Na stoms as a function of orbitals and corresponding electron concentration



$1s^2 2s^2 2p^6 3s^1$

Figure 13-3 Showing the formation of energy bands from the energy levels of isolated sodium atoms as the interatomic separation decreases. The dashed line indicates the observed interatomic separation in solid sodium. The several overlapping bands that constitute each *p* or *d* band are not indicated.

Sodium bands vs separation

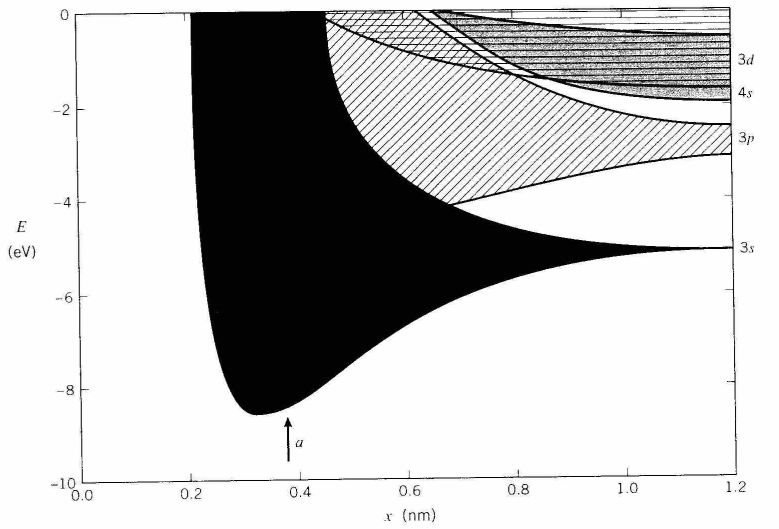


FIGURE 14-4 Outer energy bands in sodium.
The Schrödinger equation is solved for a sodium crystal treating the distance between atoms as a variable (x). At large distances the energy levels are separated, but at small distances they overlap. This explains the conductivity of metals. After J. C. Slater, "Electronic Energy Bands in Metals," *Phys. Rev.* **45**, 794 (1934).

Copper bands vs separation

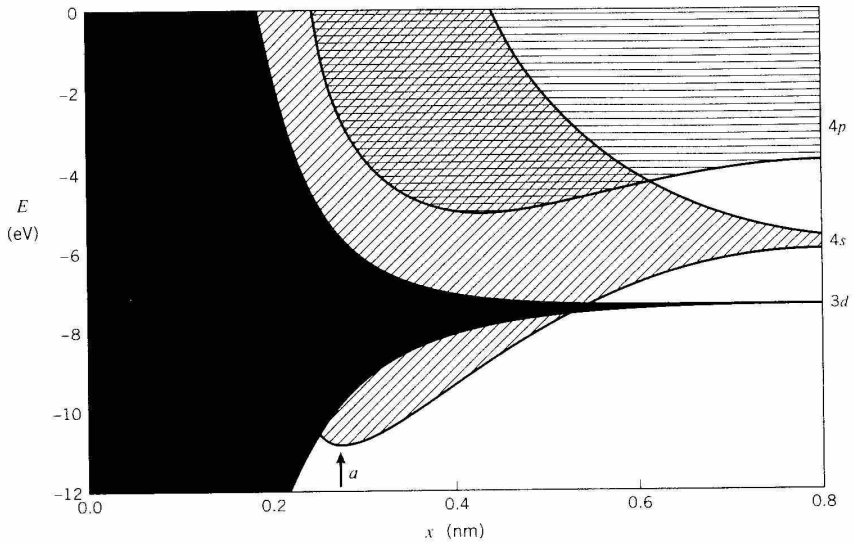


FIGURE 14-6 Energy bands of the outer electrons in copper.
After H. M. Kutter, "Energy Bands in Copper," *Phys. Rev.* **48**, 664 (1935).

