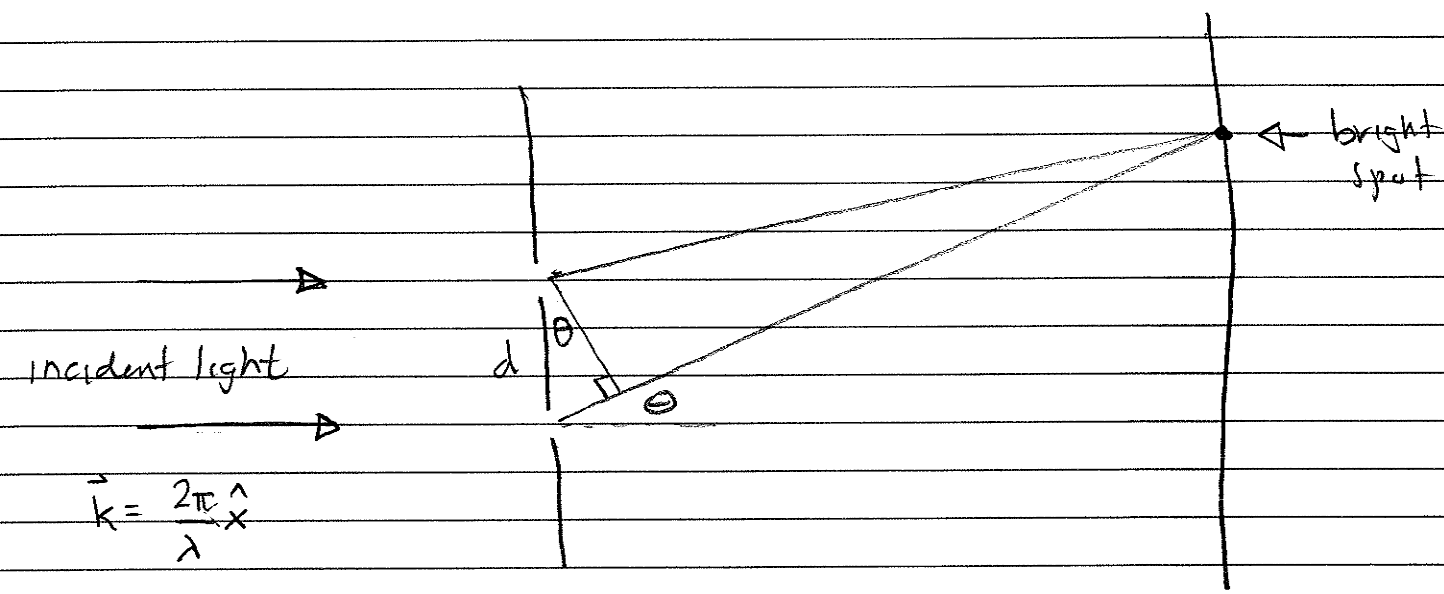
project:
D1

Diffraction

{ X rays on crystals yield intense peaks of scattered radiation for certain special λ and angles. (liquid no!)

Analogy with problem of 2 slit interference



bright spot if $d \sin\theta = \ell\lambda$

$$\vec{k}' = \frac{2\pi}{\lambda}(\cos\theta\,\hat{x} + \sin\theta\,\hat{y})$$

Only certain scattering vectors $\vec{q} = \vec{k}' - \vec{k}$ give bright spots $\quad \cos\theta - 1 = -2\sin^2\frac{\theta}{2}$

$$\vec{q} \approx \frac{2\pi}{\lambda}\frac{\ell\lambda}{d}\hat{y} = \frac{2\pi\ell}{d}\hat{y}$$

From positions of brights spots, can infer slit separation d.

