PHY 752 Electrodynamics
11-11:50 AM MWF Olin 107

Plan for Lecture 1:

Reading: Chapters 1-2 in Marder's text

1. Course structure and expectations
2. Crystal structures
   a. Real and reciprocal space lattice vectors
   b. Some examples
   c. Point symmetry properties
   d. Introduction to group theory

http://users.wfu.edu/natalie/s15phy752/

PHY 752 Solid State Physics

MWF 11-11:50 AM | **OPL 107** | **http://www.wfu.edu/~natalie/s15phy752/**

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

- General information
- Syllabus and homework assignments
- Lecture notes
- Some presentation ideas

Last modfied: Saturday, 10-Jan-2015 22:04:37 EST

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

General Information

This course is a one semester survey of Solid State Physics at the graduate level, using the textbook: **Condensed Matter Physics**, 2nd edition, by Michael P. Marder (John Wiley & Sons, Inc., 2010) -- **"MPM"**. link to errata

It is likely that your grade for the course will depend upon the following factors:

Problem sets*	45%
Presentation	10%
Exams	45%

*The schedule notes the "due" date for each assignment. Homeworks may be turned in 1 lecture past their due date without grade penalty. After that, the homework grade will be reduced by 10% for each succeeding late date. According to the honor system, all work submitted for grading purposes should represent the student's own best efforts. This means that students who work together on homework assignments should all contribute roughly equally and independently verify all derivations and results.

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Course schedule for Spring 2015

(Preliminary schedule -- subject to frequent adjustment.)

	Lecture date	MPM Reading	Topic	Assign.	Due date
1	Mon: 01/12/2015	Chap. 1 & 2	Crystal structures	#1	01/23/2015
2	Wed: 01/14/2015	Chap. 1 & 2	Some group theory		01/23/2015
	Fri: 01/16/2015	No class	NAWH out of town		
	Mon: 01/19/2015	No class	MLK Holiday		
3	Wed: 01/21/2015	Chap. 1 & 2	Some group theory		01/23/2015

January 12, 2015

PHY 752 - Problem Set #1

Read Chapter 1 & 2 in **Marder**

1. Consider a system of atoms which held together by a pairwise force of the form

$$\phi(r)=\epsilon^{-1}\left(\frac{1}{r^{12}}-\frac{1}{r^{\beta}}\right),$$

Course syllabus:
In the formal portion of the course, the following topics are usually covered:

- Crystalline structures
  - Translation vectors and reciprocal lattice vectors
  - Symmetry properties of crystals; brief introduction to group theory analysis
  - Brief survey of common structures and their properties
  - X-ray and neutron scattering analysis of crystals
- Electronic structure analysis
  - Simple model examples
  - Linear combinations of atomic orbital analyses
  - Hartree-Fock approximations
  - Density functional formalism
  - Numerical approximations and methods
- Surfaces and interfaces
  - Relationship of interface and bulk properties
  - Low energy electron diffraction analysis
  - Scanning probe analysis of surfaces
- Defects and disorder effects

Course syllabus continued:

Depending on time available the following additional formal topics are often covered:

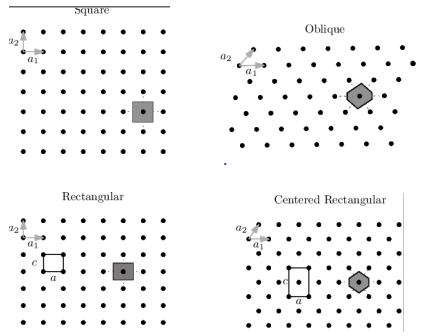
- Mechanical properties of solids
  - Cohesive properties
  - Deformation properties
  - Vibrational modes
  - Dislocations and cracks
- Electronic transport in solids
  - Semi-classical approximations and comparison with experiment
- Optical properties in solids
- Magnetic properties of solids

➔ Feedback on topics choice appreciated.

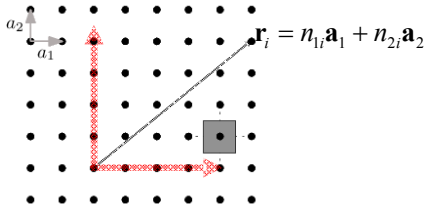
Introduction to crystalline solids

- An ideal crystal fills all space
  - Limited possibilities for crystalline forms –
    - ❑ Only 14 Bravais lattices
    - ❑ Only 32 crystallographic point groups
    - ❑ Only 230 distinct crystallographic structures
- Quantitative descriptions of crystals in terms of lattice translations vectors and basis vectors
- Use of group theory in the study of crystal structures

Two-dimensional crystals



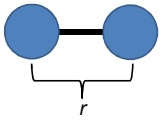
Some details –
square lattice example

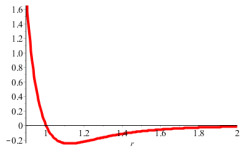


$$\mathbf{r}_i = n_{1i}\mathbf{a}_1 + n_{2i}\mathbf{a}_2$$

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

Energy associated with crystal configuration
Simple pair potential models

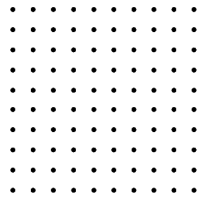


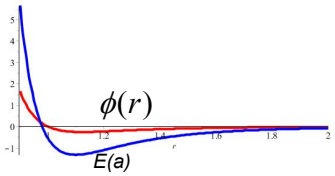


Lennard-Jones model: $\phi(r) = \frac{A}{r^{12}} - \frac{B}{r^6}$

Buckingham model: $\phi(r) = Ae^{-r/\rho} - \frac{B}{r^6}$

Energy of square lattice





$E = \sum_{j(i \neq j)} \phi(r_{ij})$

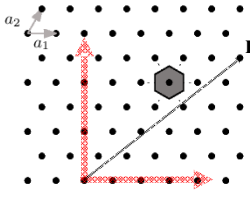
Note: This is the energy per atom assuming all atoms are identical.

