

PHYS*4150 Review

Solid State Physics

Course outline

- Free electron model
 - Drude
 - Sommerfeld
- Crystal lattices
 - Direct lattice
 - Reciprocal lattice
- Diffraction
- Semi-classical theory of metals
 - Electrons in crystal lattice
 - Bloch's theorem
 - Nearly-free electron model
- Dynamic lattice (phonons)

Metals

Periodic Table of the Elements

<div style="border: 1px solid gray; padding: 5px; display: inline-block;"> Atomic Number Symbol Name Atomic Mass </div>																	
1 1A H Hydrogen 1.008																	18 VIIIA He Helium 4.003
3 Li Lithium 6.941	4 Be Beryllium 9.012											5 B Boron 10.811	6 C Carbon 12.011	7 N Nitrogen 14.007	8 O Oxygen 15.999	9 F Fluorine 18.998	10 Ne Neon 20.180
11 Na Sodium 22.990	12 Mg Magnesium 24.305	3 IIIB Sc	4 IVB Ti	5 VB V	6 VIB Cr	7 VIIB Mn	8 VIII Fe	9 VIII Co	10 VIII Ni	11 IB Cu	12 IIB Zn	13 Al Aluminum 26.982	14 Si Silicon 28.086	15 P Phosphorus 30.974	16 S Sulfur 32.066	17 Cl Chlorine 35.453	18 Ar Argon 39.948
19 K Potassium 39.098	20 Ca Calcium 40.078	21 Sc Scandium 44.956	22 Ti Titanium 47.867	23 V Vanadium 50.942	24 Cr Chromium 51.996	25 Mn Manganese 54.938	26 Fe Iron 55.845	27 Co Cobalt 58.933	28 Ni Nickel 58.693	29 Cu Copper 63.546	30 Zn Zinc 65.38	31 Ga Gallium 69.723	32 Ge Germanium 72.631	33 As Arsenic 74.922	34 Se Selenium 78.972	35 Br Bromine 79.904	36 Kr Krypton 83.798
37 Rb Rubidium 85.468	38 Sr Strontium 87.62	39 Y Yttrium 88.906	40 Zr Zirconium 91.224	41 Nb Niobium 92.906	42 Mo Molybdenum 95.95	43 Tc Technetium 98.907	44 Ru Ruthenium 101.07	45 Rh Rhodium 102.906	46 Pd Palladium 106.42	47 Ag Silver 107.866	48 Cd Cadmium 112.411	49 In Indium 114.818	50 Sn Tin 118.711	51 Sb Antimony 121.760	52 Te Tellurium 127.6	53 I Iodine 126.904	54 Xe Xenon 131.294
55 Cs Cesium 132.905	56 Ba Barium 137.326	57-71 Lanthanide Series	72 Hf Hafnium 178.49	73 Ta Tantalum 180.948	74 W Tungsten 183.84	75 Re Rhenium 186.207	76 Os Osmium 190.23	77 Ir Iridium 192.217	78 Pt Platinum 195.085	79 Au Gold 196.967	80 Hg Mercury 200.592	81 Tl Thallium 204.383	82 Pb Lead 207.2	83 Bi Bismuth 208.980	84 Po Polonium (209)	85 At Astatine 208.987	86 Rn Radon 222.018
87 Fr Francium 223.020	88 Ra Radium 226.025	89-103 Actinide Series	104 Rf Rutherfordium (261)	105 Db Dubnium (262)	106 Sg Seaborgium (263)	107 Bh Bohrium (264)	108 Hs Hassium (265)	109 Mt Meitnerium (266)	110 Ds Darmstadtium (267)	111 Rg Roentgenium (268)	112 Cn Copernicium (269)	113 Nh Nihonium (270)	114 Fl Flerovium (279)	115 Mc Moscovium (280)	116 Lv Livermorium (281)	117 Ts Tennessine (284)	118 Og Oganesson (284)
		57 La Lanthanum 138.905	58 Ce Cerium 140.116	59 Pr Praseodymium 140.908	60 Nd Neodymium 144.242	61 Pm Promethium 144.913	62 Sm Samarium 150.36	63 Eu Europium 151.964	64 Gd Gadolinium 157.25	65 Tb Terbium 158.925	66 Dy Dysprosium 162.500	67 Ho Holmium 164.930	68 Er Erbium 167.259	69 Tm Thulium 168.934	70 Yb Ytterbium 173.055	71 Lu Lutetium 174.967	
		89 Ac Actinium 227.028	90 Th Thorium 232.038	91 Pa Protactinium 231.036	92 U Uranium 238.029	93 Np Neptunium 237.048	94 Pu Plutonium 244.064	95 Am Americium 243.061	96 Cm Curium 247.070	97 Bk Berkelium 247.070	98 Cf Californium 251.080	99 Es Einsteinium (254)	100 Fm Fermium 257.095	101 Md Mendelevium 258.1	102 No Nobelium 259.101	103 Lr Lawrencium (262)	

