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

Plan for Lecture 4:

Reading: Chapter 1.6 & 2.1 in GGGPP – electron dynamics in one dimension & introduction to crystal structures

1. Brief discussion of electron dynamics in one dimension
2. Bravais lattice structures
3. Classification of crystal structures

PHY 752 Solid State Physics

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

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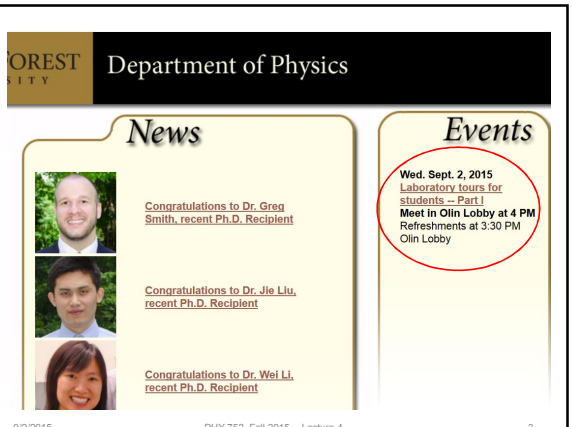
Course schedule

(Preliminary schedule -- subject to frequent adjustment.)

	Date	F&W Reading	Topic	Assignment
1	Wed, 8/26/2015	Chap. 1.1-1.2	Electrons in a periodic one-dimensional potential	#1
2	Fri, 8/28/2015	Chap. 1.3	Electrons in a periodic one-dimensional potential	#2
3	Mon, 8/31/2015	Chap. 1.4	Tight binding models	#3
4	Wed, 9/02/2015	Chap. 1.6, 2.1	Crystal structures	#4
5	Fri, 9/04/2015	Chap. 2	Group theory	
6	Mon, 9/07/2015	Chap. 2	Group theory	
7	Wed, 9/09/2015	Chap. 2	Group theory	
8	Fri, 9/11/2015			



Brief comment on electron dynamics as described by electronic band structure --

Electron velocity:

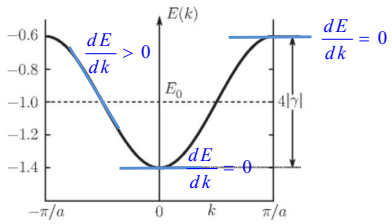
$$v(k) = \langle \psi(k,x) | \frac{p}{m} | \psi(k,x) \rangle .$$

$$\langle \psi(k,x) | \frac{p^2}{2m} + V(x) | \psi(k,x) \rangle = E(k),$$

$$\boxed{v(k) = \langle \psi(k,x) | \frac{p}{m} | \psi(k,x) \rangle = \frac{1}{\hbar} \frac{dE(k)}{dk}} ;$$

➔Band dispersion is related to electron velocity

Example of electron band dispersion in one dimension



In practice, electron transport can be well approximated by the Boltzmann equation with the main contributions coming near the Fermi level.

Electron effective mass from semi-classical analysis

$$\boxed{\frac{d(\hbar k)}{dt} = -eF} .$$ For applied force *F*

$$\frac{dv(k)}{dt} = \frac{d}{dt}\frac{1}{\hbar}\frac{dE(k)}{dk} = \frac{1}{\hbar}\frac{d^2E(k)}{dk^2}\frac{dk}{dt} = \left(\frac{1}{\hbar^2}\frac{d^2E(k)}{dk^2}\right)(-e)F .$$

1/m*

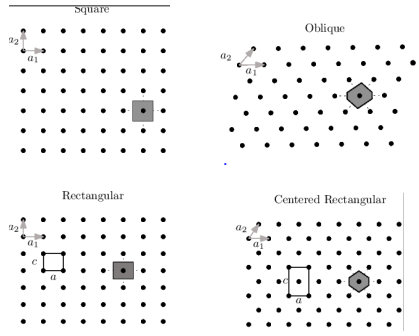
$$\boxed{\frac{1}{m^*} = \frac{1}{\hbar^2}\frac{d^2E(k)}{dk^2}} .$$

Classification of crystal structures
- 14 Bravais lattices
- 230 space groups

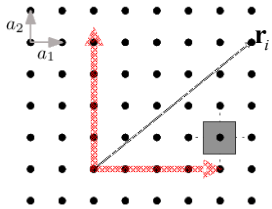
2 Geometrical Description of Crystals: Direct and Reciprocal Lattices