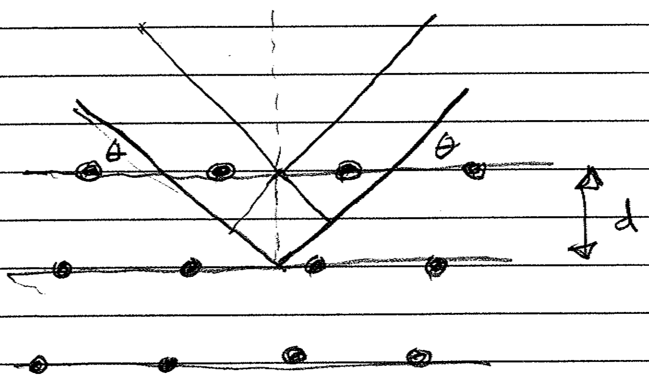
This is basically the idea of x-ray diffraction except

3d lattice of atoms $\Leftrightarrow$ 2 slits so more complicated.

project:

D2

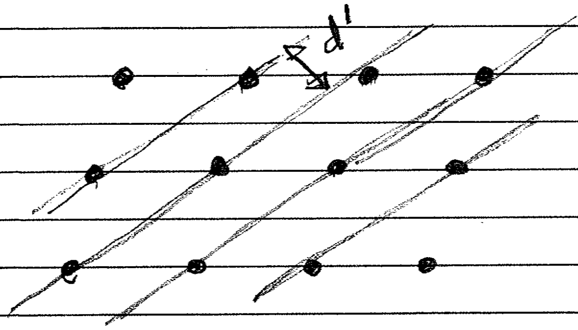
Bragg Formulation: Scattering off planes of atoms must result in constructive interference



$$2d \sin\theta = n\lambda$$

for constructive interference.

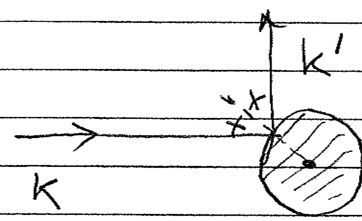
Note there are many ways to define the planes of atoms! ⇒ Many Bragg peaks



project: SC-1

Some General Remarks on Scattering

Arises in classical physics



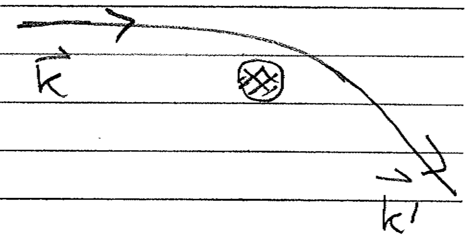
Hard sphere

Maybe you are doing

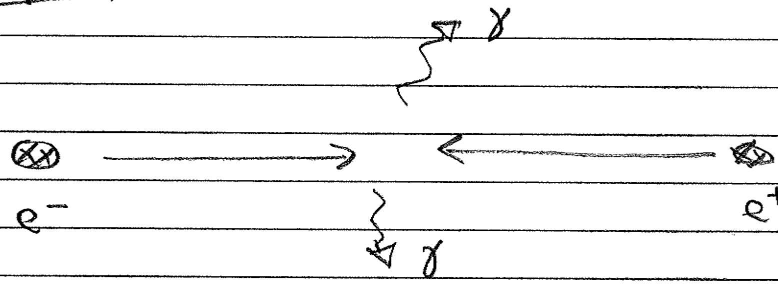
this problem in classical mechanics

Kepler problem $V(r) = 1/r$ Comet around sun

Need to solve orbit eqn (hyperbolas



Particle physics



$e^+ + e^- \to e^+ + e^-$

LEP 45 GeV 10^9

large e^- e^-

$e^- + e^- \to \mu^+ + \mu^-$

$e^+ + e^- \to q\bar{q}$

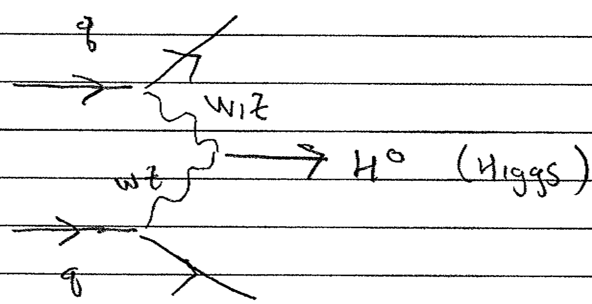
$\to$ hadrons

J/ψ $c\bar{c}$

LHC p+p

7 TeV

10^{12}



In our case $e^- +$ nucleus $\to e^- +$ nucleus $+ \gamma$ Bremstrahlung characteristic

100 keV e^- not energetic enough to produce new particles, just light

DiVOGA

project:
SC-2

How to compute these things!