Alkali Metal

Alkaline Earth

Transition Metal

Basic Metal

Semimetal

Nonmetal

Halogen

Noble Gas

Lanthanide

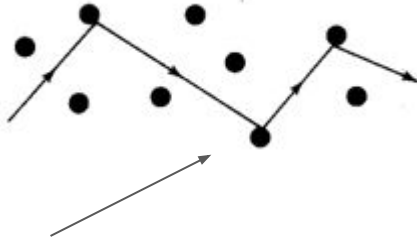
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Free electron model

Drude Model

Classical treatment of electrons in a metal

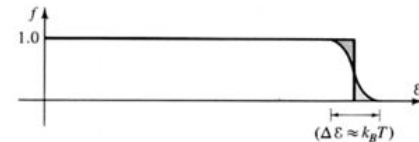
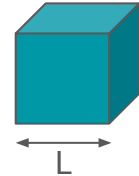


Phenomenological
scattering time τ

Sommerfeld Model

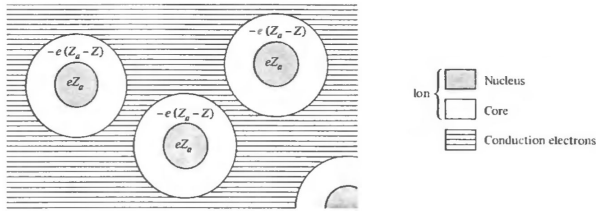
Application of Quantum mechanics and
Fermi-Dirac statistics to Drude model

$$\begin{aligned}\psi(x, y, z + L) &= \psi(x, y, z) \\ \psi(x, y + L, z) &= \psi(x, y, z) \\ \psi(x + L, y, z) &= \psi(x, y, z)\end{aligned}$$



Drude model

Classical model of free electron gas



Independent electron approx.

Free electron approx.

Classical laws of motion

DC conductivity: resistivity, current density

AC conductivity: reflectivity, transparency, plasma frequency, skin depth

Hall effect: Hall coefficient

Thermal conductivity: thermal conductivity coefficient, thermopower (Seebeck effect)

FAILURES of model

Sommerfeld model

Quantum mechanics: free electron with periodic boundary conditions

Pauli exclusion principle: Fermi-Dirac statistics, chemical potential

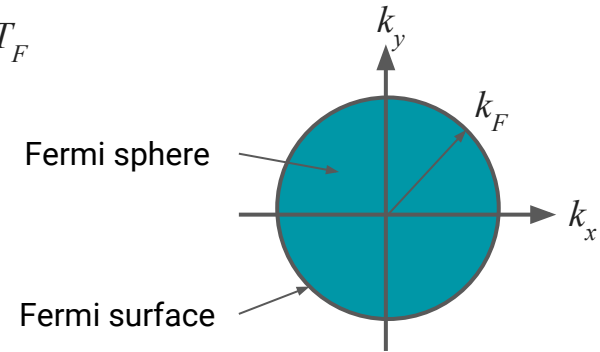
Plane-wave solutions: introduction to k-space

