

**Brief Summary of a Few Central Concepts in Condensed Matter  
Physics**

**Physics 880.06: Winter, 2003-4**

**David G. Stroud**

In these notes I give a brief survey of a few central concepts in condensed matter physics. More details can be found in a number of standard sources, e. g. Ashcroft and Mermin. These notes are a work in progress: I hope to update them from time to time.

1. Bravais Lattice.

A Bravais lattice is a network of points in d-dimensional space (usually we take  $d = 3$ ) defined by the equation

$$\mathbf{R} = \sum_{i=1}^d n_i \mathbf{a}_i, \quad (1)$$

where the  $n_i$ 's are positive or negative integers. The vectors  $\mathbf{a}_i$  are called basis vectors, and they must all be linearly independent.

For example, in a cubic lattice in  $d = 3$ , the conventional choice of the three basis vectors is  $\mathbf{a}_i = a\hat{x}_i$ , where  $\hat{x}_i$  is a unit vector in the  $i^{th}$  direction.

2. Unit Cell; Primitive Cell.

A unit cell for a crystal structure is a volume which, if translated in turn by some subset of the Bravais lattice vectors, will fill all space. The smallest possible unit cell is called the primitive cell. It is a volume which, if translated in turn by all of the Bravais lattice vectors, will fill all space. The choice of primitive cell (and of unit cell) is not unique, and may be made in any convenient way. One common choice of primitive cell is the Wigner-Seitz cell; this is that volume which is closer to a given Bravais lattice point than to any other Bravais lattice point. For example, in a simple cubic lattice, the Wigner-Seitz cell is also a cube; in a body-centered-cubic (bcc) lattice, it is a fourteen-sided polyhedron consisting of six square and eight hexagonal faces (see picture in Ashcroft and Mermin).

The conventional unit cell is the unit cell which is generally chosen. For example, in the bcc lattice, the conventional unit cell is the cube of edge  $a$ , with lattice points on the corners and one lattice point in the center of the cube. This actually has the volume of two primitive cells.

### 3. Crystal Structure.

A crystal structure is defined by a Bravais lattice and a basis of atoms. The basis of  $s$  atoms is defined by the  $s$  basis vectors and by the identities of the atoms occupying the basis sites.

Many crystal structures have a basis of just one atom, in which case there is only one basis vector which may be chosen to be zero. Some well-known

crystal structures with a basis of one atom are the face-centered cubic (fcc), body-centered cubic (bcc) and simple cubic (sc) structures.

One common crystal structure is the diamond structure (this has an fcc Bravais lattice with a basis of two identical atoms; well-known examples include C in its diamond form, Si, and Ge). The zinc-blende structure is like the diamond structure, except that the two atoms forming the basis are not identical. Examples include GaAs and InSb. The hexagonal close-packed (hcp) crystal structure has a simple hexagonal Bravais lattice with a basis of two identical atoms; examples include Mg, Zn, and Cd. The honeycomb lattice is a two-dimensional crystal structure with a triangular Bravais lattice and a basis of two atoms; the best-known example would be a single layer of C in its graphite form.

*Optional exercises: find suitable primitive vectors for the simple cubic, body-centered cubic, and face-centered cubic lattices. Find the Bravais lattice and basis vectors for the diamond, zinc-blende, and honeycomb lattices.*

#### 4. Reciprocal Lattice

The reciprocal lattice to a given Bravais lattice is also a Bravais lattice, but in “reciprocal space.” It consists of all vectors  $\mathbf{K}$  satisfying the relation

$$e^{i\mathbf{K}\cdot\mathbf{R}} = 1, \quad (2)$$

where  $\mathbf{R}$  is a lattice vector of the original Bravais lattice.