Differences down a column in the Periodic Table: IV-A Elements

same valence

4A			
CARBON		12.01	NIT
2.26	C	6	1.0
$1s^2 2s^2 2p^2$			
3.57	DIA		4.0
(4300)		1860	63
SILICON		28.086	PH
2.33	Si	14	1.8
[Ne] $3s^2 3p^2$			
5.43	DIA		7.1
1683		625	31
GERMANIUM		72.59	AR
5.32	Ge	32	5.7
[Ar] $3d^{10} 4s^2 4p^2$			
5.66	DIA		4.1
1211		360	10
TIN		118.69	AN
7.30	Sn	50	6.6
[Kr] $4d^{10} 5s^2 5p^2$			
5.82	TET	0.546	4.5
505		170	90
LEAD		207.19	BIS
11.4	Pb	82	9.8
[Xe] $4f^{14} 5d^{10} 6s^2 6p^2$			[Xe
4.95	FCC		4.1
601		88	54

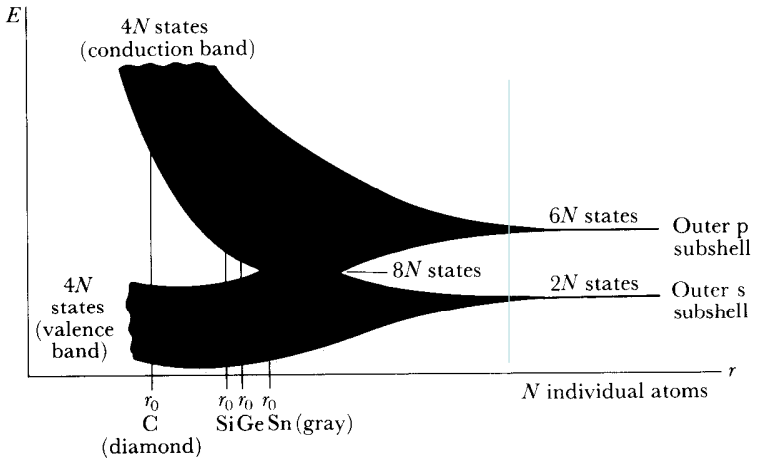


FIGURE 25.3
Gray tin, germanium, silicon, and diamond have two s and two p outer electrons and the same crystal structure. In gray Sn, the valence and conduction bands overlap, making it a metal. In Ge and Si, an energy gap of about 1 eV between those bands makes them semiconductors. In diamond, that forbidden energy gap is greater than 5 eV, making diamond an insulator.

Sandin

Lecture 20: Nearly free electron model; Kronig - Penny model

- Energy bands idea from "bonding" point of view
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Free- versus nearly free electron model

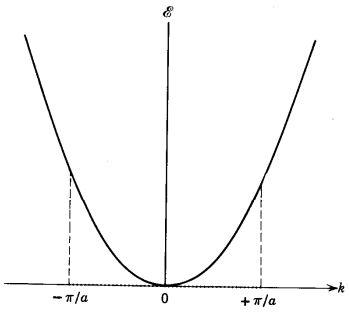
$$-\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}+\frac{\partial^2}{\partial z^2}\right)\psi_{\mathbf{k}}(\mathrm{r}) = \epsilon_{\mathbf{k}}\,\psi_{\mathbf{k}}(\mathbf{r})$$

$$\psi(x+L,y,z) = \psi(x,y,z)$$

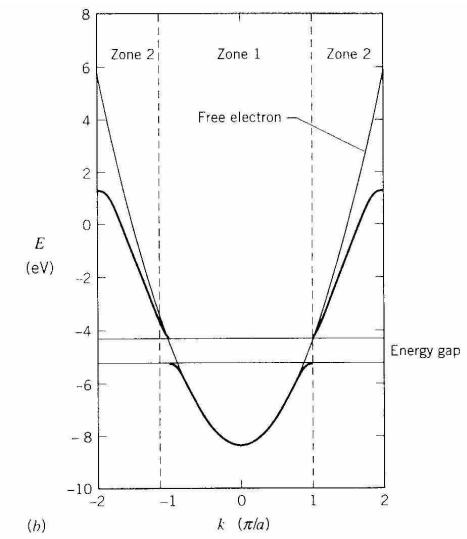
$$\boxed{\psi_{\mathbf{k}}(\mathbf{r}) = \exp\,(i\mathbf{k}\cdot\mathbf{r})\ ,}$$