Density of states

Corrections to c_V and v_0

Fermi terminology

$$E_F, k_F, v_F, T_F$$



$$\sum_{\mathbf{k}} F(\mathbf{k}) = \frac{V}{8\pi^3} \sum_{\mathbf{k}} F(\mathbf{k}) \Delta \mathbf{k} \rightarrow \frac{V}{8\pi^3} \int F(\mathbf{k}) d\mathbf{k}$$

Crystal lattices

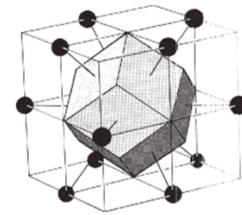
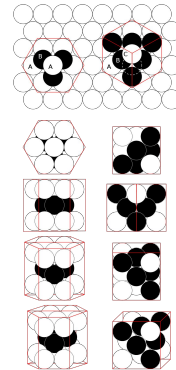
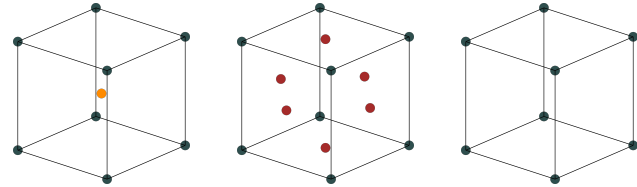
Bravais lattices: primitive vectors, lattice vectors $\rightarrow R(a_1, a_2, a_3)$, unit cell, Wigner-Seitz cell

Cubic lattices: Simple cubic, FCC, BCC

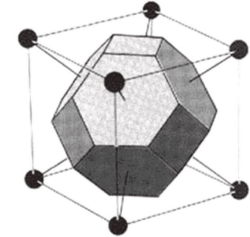
Lattice with a basis

Close-packed structures: HCP, FCC

$$\bar{R} = n_1 \bar{a}_1 + n_2 \bar{a}_2 + n_3 \bar{a}_3$$



Face Centered Cubic
Wigner-Seitz Cell



Body Centered Cubic
Wigner-Seitz Cell

Reciprocal lattice

Fourier transform of direct lattice

More k-space

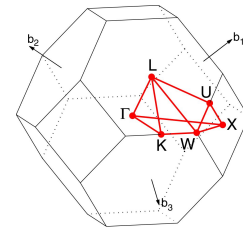
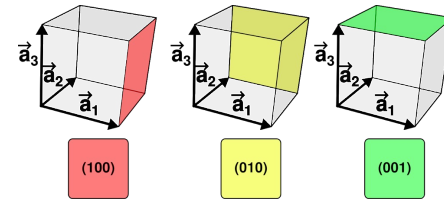
Bravais lattice: primitive vectors, reciprocal lattice vectors $\rightarrow K(b_1, b_2, b_3)$