In three dimensions, the primitive vectors of the reciprocal lattice are

$$\mathbf{b}_1 = \frac{2\pi\mathbf{a}_2 \times \mathbf{a}_3}{v_c} \quad (3)$$

$$\mathbf{b}_2 = \frac{2\pi\mathbf{a}_3 \times \mathbf{a}_1}{v_c} \quad (4)$$

$$\mathbf{b}_3 = \frac{2\pi\mathbf{a}_1 \times \mathbf{a}_2}{v_c}, \quad (5)$$

where  $v_c = |\mathbf{a}_1 \cdot \mathbf{a}_2 \times \mathbf{a}_3|$  is the volume of the primitive cell.

*Optional exercise: Show that the reciprocal of a bcc lattice is an fcc lattice. Show that the reciprocal of the reciprocal lattice is the original Bravais lattice. Show that the reciprocal of a simple hexagonal lattice is also a simple hexagonal lattice, but rotated with respect to the original one.*

The first Brillouin zone is defined to be the Wigner-Seitz cell of the reciprocal lattice.

### 5. Bloch's Theorem (for electrons)

Consider an electron moving in a potential  $U(\mathbf{r})$  which satisfies the periodicity condition

$$U(\mathbf{r} + \mathbf{R}) = U(\mathbf{r}), \quad (6)$$

where  $\mathbf{R}$  is a Bravais lattice vector. Then Bloch's theorem states that the eigenfunctions  $\psi(\mathbf{r})$  of the Schrödinger equation

$$\left( -\frac{\hbar^2}{2m} \nabla^2 + U(\mathbf{r}) \right) \psi(\mathbf{r}) = E\psi(\mathbf{r}) \quad (7)$$

are of the form

$$\psi(\mathbf{r}) = e^{i\mathbf{k}\cdot\mathbf{r}}u(\mathbf{r}), \quad (8)$$

where

$$u(\mathbf{r}) = u(\mathbf{r} + \mathbf{R}). \quad (9)$$

The vector  $\mathbf{k}$  is called the Bloch vector. Without loss of generality, one need consider  $\mathbf{k}$ 's only in the first Brillouin zone.

## 6. Fermi Surface

The Fermi surface is defined to be the surface in  $\mathbf{k}$  space which separates the regions of occupied and unoccupied states at temperature  $T = 0$ . For example, if the electrons have the dispersion relation  $E(\mathbf{k}) = \hbar^2 k^2 / (2m)$ , this surface will be a sphere. If  $\mathbf{k}$  represents the Bloch vector, then there will be a separate Fermi surface in the first Brillouin zone for each partially occupied band.

## 7. Electronic bands

Because of Bloch's theorem, the Bloch vector  $\mathbf{k}$  is always a good quantum number for the electrons. The energy levels of an electron in a periodic solid can therefore be classified into energy bands, defined by a series of functions  $E_n(\mathbf{k})$ , where  $n$  is the discrete *band index* and  $\mathbf{k}$  is the continuous Bloch vector, which can be considered as confined to the first Brillouin zone. (If  $\mathbf{k}$  is outside the first Brillouin zone, the states are equivalent to corresponding  $\mathbf{k}$  vectors in the first Brillouin zone; no new states are found by considering  $\mathbf{k}$  outside the first Brillouin zone.)

## 8. Free electron gas in d dimensions

A central concept in condensed matter physics is the idea of a free electron gas. We begin with such a gas in three dimensions ( $d = 3$ ). The electron states satisfy the Schrödinger equation (ignoring spin)  $H\psi(\mathbf{x}) = E\psi(\mathbf{x})$ , where

$$H = -\frac{\hbar^2}{2m}\nabla^2, \quad (10)$$

$m$  being the electron mass. To define normalized eigenstates, we assume a volume  $V = L^3$ , and assume periodic boundary conditions,

$$\psi(x + L, y, z) = \psi(x, y, z), \quad (11)$$

with similar conditions in the  $y$  and  $z$  directions. The allowed normalized eigenstates are

$$\psi(x, y, z) = \frac{1}{\sqrt{V}}e^{i\mathbf{k}\cdot\mathbf{r}}, \quad (12)$$

with corresponding energy

$$E(\mathbf{k}) = \frac{\hbar^2 k^2}{2m}. \quad (13)$$

The boundary conditions imply that  $k_x = 2\pi n_x/L$ ,  $k_y = 2\pi n_y/L$ ,  $k_z = 2\pi n_z/L$ , where  $n_x$ ,  $n_y$ , and  $n_z$  are positive or negative integers. Thus the allowed  $\mathbf{k}$  points lie on a simple cubic grid of density