$$k_x = 0\ ;\quad \pm\frac{2\pi}{L}\ ;\quad \pm\frac{4\pi}{L}\ ;\ \ldots\ ,$$

$$\epsilon_{\mathbf{k}} = \frac{\hbar^2}{2m}k^2 = \frac{\hbar^2}{2m}\,(k_x^2+k_y^2+k_z^2)$$



$$\varepsilon \;=\; \frac{p^2}{2m} \;=\; \frac{\hbar^2 k^2}{2m}$$



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- Energy bands idea from "bonding" point of view
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- **Periodic potential and Bloch functions**
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Periodic potential and Bloch functions

$$\Psi(x) \sim u\ e^{i(kx-\omega t)}$$

amplitude

In other words this is a variation of the electrostatic potential energy of a conduction electron in the field of positive ion cores

Bloch's theorem

$$\Psi(x) \sim u(x)\ e^{i(kx-\omega t)}$$

Amplitude varies with location

$$u(x) = u(x+a) = u(x+2a) = \ldots.$$

Periodic potential and Bloch functions

$\Psi(x) \sim u(x)\ e^{i(kx-\omega t)}$

$u(x+a) = u(x)$

$\Psi(x+a)\ e^{-i(kx+ka-\omega t)} = u(x+a)\ e^{-i(kx+ka-\omega t)}$

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

Something special happens with the phase when

$e^{ika} = 1$

$ka = +/- n\pi \qquad n = 1, 2, 3, \ldots$

$$k = \pm\frac{\pi}{a},\ \pm 2\frac{\pi}{a},\ \ldots$$

Periodic potential and Bloch functions

Consider a set of waves with +/– k-pairs, e.g. $k = \pm\frac{\pi}{a}$

$k = +\pi/a$ moves → $\qquad$ $k = -\pi/a$ moves ←

This defines a pair of waves moving right & left

Two trivial ways to superpose these waves are:

$\Psi^{+} \sim e^{ikx} + e^{-ikx} \qquad \Psi^{-} \sim e^{ikx} - e^{-ikx}$

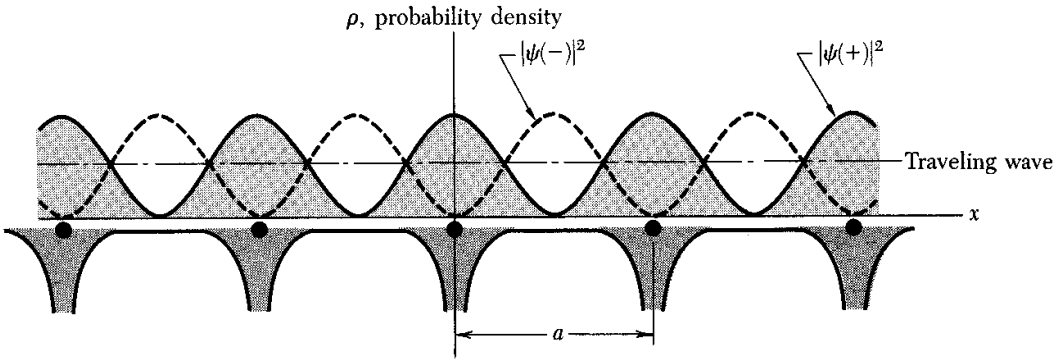
$e^{ix} = \cos(x) + i\sin(x)$

$\Psi^{+} \sim 2\cos kx \qquad \Psi^{-} \sim 2i \sin kx$

Periodic potential and Bloch functions

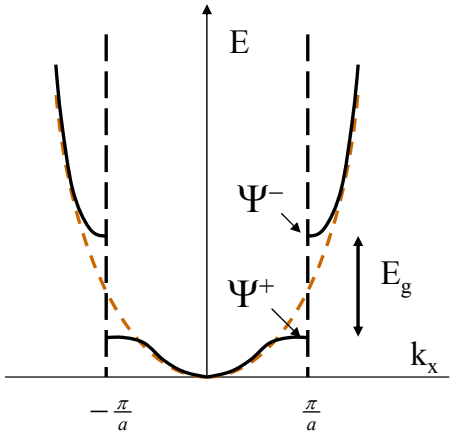
$\Psi^+ \sim 2 \cos kx$ $\qquad$ $\Psi^- \sim 2i \sin kx$

$|\Psi^+|^2 \sim 4 \cos^2 kx$ $\qquad$ $|\Psi^-|^2 \sim 4 \sin^2 kx$



(b)

Periodic potential and Bloch functions



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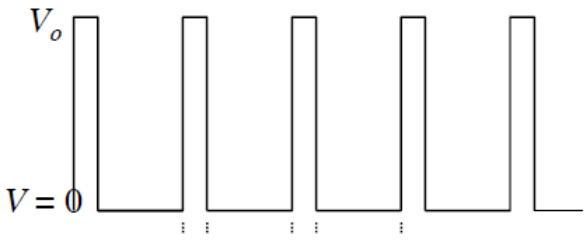
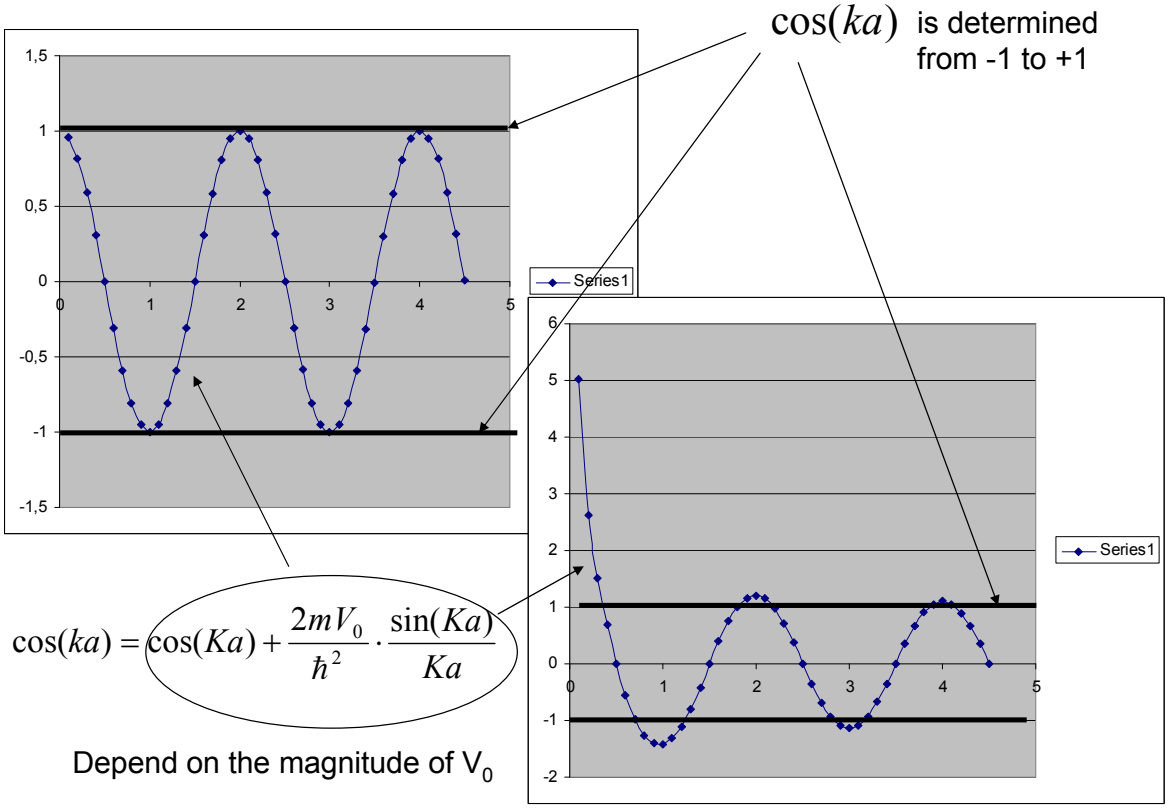
Kronig-Penney model



