

PHYS 460 - LECTURE 5

LAST LECTURE WE DISCUSSED THE ATOMIC NATURE OF MATERIALS, AND HOW ONE GOES ABOUT DESCRIBING AND CLASSIFYING DIFFERENT ATOMIC LATTICES. IN PARTICULAR, WE FOCUSED ON THE MATHEMATICAL DESCRIPTIONS OF REPEATING PATTERNS ON BRAVAIS LATTICES, WHERE THE POSITION VECTOR IN REAL SPACE OF ANY GIVEN REPEATING UNIT CAN BE DESCRIBED BY

$$\vec{r} = n_1 \vec{a}_1 + n_2 \vec{a}_2 + n_3 \vec{a}_3$$

FOR $n_i \in \mathbb{Z}$ AND $\{\vec{a}_i\}$ ANY THREE ~~NON~~COLLINEAR "LATTICE VECTORS."

WE ARE NOW MOVING TOWARDS USING THIS MATHEMATICAL FRAMEWORK TO DESCRIBE HOW THE PERIODIC NATURE OF MATERIALS AFFECTS BOTH ITS INTERNAL PROPERTIES (e.g. THE MOTION OF ELECTRONS) AND HOW THEY INTERACT WITH THE OUTSIDE WORLD (e.g. THROUGH THE SCATTERING OF LIGHT).

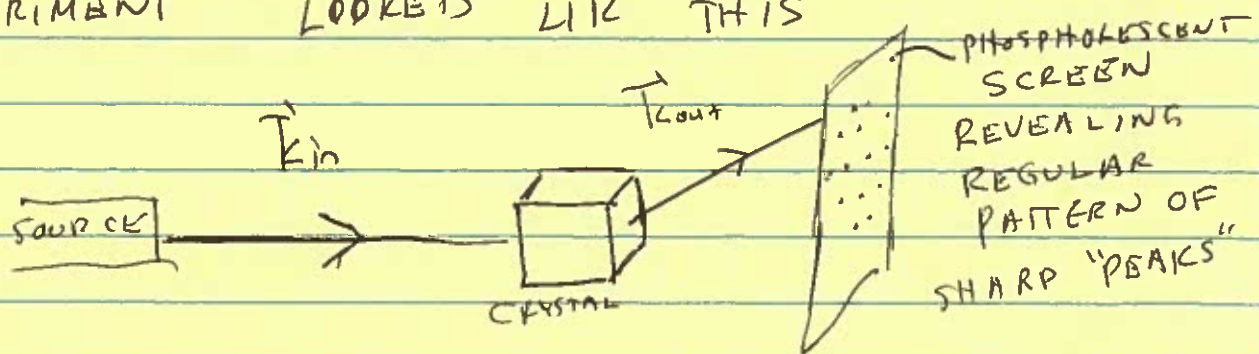
I ALLUDED AT THE END OF LAST LECTURE THAT SUCH DESCRIPTIONS ARE MORE NATURAL, NOT IN TERMS OF THE LATTICE IN "REAL" SPACE (WHAT IS KNOWN AS THE "DIRECT LATTICE"), BUT INSTEAD BY CONSIDERING THE COLLECTION OF POINTS REPRESENTING LATTICE PERIODICITIES $\rightarrow$ THE "RECIPROCAL LATTICE"

BEFORE WE GET INTO SPECIFIC DEFINITIONS, LET'S CONSIDER A COUPLE OF QUICK MOTIVATING EXAMPLES:

MOTIVATION (1) X-RAY DIFFRACTION

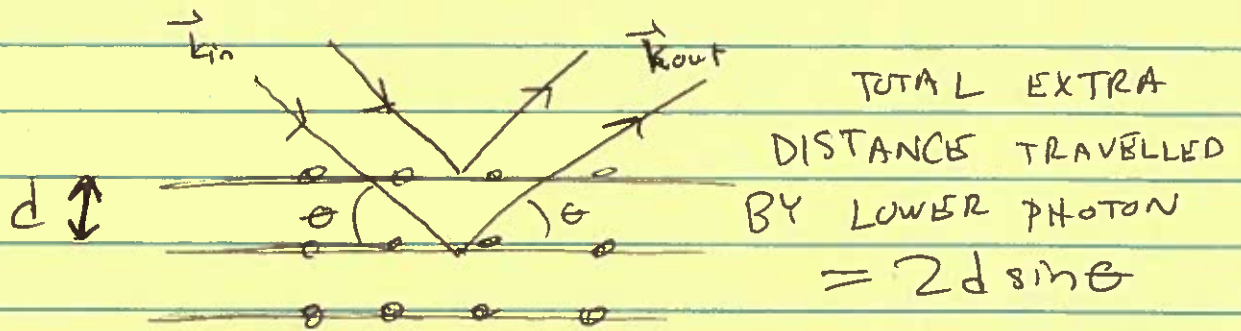
WE ALREADY DISCUSSED THE RESPONSE OF A MATERIAL TO OPTICAL LIGHT, IN THE CONTEXT OF THE DRUDE MODEL. THE RESPONSE AT THOSE WAVELENGTHS WAS GENERALLY WELL CAPTURED BY CONSIDERING MOTION OF FREE ELECTRONS (e.g. AC-SUSCEPTIBILITY AND THE PLASMA FREQUENCY). IT TURNS OUT THE RESPONSE AT HIGHER FREQUENCIES (SHORTER WAVELENGTHS) IS MUCH MORE COMPLEX. SOON AFTER THE DISCOVERY OF X-RAYS (ROENTGEN, 1895), IT WAS FOUND THAT LIGHT AT THESE SHORT WAVELENGTHS CHANGE DIRECTIONS SHARPLY, IN REGULAR WAYS THAT DEPEND STRONGLY ON THE ORIENTATION OF A CRYSTAL BEING STUDIED. MOREOVER, X-RAYS WERE ONLY FOUND TO SCATTER AT CERTAIN "MAGIC" ANGLES.