$$\rho(\mathbf{k}) = \frac{1}{(2\pi/L)^3} = \frac{V}{(2\pi)^3}. \quad (14)$$

We can now use this relation to calculate, for example, the Fermi energy,  $E_F$ , which is the energy of the maximum occupied state at  $T = 0$ . If there

are  $N$  electrons in volume  $V$ , then  $E_F$  is defined by the relation

$$2 \sum_{\mathbf{k}: E(\mathbf{k}) < E_F} (1) = N, \quad (15)$$

where the notation means that we sum up over all states such that  $E(\mathbf{k}) < E_F$ . The factor of 2 is for spin degeneracy. We turn the sum into an integral by using the transformation

$$\sum_{\mathbf{k}} \rightarrow \rho(\mathbf{k}) \int d^3k. \quad (16)$$

Using eq. (14) for the density of states, we get

$$\frac{2V}{(2\pi)^3} \int_{E(\mathbf{k}) < E_F} d^3k = N \quad (17)$$

or

$$\frac{2V}{(2\pi)^3} \left( \frac{4\pi k_F^3}{3} \right) = N, \quad (18)$$

where  $\hbar^2 k_f^2 / (2m) = E_F$ . This equation is easily solved for  $k_F$  with the result

$$k_F = (3\pi^2 n)^{1/3}, \quad (19)$$

where  $n = N/V$  is the electron density.

Other properties of the electron gas are also easily calculated. For example, the internal energy at  $T = 0$  is

$$U = \frac{2V}{(2\pi)^3} \sum_{\mathbf{k}} E(\mathbf{k}), \quad (20)$$

where the prime denotes again that the sum is carried out over all  $\mathbf{k}$  such that  $E(\mathbf{k}) < E_F$ . It is readily found that

$$U = \frac{3NE_F}{5}. \quad (21)$$

Another quantity of interest is the density of states per unit energy, denoted  $n(E)$ . By definition  $n(E)dE$  is the number of states per unit volume between energy  $E$  and energy  $E + dE$ . To calculate this, note that this is the number of states per unit volume between  $k$  and  $k + dk$ , where  $k = (2mE/\hbar^2)^{1/2}$  and therefore  $dk = (2m/\hbar^2)^{1/2}(1/2)E^{-1/2}$ .

*Optional exercise: Show that in three dimensions  $n(E) = CE^{1/2}$  and find the constant  $C$ .*

*Optional exercise: Repeat in two dimensions. Find the relation between  $k_F$  and  $n$  in two dimensions. Show that  $n(E)$  is energy independent in two dimensions and find the constant value. Repeat in one dimension.*

## 9. Finite temperature properties of the free electron gas.

At finite temperatures, the probability that an electronic state of energy  $E(\mathbf{k})$  is occupied is given by the Fermi factor,

$$f(E) = \frac{1}{e^{\beta(E-\mu)} + 1}. \quad (22)$$

For very low temperatures ( $k_B T \ll E_F$ ), the chemical potential  $\mu \sim E_F$ . Then  $f(E) \sim 1$  or  $0$  except when  $E$  is within approximately  $k_B T$  of the Fermi energy  $E_F$ . A good order of magnitude estimate of the specific heat

is then obtained by assuming that electrons between  $E_F$  and  $E_F - k_B T$  are thermally excited by an amount  $k_B T$  into previously unoccupied states. The number of such electrons is about  $n(E_F)k_B T$ . The total energy gained by each electron is  $k_B T$ , so the total increase in internal energy is about  $n(E_F)k_B^2 T^2$  per unit volume. The specific heat at constant volume is the temperature derivative of this, or

$$C_V \sim 2k_B^2 T n(E_F). \quad (23)$$

This is within a factor of two of the exact value (at very low temperatures), which is  $(\pi^2/6)k_B^2 T n(E_F)$ .