Kepler: you have done it! How to put E, B fields in QM
We did this in 115B

$\vec{p} \rightarrow \vec{p} - e/c\,\vec{A}$

$\vec{p} \cdot \vec{A}$ when squared

$\vec{A} \Rightarrow a^{+} + a$ creation/annihilation operators for photons

Basic point: Different from QM you have done so far

Fixed, known # of particle $\psi(\vec{r})$ or $\psi(\vec{r}_1, \vec{r}_2, \ldots \vec{r}_N)$

this is all we really did in 115

Now need to make provision for # particles changing!!

$\psi(\vec{r}_1) \rightarrow \psi(\vec{r}_1, \vec{r}_2)$

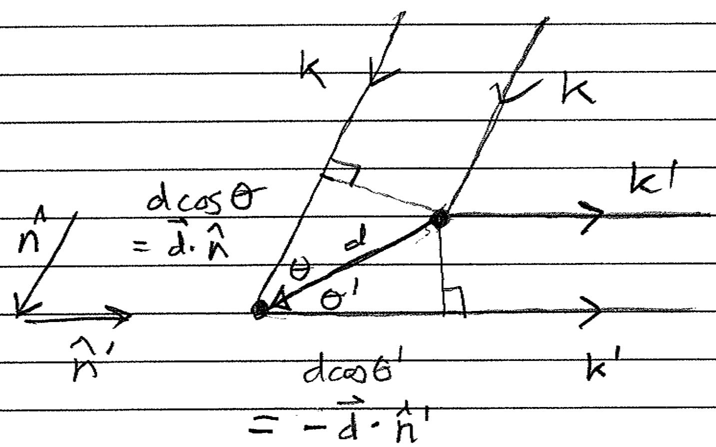
Quantum Field Theory

project:
D3

Van Laue Formulation

Instead of thinking of planes of atoms, consider crystal as identical set of atoms at $\vec{R} = n_1\vec{a}_1 + n_2\vec{a}_2 + n_3\vec{a}_3$

Consider two such scatterers



$d\cos\theta + d\cos\theta'$

$= \vec{d}\cdot(\hat{n} - \hat{n}') = m\lambda$

$\vec{d}\cdot(\vec{k} - \vec{k}') = 2\pi m$

$\left(\vec{k} = \frac{2\pi}{\lambda}\hat{n} \quad \vec{k}' = \frac{2\pi}{\lambda}\hat{n}'\right)$

