Reciprocal Space and Fourier Analysis

Additional reading

- Any book in solid state physics, in particular
  - Ashcroft and Mermin, chapters 4 and 5.
  - the oxford solid state basics, Simon, chapters 12 and 13.
- The books will cover this material in much more detail than these notes. But you don't need to know everything. In this course we will, luckily, only need the basics

Contents

Reciprocal space and Fourier analysis

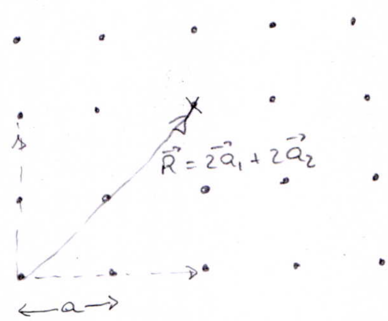
In these notes you will learn how to deal with crystalline systems. Funny enough, 99% of our work will not be in real space, but in an abstract mathematical space called reciprocal space (it look a bit like the upside-down of Stranger things).

We begin by defining a crystal and discussing some important crystal structures. this discussion will not be the most complete, since we will only need some basic facts for our course. If you want a more detailed analysis I recommend the book by Ashcroft and Mermin.

A crystal has 2 parts

$$\boxed{\text{Crystal} = \text{Bravais lattice} + \text{Basis}} \qquad (1)$$

A Bravais lattice is an infinite collection of equivalent points. One example is the square lattice



The word "equivalent" is very important: in a Bravais lattice, if an Allien moves you from one point to another, you won't even know you moved. Your surroundings are absolutely identical no matter in which point you sit.

For every lattice we may define a set of independent primitive vectors $\vec{a}_i$, such that any point in the lattice may be reached by an integer combination of the $\vec{a}_i$. that is, starting at any point you may reach any other point as

$$\boxed{\begin{gathered}\vec{R} = m_1 \vec{a}_1 + m_2 \vec{a}_2 + m_3 \vec{a}_3 \\ m_i = \text{integers.}\end{gathered}} \qquad (2)$$

[I wrote the result as if the lattice in 3D. If your lattice is 2D simply set $m_3 = 0$].

For the square lattice the obvious choice of basis vectors are

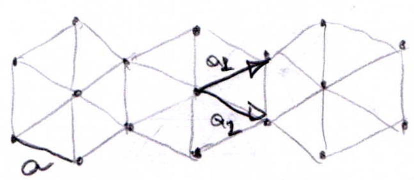
$$\vec{a}_1 = a(1,0) \qquad \vec{a}_2 = a(0,1) \qquad (3)$$

where a is the lattice spacing

Another important Bravais lattice is the hexagonal/triangular lattice

$$\vec{a}_1 = a(1,0) \qquad (4)$$

$$\vec{a}_2 = a\left(\frac{1}{2}, \frac{\sqrt{3}}{2}\right)$$



(NOT UNIQUE)

or

$$\vec{a}_1 = \frac{a}{2}(\sqrt{3}, 1) \qquad (5)$$

$$\vec{a}_2 = \frac{a}{2}(\sqrt{3}, -1)$$

This lattice has $120°$ rotation symmetry, whereas the square lattice has $90°$.