Chapter Outline head

Two-dimensional crystals



Some details –
square lattice example

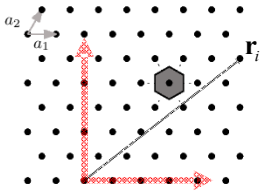


$$\mathbf{r}_i = n_{1i}\mathbf{a}_1 + n_{2i}\mathbf{a}_2$$

$$\mathbf{a}_1 = a\hat{\mathbf{x}} \qquad \mathbf{a}_2 = a\hat{\mathbf{y}}$$

Two-dimensional crystals -- continued

Hexagonal

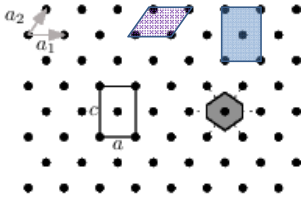


$$\mathbf{r}_i = n_{1i}\mathbf{a}_1 + n_{2i}\mathbf{a}_2$$

$$\mathbf{a}_1 = a\hat{\mathbf{x}} \qquad \mathbf{a}_2 = a\left(\frac{1}{2}\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}\hat{\mathbf{y}}\right)$$

"Conventional" versus "Primitive" unit cell

Centered Rectangular



$$\mathbf{a}_1 = a\hat{\mathbf{x}}$$
$$\mathbf{a}_2 = c\hat{\mathbf{y}}$$
$$\boldsymbol{\tau}_A = 0$$
$$\boldsymbol{\tau}_B = \frac{a}{2}\hat{\mathbf{x}} + \frac{c}{2}\hat{\mathbf{y}}$$

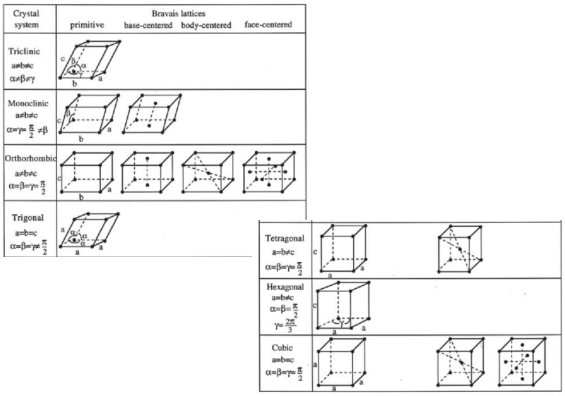
$$\mathbf{a}_1 = a\hat{\mathbf{x}}$$
$$\mathbf{a}_2 = \frac{a}{2}\hat{\mathbf{x}} + \frac{c}{2}\hat{\mathbf{y}}$$

Primitive translation vectors

$$\mathbf{t}_n = n_1\mathbf{t}_1 + n_2\mathbf{t}_2 + n_3\mathbf{t}_3;$$

Volume of primitive unit cell

$$\Omega = |\mathbf{t}_1 \cdot (\mathbf{t}_2 \times \mathbf{t}_3)|$$



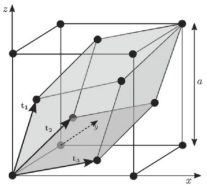
Common examples

2.2 Geometrical Description of Some Crystal Structures

Crystal Structure of Rare-Gas Solids (Face-Centered Cubic Lattice)

We begin our brief description of some crystals of interest with the case of rare-gas solids (Ne, Ar, Kr, Xe). This crystal structure (illustrated in Figure 2.4) is obtained repeating periodically in space a *face-centered cube* (fcc), i.e. a conventional cubic cell (of edge *a*) with atoms at the corners and at the center of the faces. The primitive translation vectors of the fcc Bravais lattice are

$$\mathbf{t}_1 = \frac{a}{2}(0, 1, 1), \quad \mathbf{t}_2 = \frac{a}{2}(1, 0, 1), \quad \mathbf{t}_3 = \frac{a}{2}(1, 1, 0) \tag{2.6}$$