Miller planes

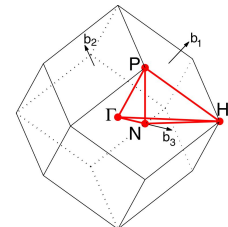
Brillouin Zones

$$e^{i\bar{K}\cdot\bar{R}} = 1$$

$$\bar{K} = n_1\bar{b}_1 + n_2\bar{b}_2 + n_3\bar{b}_3$$



FCC path: Γ -X-W-K- Γ -L-U-W-L-K|U-X



BCC path: Γ -H-N- Γ -P-H|P-N

Diffraction

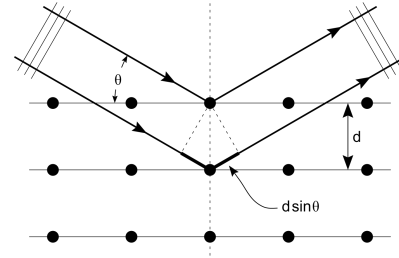
Study/measurement of crystal lattices

X-ray diffraction: direct measurement of reciprocal lattice

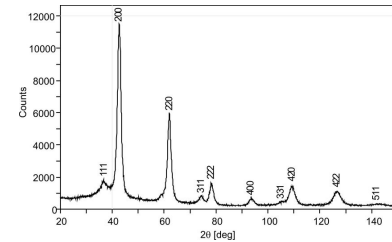
Von Laue diffraction

Powder diffraction

Structure factor: lattice with a basis, intensity of diffracted peaks



$$\bar{K} = \bar{k} - \bar{k}'$$



$$S_{\bar{K}} = \sum_j e^{i\bar{K} \cdot \bar{d}_j} \quad I_{\bar{K}} \propto |S_{\bar{K}}|^2$$

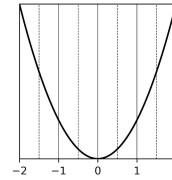
Electrons in a crystal lattice

Integration of crystal lattices with free electron model: empty lattice approximation, $2N$ electron states per B.Z., reduction to 1st B.Z. \rightarrow bands

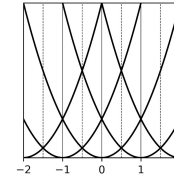
Bloch's Theorem: electrons in a periodic potential

Plane waves (FEM)

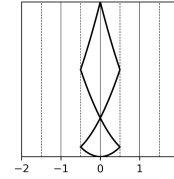
$$\psi_{n,k}(\vec{r}) = e^{i\vec{k}\cdot\vec{r}} u_{n,k}(\vec{r}) \leftarrow \text{Lattice modulation}$$



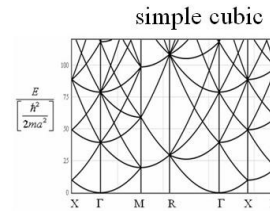
Extended



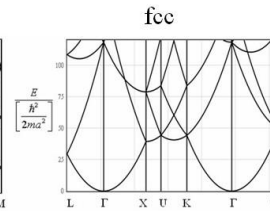
Repeated



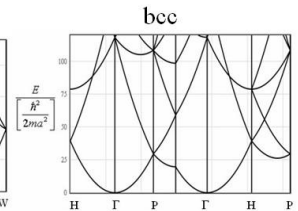
Reduced



simple cubic



fcc



bcc

$$\begin{aligned} \psi_{n,k}(\vec{r} + \vec{R}) &= e^{i\vec{k}\cdot\vec{R}} \psi_{n,k}(\vec{r}) \\ u_{n,k}(\vec{r} + \vec{R}) &= u_{n,k}(\vec{r}) \end{aligned}$$

Nearly free electron

Weak periodic potential: treat with perturbation theory

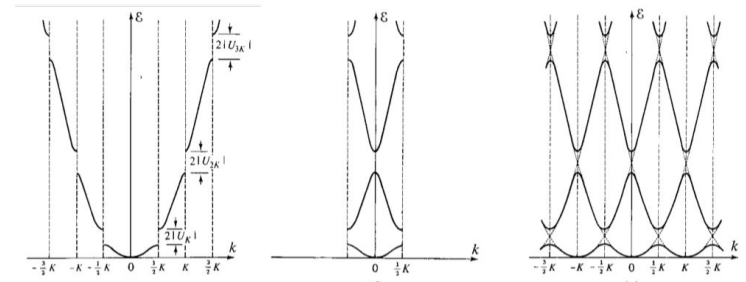
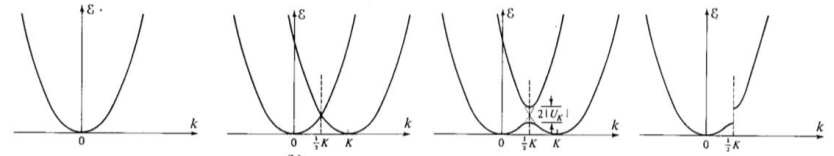
Band gap = $2|V_G|$