But $\{\vec{d}\}$ are nothing more than $\{\vec{R}\}$

Hence $\quad \vec{R}\cdot(\vec{k} - \vec{k}') = 2\pi m$

$\Rightarrow \quad e^{i(\vec{k}-\vec{k}')\cdot\vec{R}} = 1$

↑

$\Delta\vec{k}$ = Reciprocal lattice vector

project:
D4

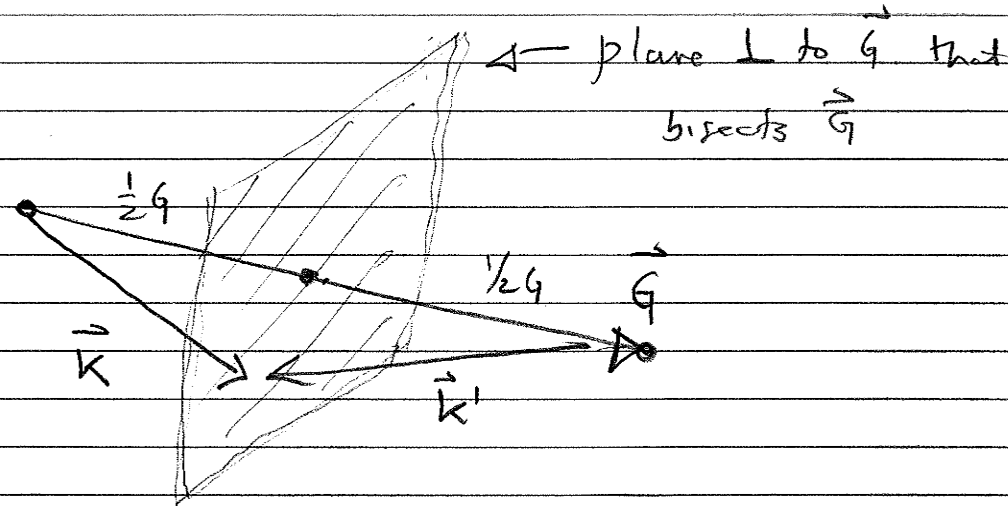
$$|\vec{k}'| = |\vec{k}| \qquad \vec{k}' = \vec{k} - \vec{G} \qquad (\text{or } \vec{k} + \vec{G}\text{, sign irrelevant})$$

$$|\vec{k} - \vec{G}| = k$$

$$k^2 - 2\vec{k}\cdot\vec{G} + G^2 = k^2$$

$$\vec{k}\cdot\hat{G} = \frac{1}{2} G$$

Component of $\vec{k}$ along $\hat{G}$ is 1/2 of length of $\vec{G}$



Laue condition: $\vec{k}$ lies on plane ⊥ to $\vec{G}$ and bisecting $\vec{G}$

"Bragg Plane"

DIVOGA

project:

E-1

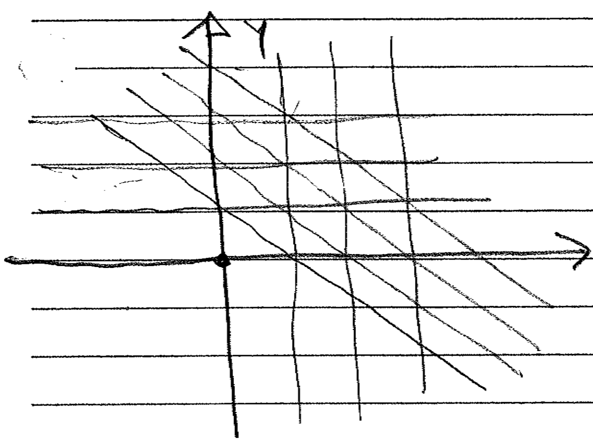
Ewald Construction

Consider an incident x-ray of wave vector $\vec{k}$.

It can give a Bragg peak if its tip lies on a Bragg plane.

Most likely this will not happen: Suppose you have a collection of 2D planes and pick some vector $\vec{k}$. What chance does its tip have of lying in a plane? Very small!

Easier to picture in lower d



I give you a (infinite) collection of lines. Put tail of arrow at origin, ~~and~~ what is chance head will lie on line?

very unlikely: lines are 1d objects in 2d world.

PROBLEM:

$\Rightarrow$ Expect NO BRAGG PEAKS!

project:
E-2

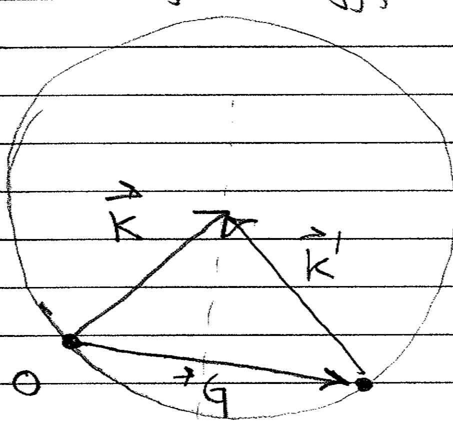
Sol'n: Allow many $\vec{k}$ either by allowing $|\vec{k}|$ or directn of $\vec{k}$ to vary