Nearest neighbor distance between fcc lattice points: $a/\sqrt{2}$ (12)

https://en.wikipedia.org/wiki/Periodic_table_(crystal_structure)%29

Crystal structure of elements in the periodic table

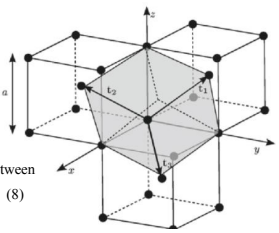
1 H HEX																	2 He HCP
3 Li BCC	4 Be HCP											5 B RHO	6 C HEX	7 N HEX	8 O CUB	9 F CUB	10 Ne FCC
11 Na BCC	12 Mg HCP											13 Al FCC	14 Si CUB	15 P ORTH	16 S ORTH	17 Cl ORTH	18 Ar FCC
19 K BCC	20 Ca FCC	21 Sc HCP	22 Ti HCP	23 V BCC	24 Cr BCC	25 Mn BCC	26 Fe BCC	27 Co HCP	28 Ni FCC	29 Cu FCC	30 Zn HCP	31 Ga ORTH	32 Ge CUB	33 As RHO	34 Se HEX	35 Br ORTH	36 Kr FCC
37 Rb BCC	38 Sr FCC	39 Y HCP	40 Zr HCP	41 Nb BCC	42 Mo BCC	43 Tc HCP	44 Ru HCP	45 Rh FCC	46 Pd FCC	47 Ag FCC	48 Cd HCP	49 In TETR	50 Sn TETR	51 Sb RHO	52 Te HEX	53 I ORTH	54 Xe FCC
55 Cs BCC	56 Ba BCC	*	72 Hf HCP	73 Ta BCC/TETR	74 W BCC	75 Re HCP	76 Os HCP	77 Ir FCC	78 Pt FCC	79 Au FCC	80 Hg RHO	81 Tl HCP	82 Pb FCC	83 Bi RHO	84 Po CUB/RHO	85 At [FCC]	86 Rn FCC
87 Fr [BCC]	88 Ra BCC	**	104 Rf [HCP]	105 Db [BCC]	106 Sg [BCC]	107 Bh [HCP]	108 Hs [HCP]	109 Mt [FCC]	110 Ds [BCC]	111 Rg [BCC]	112 Cn [HCP]	113 Uut	114 Fl	115 Uup	116 Lv	117 Uus	118 Uuo

Crystal Structure of Alkali Metals (Body-Centered Cubic Lattice)

The crystal structure of alkali metals (see Figure 2.5) is obtained repeating periodically in space a body-centered cube (bcc), i.e. a conventional cubic cell with atoms at the corners and at the center of a cube of edge a. The primitive translation vectors of the bcc Bravais lattice are

$$\mathbf{t}_1 = \frac{a}{2}(-1,1,1), \quad \mathbf{t}_2 = \frac{a}{2}(1,-1,1), \quad \mathbf{t}_3 = \frac{a}{2}(1,1,-1). \tag{2.7}$$

Notice that $\mathbf{t}_1+\mathbf{t}_2+\mathbf{t}_3 = (a/2)(1,1,1)$, and $\mathbf{t}_2+\mathbf{t}_3 = a(1,0,0)$, $\mathbf{t}_1+\mathbf{t}_3 = a(0,1,0)$, and $\mathbf{t}_1+\mathbf{t}_2 = a(0,0,1)$. The atom at the origin has 8 nearest neighbors in the positions



Nearest neighbor distance between bcc lattice points: $a\sqrt{3}/2$ (8)

2.4 Reciprocal Lattices

2.4.1 Definitions and Basic Properties

For the study of crystals, besides *the direct lattice in the ordinary space*, it is important to consider also the *reciprocal lattice in the dual (or reciprocal) space*.

Given a crystal with primitive translation vectors $\mathbf{t}_1, \mathbf{t}_2, \mathbf{t}_3$ in the direct space, we consider the three primitive vectors $\mathbf{g}_1, \mathbf{g}_2, \mathbf{g}_3$ in the reciprocal space, defined by the relations

$$\mathbf{t}_i \cdot \mathbf{g}_j = 2\pi\delta_{ij} \tag{2.16a}$$

$$\mathbf{g}_1 = \frac{2\pi}{\Omega}\mathbf{t}_2\times\mathbf{t}_3, \quad \mathbf{g}_2 = \frac{2\pi}{\Omega}\mathbf{t}_3\times\mathbf{t}_1, \quad \mathbf{g}_3 = \frac{2\pi}{\Omega}\mathbf{t}_1\times\mathbf{t}_2, \quad \text{and} \quad \Omega = \mathbf{t}_1\cdot(\mathbf{t}_2\times\mathbf{t}_3), \tag{2.17}$$

