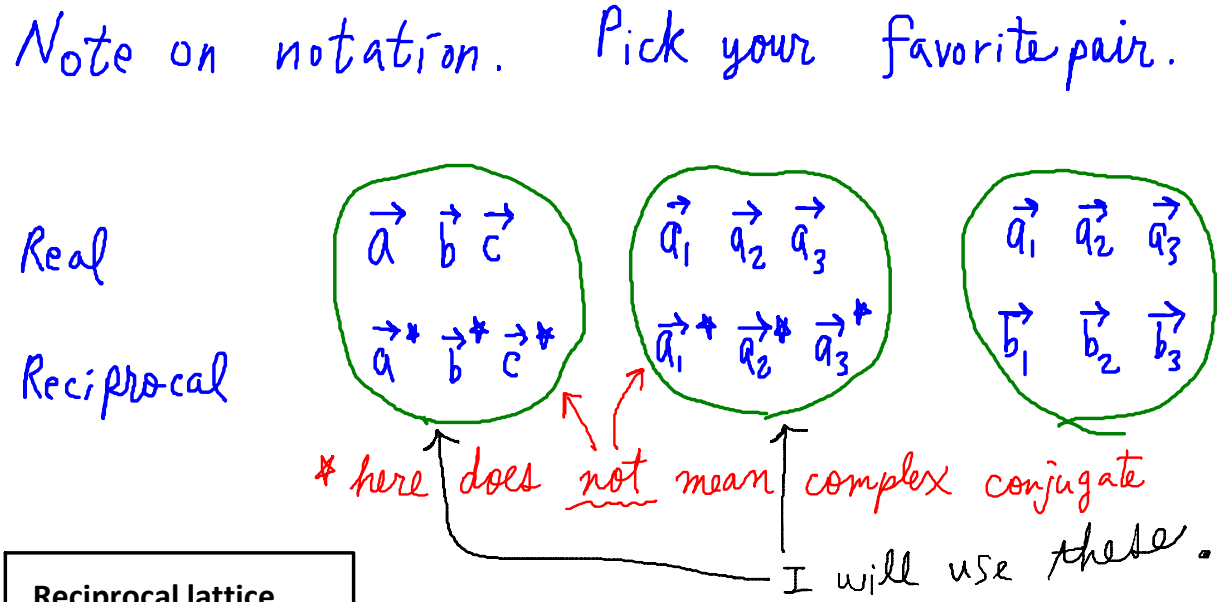
Lecture 04

Thursday, January 19, 2012



Reciprocal lattice

Has the same symmetry as the real lattice.
Its reciprocal is the real lattice.

Real lattice: $\vec{R} = l\,\vec{a} + m\,\vec{b} + n\,\vec{c}$

Reciprocal lattice: $\vec{G} = l\,\vec{a}^* + m\,\vec{b}^* + n\,\vec{c}^*$

notation: $\vec{K}$ in place of $\vec{G}$ is often used, also.

The first Brillouin zone

The Wigner Seitz cell in the reciprocal lattice.
Very important for this course and also in general.
In short, we may call it the Brillouin zone (BZ), as the "first" is implied then by convention.

Note that any two BZs in the reciprocal space are completely equivalent to each other. What does this mean? Note that the reciprocal space is the wave-vector/momentum space.

In **one dimension**, the BZ is simply the interval $(-\pi/a, \pi/a)$, if a is the lattice constant of the crystal.