Laue Method / Ewald Construction

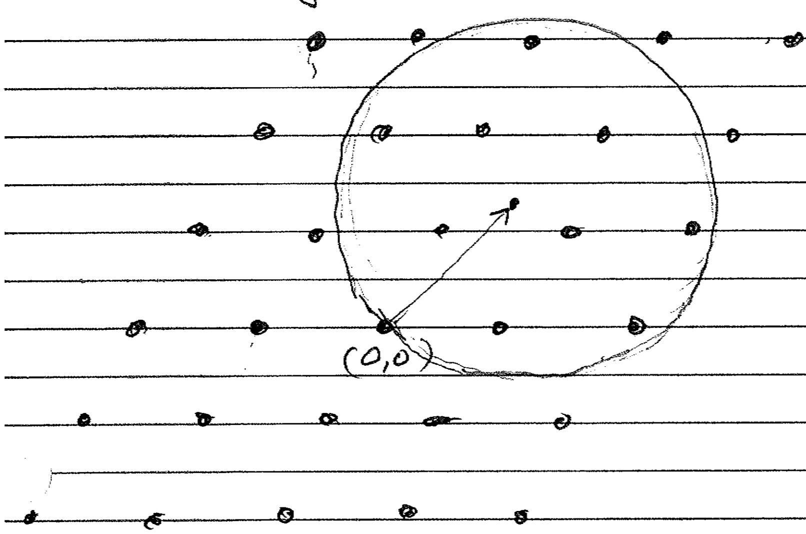
Given incident $\vec{k}$.
Draw sphere centered at tip of $\vec{k}$ (so that it passes through origin)

Will get Bragg peak if a $\vec{G}$ lies on sphere

$$\vec{k}' = \vec{k} - \vec{G}$$



Can again see that it is unlikely there will be such a $\vec{G}$



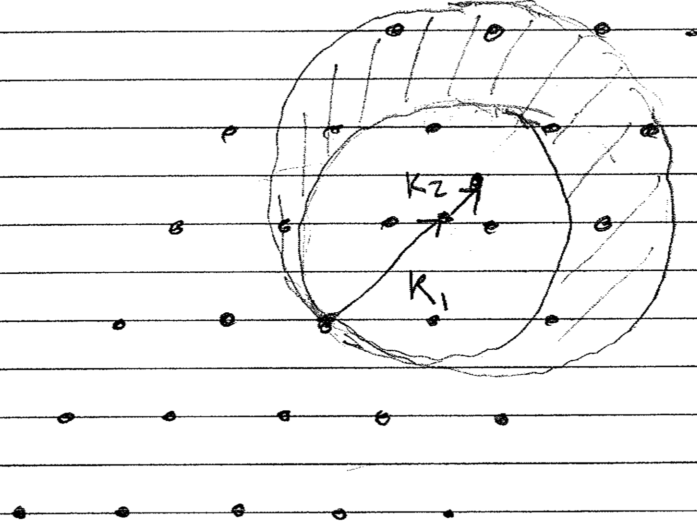
← ~~typical~~ collection of $\vec{G} = n_1 \vec{b}_1 + n_2 \vec{b}_2$

typical $\vec{k}$ will not intersect any $\vec{G}$.

project:
E3

Use non monochromatic Beam $k_1 < k < k_2$

(such as produced by Bremstrahhlung)



Now have 3d space in which to find $\vec{G}$ and there will be non zero probability

Rotating crystal method : Fixed $|\vec{k}|$, but crystal orientation is changed

As $\{\vec{a}_i\}$ are rotated the $\{\vec{b}_i\}$ also trace paths in reciprocal space. Those paths will hit Bragg sphere and give Bragg peaks