Example: fcc bravais lattice

$$\mathbf{t}_1 = \frac{a}{2}(0,1,1), \quad \mathbf{t}_2 = \frac{a}{2}(1,0,1), \quad \mathbf{t}_3 = \frac{a}{2}(1,1,0).$$

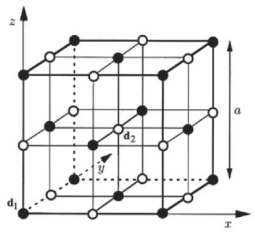
$$\mathbf{g}_1 = \frac{2\pi}{a}(-1,1,1), \quad \mathbf{g}_2 = \frac{2\pi}{a}(1,-1,1), \quad \mathbf{g}_3 = \frac{2\pi}{a}(1,1,-1).$$

Crystal basis vectors

$$\text{Crystal structure} \Longrightarrow \begin{cases} \mathbf{t}_1, \mathbf{t}_2, \mathbf{t}_3 & \text{(primitive translation vectors)} \\ \mathbf{d}_1, \mathbf{d}_2, \ldots, \mathbf{d}_v & \text{(basis of equal or different atoms)} \end{cases}.$$

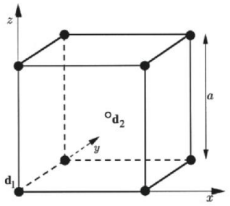
Example – NaCl having fcc lattice with a basis

$$\mathbf{t}_1 = \frac{a}{2}(0,1,1), \quad \mathbf{t}_2 = \frac{a}{2}(1,0,1), \quad \mathbf{t}_3 = \frac{a}{2}(1,1,0)$$
$$\mathbf{d}_1 = 0, \quad \mathbf{d}_2 = \frac{a}{2}(1,1,1)$$



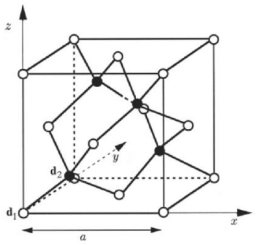
Example – CsCl having sc lattice with a basis

$$\mathbf{t}_1 = a(1,0,0), \quad \mathbf{t}_2 = a(0,1,0), \quad \mathbf{t}_3 = a(0,0,1)$$
$$\mathbf{d}_1 = 0, \quad \mathbf{d}_2 = \frac{a}{2}(1,1,1)$$



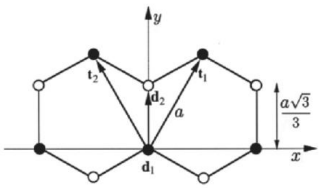
Example – diamond having fcc lattice with a basis

$$\mathbf{t}_1 = \frac{a}{2}(0,1,1), \quad \mathbf{t}_2 = \frac{a}{2}(1,0,1), \quad \mathbf{t}_3 = \frac{a}{2}(1,1,0)$$
$$\mathbf{d}_1 = 0, \quad \mathbf{d}_2 = \frac{a}{4}(1,1,1)$$



Two-dimensional graphene

$$\mathbf{t}_1 = a\left(\frac{1}{2}, \frac{\sqrt{3}}{2}, 0\right), \quad \mathbf{t}_2 = a\left(-\frac{1}{2}, \frac{\sqrt{3}}{2}, 0\right)$$
$$\mathbf{d}_1 = 0, \quad \mathbf{d}_2 = a\left(0, \frac{\sqrt{3}}{3}, 0\right)$$



Graphite lattice

$$\mathbf{t}_1 = a\left(\frac{1}{2}, \frac{\sqrt{3}}{2}, 0\right), \quad \mathbf{t}_2 = a\left(-\frac{1}{2}, \frac{\sqrt{3}}{2}, 0\right), \quad \mathbf{t}_3 = c(0, 0, 1)$$
$$\mathbf{d}_1 = 0, \quad \mathbf{d}_2 = a\left(0, \frac{\sqrt{3}}{3}, 0\right), \quad \mathbf{d}_3 = c\left(0, 0, \frac{1}{2}\right), \quad \mathbf{d}_4 = \left(0, a\frac{2\sqrt{3}}{3}, \frac{c}{2}\right)$$