Institutt for fysikk, NTNU TFY4340 Mesoscopic Physics Spring 2010

Lecture notes, week 3 (January 19)

## SOLID STATE PHYSICS UPDATE

Crystal structure

A Bravais lattice is formed by all possible lattice vectors

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

where  $n_i = 0, \pm 1, \pm 2, ...$ , and  $a_1, a_2$ , and  $a_3$  are primitive vectors. A primitive unit cell is spanned by the primitive vectors:



The primitive cell has volume

$$V_3 = |(\boldsymbol{a}_1 \times \boldsymbol{a}_2) \cdot \boldsymbol{a}_3|.$$

(Subscript 3 indicates a 3–dimensional volume.) In a 2–dimensional system (2D), the "volume" (i.e., area) of the primitive cell is

$$V_2 = A = |\boldsymbol{a}_1 \times \boldsymbol{a}_2|.$$

Example: 2D triangular lattice.



Primitive vectors:

$$a_1 = a\hat{x}$$
  

$$a_2 = \frac{a}{2}\hat{x} + \sqrt{a^2 - (a/2)^2}\hat{y} = \frac{a}{2}\hat{x} + \frac{\sqrt{3}a}{2}\hat{y}$$

Area of primitive cell:

$$V_2 = A = |\mathbf{a}_1 \times \mathbf{a}_2| = |\frac{\sqrt{3}a^2}{2}\hat{z}| = \frac{\sqrt{3}a^2}{2}.$$

Example: 3D face-centered cubic (FCC) lattice.



Primitive vectors:

$$egin{array}{rcl} {m a}_1 &=& rac{a}{2}\,(\hat{x}+\hat{y}) \ {m a}_2 &=& rac{a}{2}\,(\hat{x}+\hat{z}) \ {m a}_3 &=& rac{a}{2}\,(\hat{y}+\hat{z}) \end{array}$$

Primitive cell volume:

$$V_3 = |(\boldsymbol{a}_1 \times \boldsymbol{a}_2) \cdot \boldsymbol{a}_3| = \frac{a^3}{8} |(-\hat{y} - \hat{z}) \cdot (\hat{y} + \hat{z})| = \frac{a^3}{8} |-2| = \frac{a^3}{4}$$

This is the volume pr lattice point in the FCC Bravais lattice.

A Wigner–Seitz cell is the region of space around a given lattice point P which is closer to P than to all the other lattice points.

Example: 2D triangular lattice.



In other words, the 2D triangular lattice has a hexagonal Wigner–Seitz cell.

The reciprocal lattice of a Bravais lattice consists of all the (wave–)vectors  $\boldsymbol{K}$  that correspond to plane waves

 $e^{i \boldsymbol{K} \cdot \boldsymbol{r}}$ 

with the periodicity of the Bravais lattice, i.e.,

$$e^{i\boldsymbol{K}\cdot(\boldsymbol{r}+\boldsymbol{R})}=e^{i\boldsymbol{K}\cdot\boldsymbol{r}}.$$

which implies that  $\mathbf{K} \cdot \mathbf{R} = 0, \pm 2\pi, \pm 4\pi, \dots$  Hence,

$$\boldsymbol{K} = m_1 \boldsymbol{b}_1 + m_2 \boldsymbol{b}_2 + m_3 \boldsymbol{b}_3,$$

with integer-valued  $m_i$  and the following relations between the primitive reciprocal lattice vectors  $b_i$ and the primitive real space lattice vectors  $a_i$ :

$$b_1 = \frac{2\pi}{V} (\boldsymbol{a}_2 \times \boldsymbol{a}_3)$$
  

$$b_2 = \frac{2\pi}{V} (\boldsymbol{a}_3 \times \boldsymbol{a}_1)$$
  

$$b_3 = \frac{2\pi}{V} (\boldsymbol{a}_1 \times \boldsymbol{a}_2)$$

Here,  $V = V_3 = |(\mathbf{a}_1 \times \mathbf{a}_2) \cdot \mathbf{a}_3|$ , as above. One also has the relation  $\mathbf{b}_i \cdot \mathbf{a}_j = 2\pi \delta_{ij}$  between primitive reciprocal and direct lattice vectors. Here,  $\delta_{ij}$  is the Kronecker delta, i.e.,  $\delta_{ij} = 1$  if i = j and  $\delta_{ij} = 0$  if  $i \neq j$ .

Brillouin zones:

The Wigner-Seitz cell in reciprocal space, around the origin  $\mathbf{K} = 0$ , is by definition the *first Brillouin* zone (1BZ). [More generally, the *n*-th BZ corresponds to the region of K-space with K = 0 as the *n*-th nearest neighbour.]