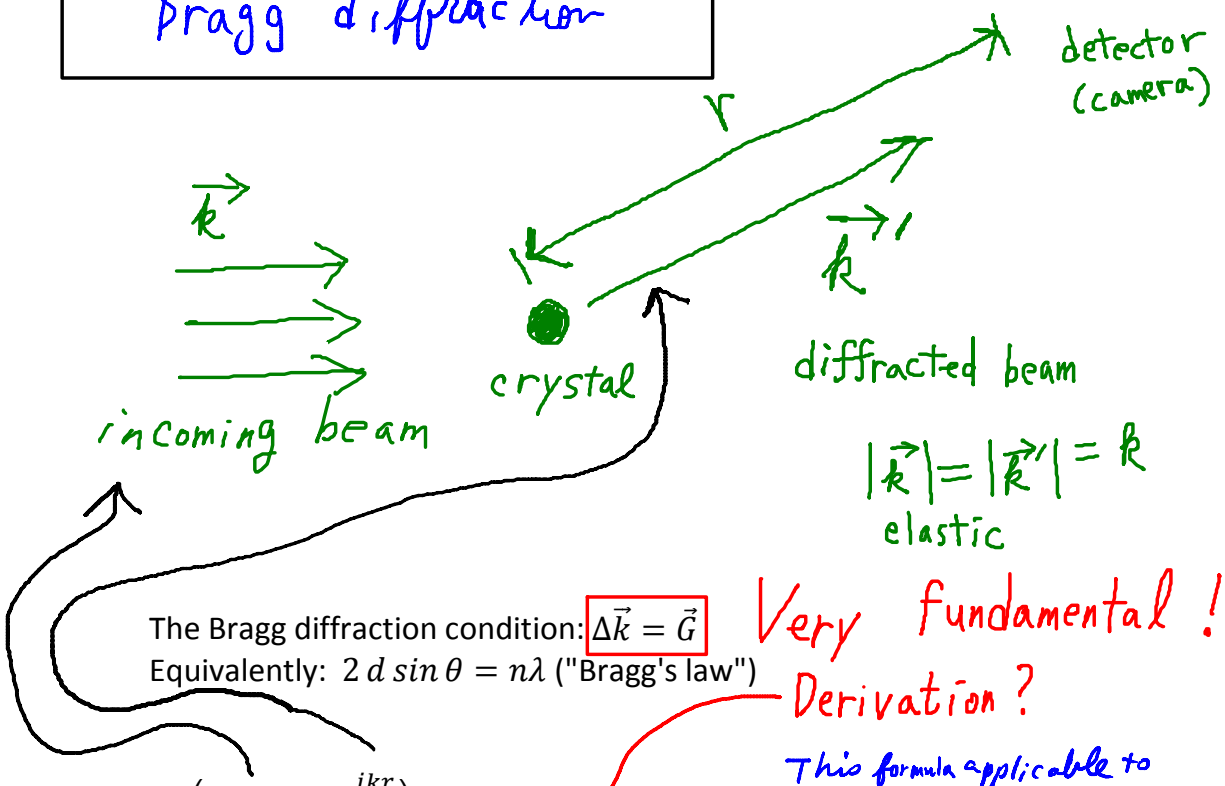
In **two dimensions**, the BZ is a square, a hexagon, a rectangle, a stretched hexagon, or a corner cut parallelogram.

In **three dimensions**, the BZ can look quite pretty.

In the following, the theory of diffraction will be given. Please read it carefully as it is a very detailed account. In a homework problem, I think I will present a slightly different point of view, which will still get the same essential results.

Elementary theory of diffraction by crystal

Bragg diffraction



The Bragg diffraction condition: $\Delta\vec{k} = \vec{G}$ Very fundamental !

Equivalently: $2\,d\,\sin\theta = n\lambda$ ("Bragg's law")

Derivation ?

$$\psi = A\left(e^{i\vec{k}\cdot\vec{r}} + f\frac{e^{ikr}}{r}\right)$$

This formula applicable to electron, neutron diffraction

$$f = -\frac{m}{2\pi\hbar^2}\int e^{i(-\vec{k}'+\vec{k})\cdot\vec{r}'}V(\vec{r}')d\vec{r}'$$

The first order Born approximation (cf. any QM book).

but not to X-ray diffraction. However, the results are still applicable to X-ray. See "atomic form factor" later.

Here, $V(\vec{r}')$ is the potential due to the crystal.

So, $V(\vec{r}') = \sum_{\vec{R}}' V_b(\vec{r}' - \vec{R})$, where $V_b(\vec{r}' - \vec{R})$ is the potential due to the basis at lattice vector $\vec{R}$.

Define $\vec{k}' - \vec{k} = \Delta\vec{k}$

Notation $\vec{q}$ is often used in place of $\Delta\vec{k}$.

Then, $f \propto \int e^{-i(\vec{k}'-\vec{k})\cdot\vec{r}'}V(\vec{r}')d\vec{r}' = \int e^{-i\Delta\vec{k}\cdot\vec{r}'}\sum_{\vec{R}}V_b(\vec{r}' - \vec{R})\,d\vec{r}'$

$= \int e^{-i\Delta\vec{k}\cdot(\vec{s}+\vec{R})}\sum_{\vec{R}}'V_b(\vec{s})d\vec{s} = \sum_{\vec{R}}e^{-i\Delta\vec{k}\cdot\vec{R}}\int e^{-i\Delta\vec{k}\cdot\vec{s}}V_b(\vec{s})d\vec{s}$

$(\vec{s} = \vec{r}' - \vec{R})$

independent of $\vec{R}$!

