Solid State Physics: Midterm 2 Review

November 4, 2018

1 Crystal Structure

1.1 Basics of Crystal Structure

- A *lattice* is an infinite set of points defined by integer sums of a set of linearly independent *primitive lattice vectors*.
- Alternatively: A *lattice* is an infintie discrete set of vectors where addition of any two vectors in the set gives a third vector in the set, or a *lattice* is an infinite discrete set of points where the environment of any given point is equivalent to the environment of any other point.
- Lattice points may be described in three dimensions as

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

- In 2+ dimensions, the choice of primitice lattice vectors is not unique.
- A *unit cell* is the repeated motif which is the elementary building block of any periodic structure. When many identical unit cells are tiled together, they completely fill all of space and reconstruct the full structure.
- A *primitive unit cell* is a unit cell containing exactly one lattice point.
- A *conventional unit cell* is a typically less-minimal unit cell, often with orthogonal axes, chosen due to ease of use.
- A *Wigner-Seitz cell* is constructed by including all points in space that are closer to a given lattice point than any other lattice point. Approach: choose a lattice cell and draw lines to all possible neighbors. Perpendicular bisectors of these lines bound the Wigner-Seitz cell.
- The description of the unit cell with respect to the associated lattice point is known as the *basis*.
- The positions of atoms can be described by

$$\mathbf{R} = \mathbf{R}_{lattice} + \mathbf{R}_{basis}$$

1.2 Three-Dimensional Lattices

The simplest example is the *simple cubic* lattice.

- The primitive unit cell is typically a cube, where each corner contributes 1/8 lattice point.
- *Tetragonal* and *orthorhombic* lattices have two and three different primitive lattice vector lengths, respectively.
- A point in the lattice may be written as $[uvw]$ where

$$[uvw] = u\mathbf{a}_1 + v\mathbf{a}_2 + w\mathbf{a}_3$$

- In the case of orthogonal axes, $\mathbf{a}_1$ is assumed to be in the $\hat{x}$ direction, etc.