$$\cos(ka) = \cos(Ka) + \frac{2mV_0}{\hbar^2} \cdot \frac{\sin(Ka)}{Ka}$$

Kronig-Penney model



Kronig-Penney model

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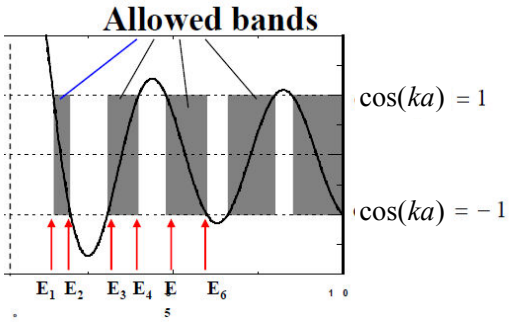
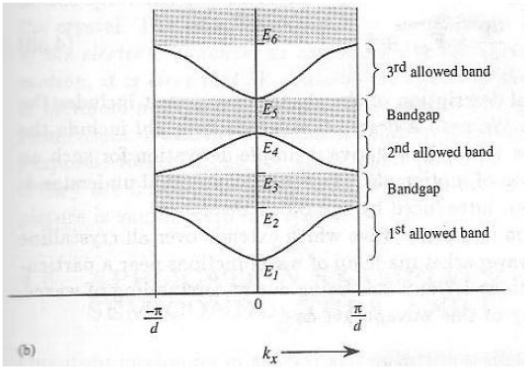
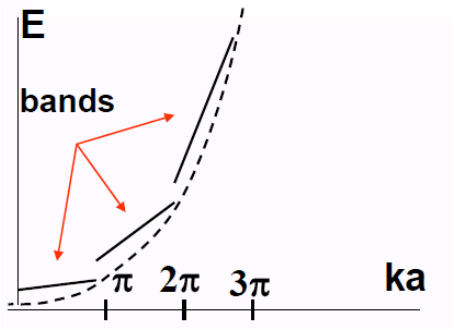


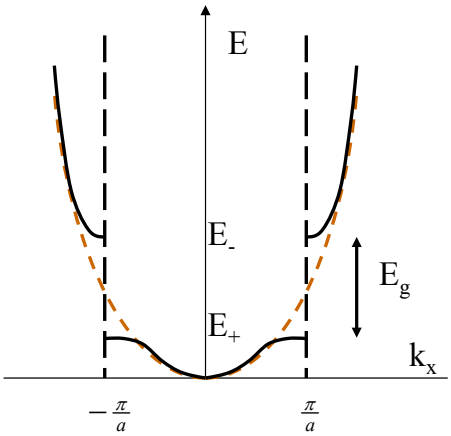
The allowed and forbidden bands are plotted in the E vs. k relation.



Kronig-Penney model

In between the two energies there are no allowed energies; i.e., an energy gap exists. We can sketch these 1-D results schematically:





The periodic potential U(x) splits the free-electron E(k) into "energy bands" separated by gaps at each BZ boundary.