581 semester review – Dr. Colton – Winter 2012

Big Themes

- Quasi particles ("collective excitations", "quantized oscillations")
  - Phonons
  - Photons
  - Electrons in solids ($m_e \neq m$)
  - Holes
  - Excitons
  - Polaritons
  - Plasmons
  - Polarons (not discussed; see Ch. 14, pp. 420-422)
  - Magnons (not discussed; see Ch. 12, pp. 330-335)
- Dispersion relations, and how to calculate them
  - Phonons, ω vs. k
  - Electrons, E vs. k
- Connection with other areas of physics
  - Thermodynamics
  - Quantum mechanics
  - Electrodynamics
- Mathematical techniques
  - Calculus, 1D and multivariable
  - Complex numbers
  - Fourier analysis
  - Linear algebra
- Models of reality (not a complete list, I am sure)
  - Phonons:
    - Balls & springs
    - Debye
    - Einstein
    - Simple scattering model
  - Electrons:
    - Free electrons
    - Simple scattering model
    - Kronig-Penney
    - Empty lattice
    - Nearly free electron
    - Hydrogen atom (electrons/donor ions; also electrons/holes as excitons)
    - Lorentz model

Chapter 1 – Crystal Structure

- Crystal = Lattice + basis
  - Symmetries (translation, rotation, reflection)
  - Lattice vectors
  - Primitive lattice vectors
- Lattice types ("Bravais")… especially sc, fcc, bcc, hexagonal
- Primitive unit cell
  - Conventional unit cell for fcc, bcc
- Crystal planes, Miller indices
- Examples of crystal structures… especially fcc, bcc, NaCl, CsCl, hcp, diamond, zinc-blende

Chapter 2 – Wave Diffraction and the Reciprocal Lattice

- X-ray diffraction ("Bragg diffraction") as interference from planes of atoms
- Reciprocal lattice as Fourier transform of real space lattice

    - Reciprocal lattice vectors
    - Primitive reciprocal lattice vectors
- Brillouin zones, first Brillouin zone for common crystals… especially fcc, bcc, NaCl, hcp, diamond, zinc-blende
- Generalized Bragg diffraction, using reciprocal lattice vectors, $\Delta\mathbf{k} = \mathbf{G}$
- Structure factor, atomic form factors – how they impact observed diffraction spots
- Temperature dependence of x-ray diffraction pattern (Debye-Waller factor)

Chapter 3A – Crystal Binding

- Crystal binding (van der Waals, ionic, covalent, metallic, hydrogen)
- Cohesive energy
    - Lenard-Jones potential for van der Waals
    - Madelung potential for ionic
        - Madelung constant α
- Equilibrium lattice constant
- Compressibility/bulk modulus

Chapter 3B – Elastic Constants

- Long wavelength sound waves (solid as elastic continuum)
- Stress/strain tensors (2^{nd} rank)
    - Physical meaning (fractional volume change as trace of strain tensor, etc.)
- Stiffness/compliance tensors (4^{th} rank, but expressed as 6×6 matrix)
    - Stiffness constants for cubic crystals (C_{11}, C_{12}, C_{44})
- How to get velocities of sound waves in cubic crystals in various directions (longitudinal and transverse)
    - Table of "effective elastic constants" for [100], [110], and [111] directions.

Chapter 4 – Phonons 1. Crystal Vibrations

- Balls & springs models, including 2 or more atoms/basis
    - Boundary conditions (periodic vs. other)
- Dispersion curves, ω vs. k
    - Acoustic and optical branches
    - Determining number/type of branches for various numbers of atoms in primitive cell, various dimensions
    - Physical meaning of waves at zone center and at zone edge
- Reduced zone scheme (first Brillouin zone)
- Phonons! (quantization of the vibrational modes)
    - Spacing between points in First B.Z. is $L/2\pi$ ($(L/2\pi)^3$ in 3D)
- Phonon scattering, conservation of crystal momentum (momentum ± a RLV×$\hbar$)

Chapter 5 – Phonons 2. Thermal Properties

- Bose-Einstein distribution function
    - How to calculate total number of particles
    - How to calculate total energy
- Density of states $\mathcal{D}(E)$ (how to calculate in 1D, 2D, and 3D)
- Debye model
- How to calculate total energy and heat capacity in the Debye model
    - Low temperature limit ($\sim T^3$)
    - High temperature limit (constant, matches Dulong-Petit value from equipartition theorem)
- Einstein model
- Thermal conductivity – phonon scattering model
    - Scattering time, mean free path
    - Mechanisms contributing to τ: surfaces, defects, electrons, phonons

    - Temperature dependence (low T = dominated by C_V dependence on T; high T = dominated by τ dependence on T)

Chapter 6 – Free Electron Fermi Gas

- Metal = box containing a "gas" of free electrons
- Density of states (1D, 2D, and 3D)
- Fermi-Dirac distribution function
    - Chemical potential and Fermi energy ("Fermi level")
    - How to calculate total number of particles
    - How to calculate the chemical potential
        - For zero temperature, two methods (Fermi energy)
        - For non-zero temperatures
    - How to calculate total energy
- Heat capacity of free electron gas
    - Low temperature limit (~T)
- Electrical and thermal conductivity – electron scattering model
    - Scattering time, mean free path, drift velocity, Ohm's Law
    - Wiedermann-Franz Law, Lorentz number
- Hall effect

Chapter 7 – Energy bands

- Bloch theorem ("Bloch functions", "Bloch waves")
- Band structures, E vs. k
    - Reduced zone scheme (first B.Z.)
- Zone edge as Bragg diffraction of electron waves (standing waves)
- Band structure calculation 0: Free electrons (discussed in last chapter)
- Band structure calculation 1: Kronig-Penney model (1D)
- Band structure calculation 2: Empty lattice approximation
- Band structure calculation 3: Central equation
    - Fourier transform of Schroedinger equation
    - Expanding U in Fourier components U_G
- Band structure calculations 4: Perturbation theory ("Nearly free electron model")
    - States connect to other states with same k (reduced zone)
    - Degenerate perturbation theory when states with same k have same energy
    - Energy gaps; parabolic bands going away from the gaps
- Metals vs. insulators (and semiconductors) – which category a given material will be in

Chapters 8 and 17 – Semiconductors/ Semiconductor Devices

- Energy gaps ("band gaps"), direct and indirect
    - General picture of band structure for Si and GaAs as prototypical semiconductors
- Valence and conduction bands
- Effective mass
- Holes
- Intrinsic semiconductors
    - Thermal promotion of electrons from VB to CB, intrinsic concentration n_i
    - Chemical potential/Fermi energy (equation)
- Mobility
- Doped semiconductors
    - Donors vs. acceptors; n- vs. p-type
    - Binding energy and Bohr radius of electrons/holes
    - Thermal promotion of electrons from donor level to CB (or holes from acceptor level to VB)
    - Chemical potential/Fermi energy (qualitatively)
- Junctions
    - p-n ("diode", "diode drop")

    - semiconductor-metal (“Schottky”)
- Transistors, bipolar and FET

Chapters 14 – 16 (selected section) – Optical Properties of Solids

- Electromagnetic theory
    - Polarization
    - Susceptibility
    - Relative permittivity (aka dielectric constant)
    - Index of refraction
- Optical reflectance
- Kramers-Kronig relations
- Lorentz model
    - UV: electrons bound to atoms
    - IR: ions, coupling to phonons
        - Polaritons
    - Metals (not bound)
        - Plasma oscillations, plasmons