This result motivates the following definition.

$$f_b(\Delta\vec{k}) \equiv -\frac{m}{2\pi\hbar^2}\int e^{-i\Delta\vec{k}\cdot\vec{r}}V_b(\vec{r})d\vec{r}$$

Which leads to a nice separation of f into two terms!

$$f = f_b(\Delta\vec{k})\sum_{\vec{R}}e^{-i\Delta\vec{k}\cdot\vec{R}}$$

$$f = f_b(\Delta\vec{k}) \sum_{\vec{R}} e^{-i\Delta\vec{k}\cdot\vec{R}}$$

basis property — lattice property

Meaning of f? As shown above, f is the amplitude of the wave function corresponding to the diffracted wave. We call f the **scattering amplitude**. This is the key quantity in the theory. The measured diffraction intensity I_d at distance r, for a given unit flux ($|A| = 1$) of incoming beam of quantum particles is given by $I = \frac{|f|^2}{r^2}$. The inverse-square attenuation is easy to understand. The crucial physics is contained in $|f|^2$. [In Kittel, the notation F is used instead of f.]

First let us look at the lattice sum, $L = \sum_{\vec{R}} e^{-i\Delta\vec{k}\cdot\vec{R}}$. Then, $f = f_b L$, where all quantities here are functions of Δk, even though not explicitly noted.

It is helpful to consider a one-dimensional problem, first.

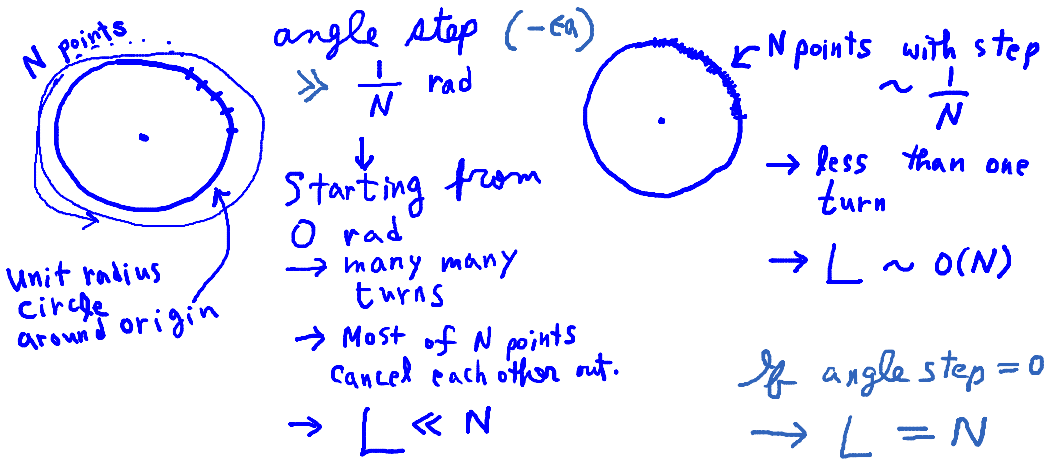
Real BL: $R = na$. Reciprocal BL: $G = 2\pi m/a$.

$$L = \sum_{n=0}^{N-1} e^{-i\Delta kna}$$

Yeah! Proof for 1D!

Note that when $\Delta k = G = \frac{2\pi m}{a}$, the summand is always 1, and so $L = N$. One can prove rigorously that L is peaked around $\Delta k = G$ with the peak width $= O\left(\frac{1}{N}\right)$. I.e., the peak will be extremely sharp for a macroscopic crystal. [Or, the peak may be broad, if the crystal is poor quality.]

Why does L behave this way? Graphically, L is the sum of position vectors equally spaced on a unit radius circle around the origin. The difference $\epsilon = \Delta k - G$ has the geometric meaning of $-\epsilon a$ corresponding to the successive angular step between adjacent vectors summed by L. For $\epsilon < 0$, the following diagram shows why L behaves the way it does (and similarly for $\epsilon > 0$). [Note that in this discussion only ϵ modulo 2π is important. So, we can take, without loss of generality, $-\pi < \epsilon \leq \pi$. In the diagram, we only consider $\epsilon < 0$.]



Now, let us consider a general dimension D. Let the real BL be spanned by $\{\vec{a}_l\}, l = 1,2,\ldots D$. $\vec{R} = \sum_l n_l \vec{a}_l$ (n_l = integer). Let $\Delta\vec{k} = \sum_l x_l \vec{a}^*_l$. Showing the diffraction condition $\Delta\vec{k} = \vec{G}$ is equivalent to showing that each x_l is an integer. This is quite straightforward, if we use $\vec{a}_l \cdot \vec{a}^*_m = 2\pi\delta_{lm}$: $L = \sum_{\vec{R}} e^{-i\Delta\vec{k}\cdot\vec{R}} = \sum_{\vec{R}} e^{-i\sum_l x_l n_l 2\pi} = \left(\sum_{n_1} e^{-i2\pi x_1 n_1}\right)\left(\sum_{n_2} e^{-i2\pi x_2 n_2}\right)\ldots\left(\sum_{n_D} e^{-i2\pi x_D n_D}\right)$. Here, each sum is functionally the same form as the sum that we examined for the one dimensional case. So, we have the diffraction condition $x_l =$ integer. So, in any dimensions, we get the celebrated **Bragg diffraction** formula.