For square lattice with lattice constant a:

$E \approx 4\phi(a) + 4\phi(\sqrt{2}a) + 4\phi(2a) + 8\phi(\sqrt{5}a) + \ldots$

Two-dimensional crystals -- continued

Hexagonal



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

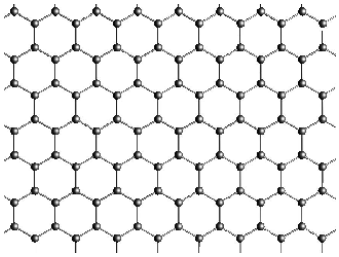
$\mathbf{a}_1 = a\hat{\mathbf{x}} \qquad \mathbf{a}_2 = a\left(\frac{1}{2}\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}\hat{\mathbf{y}}\right)$

For hexagonal lattice with lattice constant a:

$E \approx 6\phi(a) + 6\phi(\sqrt{3}a) + 6\phi(2a) + \ldots$

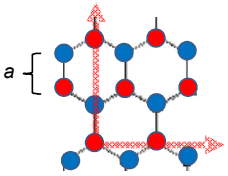
Two-dimensional crystals -- continued

Honeycomb lattice (graphene sheet)



Example of lattice with a "basis"

Honeycomb lattice (graphene sheet)



red atoms:

$$\mathbf{r}_i = \boldsymbol{\tau}_{\text{red}} + n_{1i}\mathbf{a}_1 + n_{2i}\mathbf{a}_2$$

blue atoms:

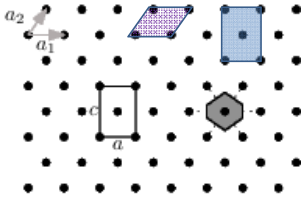
$$\mathbf{r}_i = \boldsymbol{\tau}_{\text{blue}} + n_{1i}\mathbf{a}_1 + n_{2i}\mathbf{a}_2$$

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

$$\boldsymbol{\tau}_{\text{red}} = 0 \qquad \boldsymbol{\tau}_{\text{blue}} = a\hat{\mathbf{y}}$$

"Conventional" versus "Primitive" unit cell

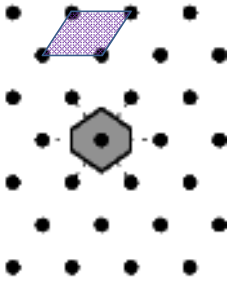
Centered Rectangular



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

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

Wigner-Seitz cell



Note that primitive cell and Wigner-Seitz cell have the same volume.

Generalization to 3-dimensions

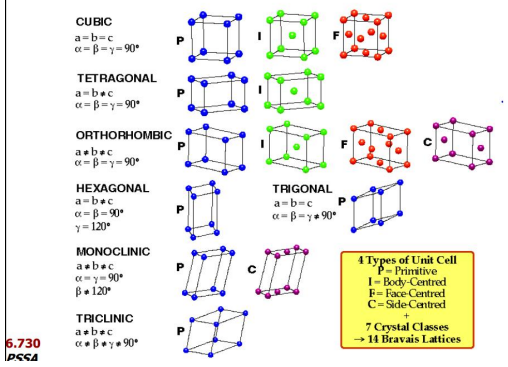
$$\mathbf{r}_i = \boldsymbol{\tau}_{\text{type}} + n_{1i}\mathbf{a}_1 + n_{2i}\mathbf{a}_2 + n_{3i}\mathbf{a}_3$$

basis vector

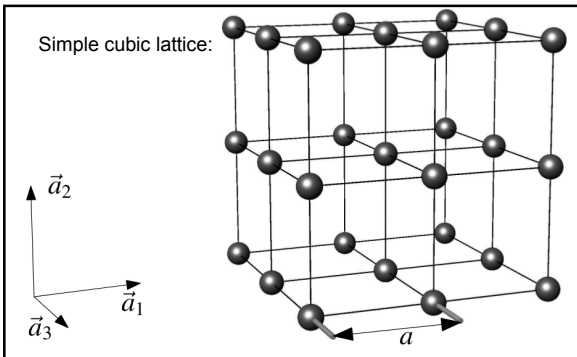
Bravais lattice

From http://web.mit.edu/6.730

3D: 14 Bravais Lattices

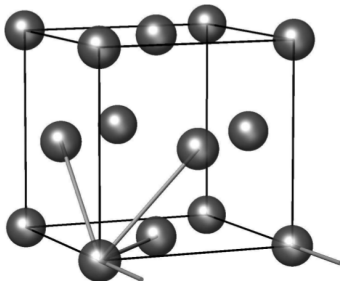


Simple cubic lattice:



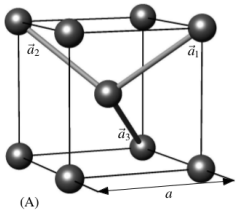
$$\vec{a}_1 = a(1\ 0\ 0),\ \vec{a}_2 = a(0\ 1\ 0),\ \vec{a}_3 = a(0\ 0\ 1)$$

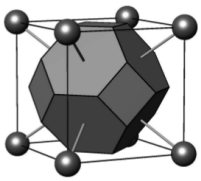
Face-centered cubic lattice



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

Body centered cubic lattice





Wigner-Seitz cell

$$\vec{a}_1 = \frac{a}{2}(1\ 1\ -1)\quad \vec{a}_2 = \frac{a}{2}(-1\ 1\ 1)\quad \vec{a}_3 = \frac{a}{2}(1\ -1\ 1)$$