### 10. Lattice vibrations.

The atoms in a crystal do not actually sit statically on their lattice sites, but vibrate around those sites. This occurs even at temperature  $T = 0$  (because of zero-point motion). In a periodic crystal, the vibrations are Bloch waves which have definite wave vectors  $\mathbf{k}$  and definite frequencies  $\omega$ . The relation between  $\omega$  and  $\mathbf{k}$  can be worked out from the *harmonic Hamiltonian*  $H_{harm}$ , which is applicable when the amplitude of the oscillations is small. We describe this for the case of one atom per unit cell.

$H_{harm}$  is the sum of a kinetic energy and a potential energy:

$$H_{harm} = K + U_{harm}, \quad (24)$$

where the kinetic energy is

$$K = \sum_{\mathbf{R}} \frac{\mathbf{P}_{\mathbf{R}} \cdot \mathbf{P}_{\mathbf{R}}}{2M}, \quad (25)$$

and the potential energy is

$$U_{harm} = U_0 + \frac{1}{2} \sum_{\mathbf{R}, \mathbf{R}'} \sum_{\alpha\beta} D_{\alpha\beta}(\mathbf{R} - \mathbf{R}') u_{R\alpha} u_{R'\beta}. \quad (26)$$

Here  $U_0$  is the static potential energy,  $\mathbf{P}_{\mathbf{R}}$  is the momentum operator of the  $\mathbf{R}^{th}$  atom,  $\mathbf{u}_{\mathbf{R}}$  is the operator describing the displacement of the  $\mathbf{R}^{th}$  atom from its equilibrium position, and the subscripts  $\alpha$  and  $\beta$  denote Cartesian components. The quantity  $D_{\alpha\beta}(\mathbf{R} - \mathbf{R}')$  is called the *dynamical matrix*. It depends only on the difference  $\mathbf{R} - \mathbf{R}'$  in a periodic crystal, and not on  $\mathbf{R}$  and  $\mathbf{R}'$  individually.

$H_{harm}$  can be treated as a classical Hamiltonian, and the classical equations of motion can be written down. They take the form

$$M\ddot{u}_{R\alpha} = - \sum_{\mathbf{R}'\beta} D_{\alpha\beta}(\mathbf{R} - \mathbf{R}') u_{R'\beta}, \quad (27)$$

where the dot denotes a time derivative. The solutions take the form

$$u_{R\alpha}(t) = u_{\alpha 0} \exp(i\mathbf{k} \cdot \mathbf{R} - i\omega t), \quad (28)$$

where the squared frequencies  $\omega^2(\mathbf{k})$  are solutions of the  $3 \times 3$  determinantal equation

$$\det|D_{\alpha\beta}(\mathbf{k}) - M\omega^2(\mathbf{k})\delta_{\alpha\beta}| = 0. \quad (29)$$

The matrix  $D_{\alpha\beta}(\mathbf{k})$ , also known as the dynamical matrix, is just the Fourier transform of  $D_{\alpha\beta}(\mathbf{R} - \mathbf{R}')$ :

$$D_{\alpha\beta}(\mathbf{k}) = \sum_{\mathbf{R}} \exp(-i\mathbf{k} \cdot \mathbf{R}) D_{\alpha\beta}(\mathbf{R}). \quad (30)$$

For each  $\mathbf{k}$ , there are three functions  $\omega^2(\mathbf{k})$ , which describe the *dispersion relations* for lattice vibrations in the crystal. If there are  $N$  atoms in the crystal, then there are  $3N$  modes. One needs to consider only  $\mathbf{k}$  in the first Brillouin zone (BZ); all modes outside the first Brillouin zone turn out to be equivalent to modes within the first BZ.

There can be pure longitudinal modes ( $\mathbf{k} \parallel \mathbf{u}$ ) and pure transverse modes ( $\mathbf{k} \perp \mathbf{u}$ ). However, in general, the modes need not be either pure longitudinal or pure transverse.