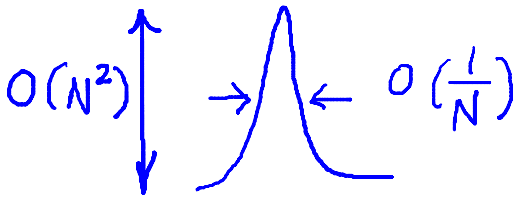
$\Delta\vec{k} = \vec{G}$

Yeah! Now proved for any dimension.

NOTE:

1) Although we used the first Born approximation to derive this important result, the result is actually a general property of the problem and remains valid to all orders. It is the result of the **discrete translation symmetry** of the Bravais lattice, and thus the crystal.
2) The first order Born approximation result is summarized as $f = \sum_{\vec{R}} f_b e^{-i\Delta\vec{k}\cdot\vec{R}}$. The physical content of this expression? The scattering amplitude off of the basis at the origin is by assumption f_b. For a basis at $\vec{R}$, the factor $e^{-i\Delta\vec{k}\cdot\vec{R}} = e^{i(\vec{k}\cdot\vec{R}-\vec{k}'\cdot\vec{R})}$ accounts for the difference in phase due to the path difference. By the first order Born approximation, we are not considering possible processes such as $\vec{k} \to \vec{k}'' \to \vec{k}'$. These and other multiple scattering events are always there, and become important to consider in some experiments.
3) The basis-dependent function $f_b \propto \int e^{-i\Delta\vec{k}\cdot\vec{r}} V_b(\vec{r}) d\vec{r}$ contains important physics about **charge or spin structure** of electrons (X-ray, electron, or neutron scattering) or nuclei (neutron scattering). In the case of coupling to charge, one can set $f_b \propto \int e^{-i\Delta\vec{k}\cdot\vec{r}} n(\vec{r}) d\vec{r}$ where $n(\vec{r})$ is the charge density of the basis. In the case of coupling to spin, the spin density of the basis should be used.
4) $\Delta\vec{k} = \vec{G}$ means $\vec{a}_i \cdot \Delta\vec{k} = 2\pi \times$ integer. This set of equations is called **Laue equations**.

Diffraction peak



Diffraction intensity $\propto |f|^2/r^2$. Thus, the peak intensity $\propto N^2$, and the peak width $\propto 1/N$. The intensity scaling as N^2 is of course something very common in

physics whenever "coherence" is involved (e.g. in laser). Thus, for a very good crystal, the peak will be very strong and the width will be negligible (the actual width being determined by the instrumental resolution or the thermal broadening). For a poor crystal, the peak width can indicate the sizes of single crystalline grains that make up the crystal.

The fact that the width of the diffraction peak scales like $1/N$, while the intensity scales like N^2, makes sense if you think about the energy consideration of the photon (or any incoming quantum particle). Each atom has a certain probability to diffract, and thus re-direct the energy of, photons. So, the total diffracted energy must scale as N. The energy of the diffracted peak is proportional to the integral of the diffraction peak and thus does scale as N, as expected.

One last thing. This discussion implicitly assumed a one dimensional crystal. In a three dimensional crystal, the diffraction peak is a function of three different variables (Δk_{a^*}, Δk_{b^*}, and Δk_{c^*}), where $\Delta k_a{}^*$ is the component of the vector $\Delta\vec{k}$ along the $\vec{a}^*$ axis and so on. As we saw in the last section, the total sum of exponential in three dimensions separates into the product of three sums, each of which can be thought of as mathematically equivalent to that for a one dimensional lattice. Thus, the intensity of the diffraction peak then scales as $(N_a N_b N_c)^2$ if we assume that the crystal is in a shape of a parallelepiped with N_a lattice points along the $\vec{a}$ axis, N_b lattice points along the $\vec{b}$ axis, and N_c lattice points along the $\vec{c}$ axis. The width of the diffraction peak scales as N_a along the Δk_{a^*} axis, as N_b along the Δk_b^* axis, and as N_c along the Δk_c^* axis.