Institutt for fysikk, NTNU
TFY4340 Mesoscopic Physics
Spring 2010

Lecture notes, week 3 (January 19)

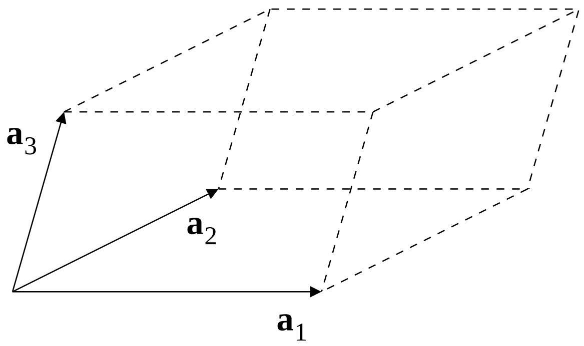
SOLID STATE PHYSICS UPDATE

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 $n_i = 0, \pm1, \pm2, \ldots$, and $\boldsymbol{a}_1$, $\boldsymbol{a}_2$, and $\boldsymbol{a}_3$ are primitive vectors. A primitive unit cell is spanned by the primitive vectors:



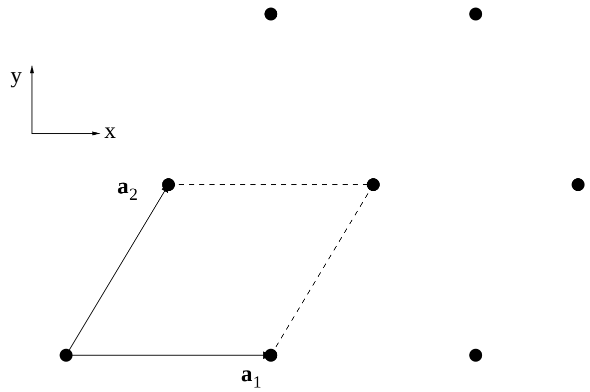
The primitive cell has volume

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

(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.



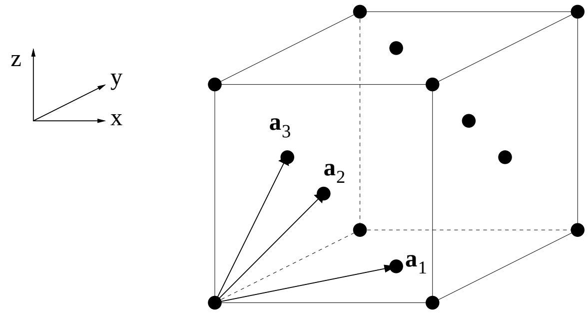
Primitive vectors:

$$\begin{aligned}\boldsymbol{a}_1 &= a\hat{x}\\ \boldsymbol{a}_2 &= \frac{a}{2}\hat{x}+\sqrt{a^2-(a/2)^2}\hat{y}=\frac{a}{2}\hat{x}+\frac{\sqrt{3}a}{2}\hat{y}\end{aligned}$$

Area of primitive cell:

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

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



Primitive vectors:

$$\begin{aligned}\boldsymbol{a}_1 &= \frac{a}{2}(\hat{x}+\hat{y})\\ \boldsymbol{a}_2 &= \frac{a}{2}(\hat{x}+\hat{z})\\ \boldsymbol{a}_3 &= \frac{a}{2}(\hat{y}+\hat{z})\end{aligned}$$

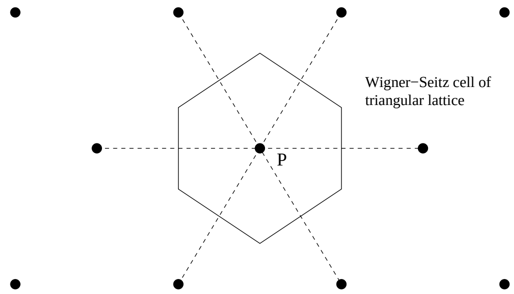
Primitive cell volume:

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

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 $\boldsymbol{K}\cdot\boldsymbol{R} = 0, \pm 2\pi, \pm 4\pi, \ldots$. 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 $\boldsymbol{b}_i$ and the primitive real space lattice vectors $\boldsymbol{a}_i$:

$$\begin{aligned} \boldsymbol{b}_1 &= \frac{2\pi}{V}\,(\boldsymbol{a}_2\times\boldsymbol{a}_3) \\ \boldsymbol{b}_2 &= \frac{2\pi}{V}\,(\boldsymbol{a}_3\times\boldsymbol{a}_1) \\ \boldsymbol{b}_3 &= \frac{2\pi}{V}\,(\boldsymbol{a}_1\times\boldsymbol{a}_2) \end{aligned}$$

Here, $V = V_3 = |\,(\boldsymbol{a}_1\times\boldsymbol{a}_2)\cdot\boldsymbol{a}_3|$, as above. One also has the relation $\boldsymbol{b}_i\cdot\boldsymbol{a}_j = 2\pi\delta_{ij}$ between primitive reciprocal and direct lattice vectors. Here, δ_{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 $\boldsymbol{K} = 0$, 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, $V(\boldsymbol{r}+\boldsymbol{R}) = V(\boldsymbol{r})$, 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 ψ 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

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

Once more, the n_i are integer–valued.

Spin degeneracy

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

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

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

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

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

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