Material types

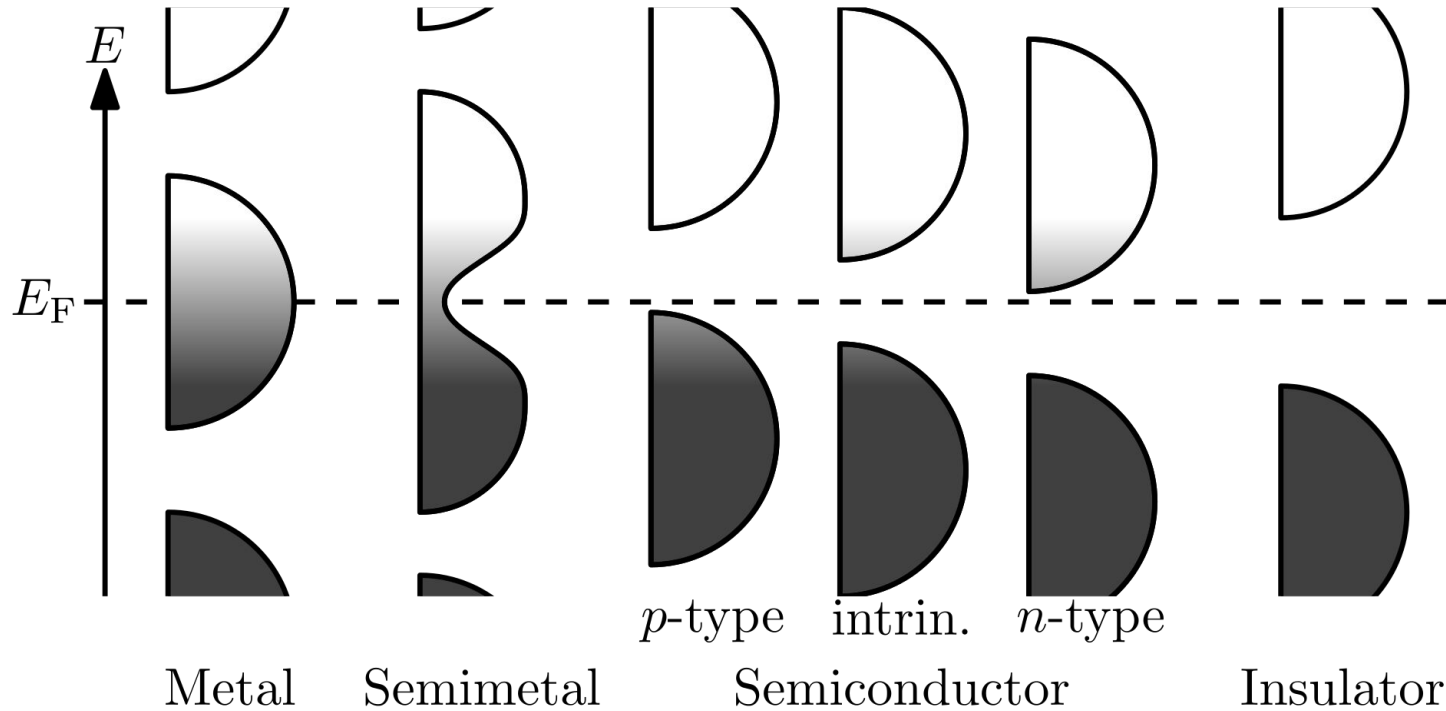
Insulator requires even # of electrons

Filled bands are inert

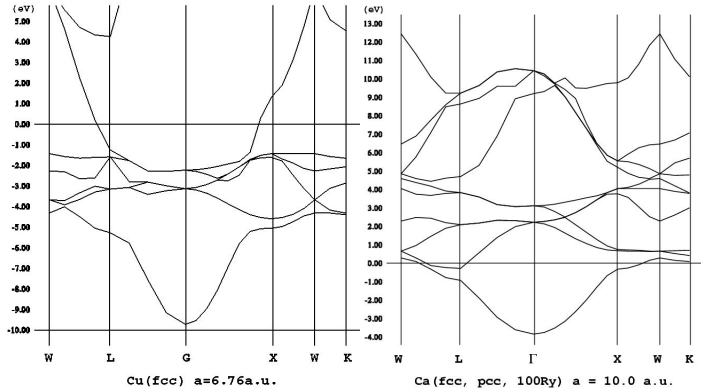
$$V(x) = \sum_{\bar{G}} V_{\bar{G}} e^{i\bar{G}\cdot\bar{r}}$$



Materials

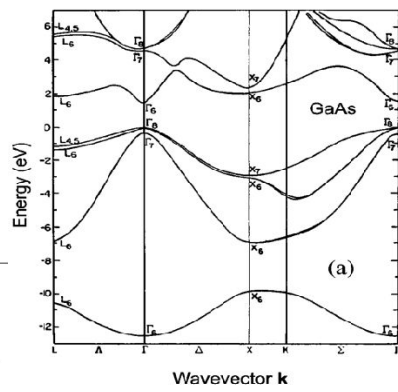


Band structure

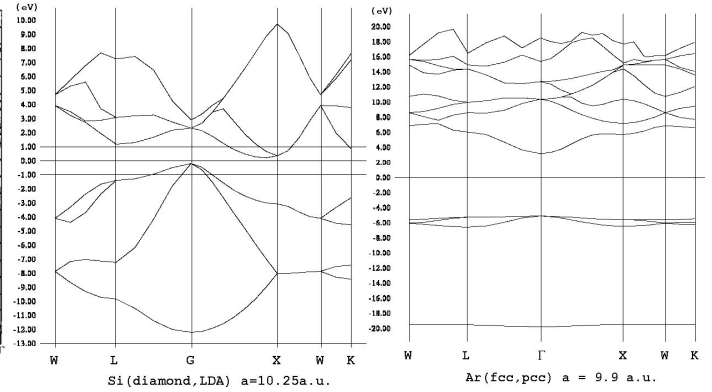


Metal

Semi-metal



Semiconductor
(direct)



Semiconductor
(indirect)

Insulator

Dynamic lattice

Harmonic lattice approximation

Dynamical matrix: dispersion curves, 1D monatomic, diatomic lattice, optic and acoustic modes, generalize to 3D