We will mainly discuss experiments that involve transport of electrons in semiconductors like silicon, Si, and gallium arsenide, GaAs. The crystal structure of Si is the *diamond* lattice, i.e., two FCC sublattices, one centered at the origin, and the other shifted an amount (a/4, a/4, a/4) with respect to the first one. Gallium arsenide has the *zincblende* lattice structure, with an FCC Ga lattice centered at (0, 0, 0) and an FCC As lattice centered at (a/4, a/4, a/4). The reciprocal lattice of the FCC lattice is the body–centered cubic (BCC) lattice.

## Electrons in solid state crystals

Several factors complicate the quantum-mechanical description of electrons in a crystal:

- the periodic potential,  $V(\mathbf{r} + \mathbf{R}) = V(\mathbf{r})$ , due to the ionic lattice
- there are *many* electrons, interacting with each other (Coulomb repulsion)
- the lattice is not static, but vibrating, even at zero temperature (T = 0) (the ground state of a harmonic oscillator has energy  $E = \hbar \omega/2$ )
- the crystal is not perfect, there are impurities and other lattice defects
- the temperature in a real system is not zero

- the electron spin couples to its orbital motion, so-called spin-orbit coupling
- and so on

We start by making the most drastic simplifications and neglect *all* the complications listed above and assume that we have *free, non-interacting* electrons moving around in our crystal. I.e., the potential is simply a constant, and we may as well put V = 0. However, we retain the fact that electrons are *fermions*, so that a given single–particle quantum state may at most be occupied by a single electron. This is the *Pauli exclusion principle*. A "single–particle quantum state" is a solution  $\psi$  of the (time independent) single–particle Schrödinger equation (SE)

$$\left[-\frac{\hbar^2}{2m}\nabla^2 + V(\boldsymbol{r})\right]\psi(\boldsymbol{r}) = E\psi(\boldsymbol{r}).$$

For simplicity, we let our "constant potential crystal" be a cube with volume  $V = L^3$ . Concerning boundary conditions, we may choose between (a) vanishing wave function,  $\psi = 0$ , at the edges of the cube, or (b) periodic boundary conditions (PBC),  $\psi(x + L, y, z) = \psi(x, y, z)$  etc. With PBC, the eigensolutions are plane waves,

$$\psi(x, y, z) = C e^{i \boldsymbol{k} \cdot \boldsymbol{r}},$$

with wave vectors

$$\mathbf{k} = k_x \hat{x} + k_y \hat{y} + k_z \hat{z} = \frac{2\pi}{L} \left( n_1 \hat{x} + n_2 \hat{y} + n_3 \hat{z} \right)$$

Once more, the  $n_i$  are integer-valued.

## Spin degeneracy

Electrons have spin S, with  $S = |S| = \sqrt{s(s+1)}\hbar = \sqrt{3/4}\hbar$  and  $S_z = m_s\hbar = \pm\hbar/2$ . Thus, we have 2 possible spin states for each "orbital state"  $\psi(\mathbf{r})$ :  $\xi(+)$  for a "spin up" electron and  $\xi(-)$  for a "spin down" electron.

*Energy eigenvalus* Inserting the plane wave solution into the SE yields the familiar free–electron energy eigenvalues

$$E(\boldsymbol{k}) = \frac{\hbar^2 k^2}{2m}.$$

The function  $E(\mathbf{k})$  is also known as the *dispersion relation*. If the system is sufficiently small, the energy spectrum is *discrete*, with a separation between the energy levels proportional to  $1/L^3$ . In a macroscopic system, with a large value of L, we have an approximately *continuous* energy spectrum.

## Density of states

Having determined the dispersion relation  $E(\mathbf{k})$ , we are able to calculate the density of states (DOS), both in k-space and as a function of the energy E. Carrying on with the free-electron model, we see that there is one allowed value of the wave vector  $\mathbf{k}$  in a cube of volume  $(2\pi/L)^3$  in k-space. Taking spin degeneracy into account, this means that there are 2 allowed states in this volume. Hence, the DOS in k-space is

$$D(\mathbf{k}) = \frac{2}{(2\pi/L)^3} = \frac{V}{4\pi^3}.$$

Within a sphere of radius k, the number of allowed states is then

$$N(k) = D(\mathbf{k}) \cdot V_k = \frac{V}{4\pi^3} \cdot \frac{4}{3}\pi k^3 = \frac{V}{3\pi^2}k^3.$$

Hence, since  $k = \sqrt{2mE/\hbar^2}$ , the number of allowed states with energy less than E is

$$N(E) = \frac{V}{3\pi^2} \cdot \left(\frac{2mE}{\hbar^2}\right)^{3/2}.$$