$3 \cdot N_b \cdot N$ normal modes: N modes per Brillouin zone per branch

Phonons

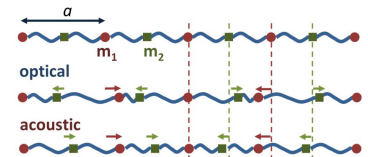
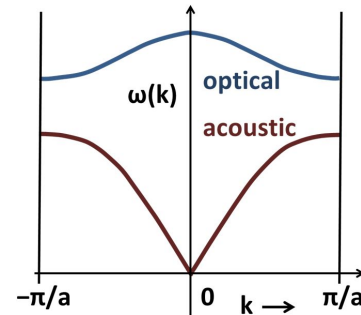
$$\text{Energy} = \hbar \omega_{n,k}$$

$$n_{s,k} = \frac{1}{e^{\hbar \omega_{s,k}/k_B T} - 1}$$

Occupancy: # of phonons in state s,k

$$\varphi^0(l, l') = \left. \frac{\partial^2 W}{\partial u_l \partial u_{l'}} \right|_0$$

$$\hat{D}_{\alpha, \alpha'}^{\mu, \mu'}(\bar{k}) = \frac{1}{\sqrt{M_\alpha M_{\alpha'}}} \sum_m \varphi_{\alpha, \alpha'}^{\mu, \mu'}(m) e^{i\bar{k} \cdot \bar{R}_m^0}$$



Final Exam:
Wed. April 17, 8:30-10:30am, MacN318