A TYPICAL "X-RAY DIFFRACTION" EXPERIMENT LOOKED LIKE THIS



ROENTGEN
NOBEL PRIZE
1901

WAS ABLE TO EXPLAIN THIS PATTERN BY CONSIDERING CONSTRUCTIVE INTERFERENCE CONDITIONS FROM SCATTERING OFF FAMILIES OF PARALLEL ATOMIC PLANES:



$\therefore$ PEAKS OCCUR WHEN SCATTERED BEAMS ARE IN-PHASE

$\rightarrow$

$$2d \sin \theta = n\lambda, n \in \mathbb{Z}$$

BRAGG'S LAW

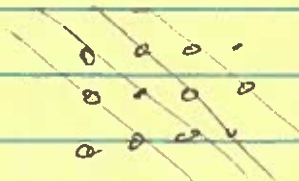
IT IS IMPORTANT TO NOTE:

- (A) THAT THE REGULARITY OF ATOM SPACINGS WAS IMPORTANT. OTHERWISE THERE WOULD HAVE BEEN NO CONSTRUCTIVE INTERFERENCE
- (B) SPECIFICALLY, THE EXISTENCE OF REGULARLY SPACED PLANES IS FUNDAMENTAL. ANGLE IS SET BY SPACING, d

AND

- (C) THERE ARE AN INFINITE NUMBER OF SUCH PLANES IN ANY BRavais LATTICE

P.S



$\rightarrow$ STRONG MOTIVATION FOR DEVELOPING MEANS OF DISCUSSING PLANE SPACING (i.e. PERIODICITY)

BRAGG
NOBEL PRIZE
1915

MOTIVATION (2) : PERIODICITY OF CRYSTAL PROPERTIES

AS THE FUNDAMENTAL STRUCTURE OF A CRYSTAL IS PERIODIC IN SPACE, IT IS REASONABLE TO EXPECT OTHER MATERIAL PROPERTIES (e.g. ELECTRON DENSITY) AND SAMPLE RESPONSE (e.g. COLLECTIVE MOTION OF ATOMS) TO VARY WITH THE SAME PERIODICITY.

SPECIFICALLY, IF ATOMIC POSITIONS ARE DESCRIBED BY THE BRAVAIS LATTICE

$$\vec{R} = n_1 \vec{a}_1 + n_2 \vec{a}_2 + n_3 \vec{a}_3, \quad n_i \in \mathbb{Z}$$

THEN ONE MIGHT EXPECT ANY WAVE INSIDE THE CRYSTAL (e.g. ELECTRONS!) TO BE BOUND BY THE CONDITION

$$\psi(\vec{r} + \vec{R}) = \psi(\vec{r})$$

$$\Rightarrow \psi_0 e^{i\vec{k} \cdot (\vec{r} + \vec{R})} = \psi_0 e^{i\vec{k} \cdot \vec{r}}$$

$$\Rightarrow e^{i\vec{k} \cdot \vec{R}} = 1$$

AS $\vec{R}$ IS DETERMINED BY THE CRYSTAL STRUCTURE, THIS STATEMENT IMPLIES THAT ONLY CERTAIN SPECIAL WAVELENGTHS, $\vec{k}$, ARE SUPPORTED INSIDE A PERIODIC CRYSTAL

→ IT TURNS OUT BOTH THESE PERIODIC WAVELENGTH CONDITIONS AND PERIODIC PLANES ARE CAPTURED BY ONE MATHEMATICAL CONSTRUCT: THE RECIPROCAL LATTICE

THE RECIPROCAL LATTICE

DEFINITION: THE "RECIPROCAL LATTICE" OF A GIVEN BRAVAIS LATTICE, $\{\vec{R}\}$, IS THE COLLECTION OF POINTS, $\{\vec{G}\}$, WHICH SATISFY THE RELATION

$$e^{i\vec{G} \cdot \vec{R}} = 1$$

FOR ALL POSITIONS IN $\vec{R}$ ↑ "DIRECT LATTICE"

NOTE: • SINCE ELEMENTS OF $\vec{R}$ HAVE UNITS OF LENGTH, THIS DEFINITION IMPLY ELEMENTS OF $\vec{G}$ HAVE UNITS OF INVERSE LENGTH

• GIVEN OUR DISCUSSION OF MOTIVATION ②, IT IS IN FACT NATURAL TO THINK OF THE COLLECTION OF ALL WAVEVECTORS CONSISTENT WITH PERIODIC STRUCTURE, $\vec{R}$.

• FURTHER, SINCE THE MOMENTUM OF A WAVE IS $\vec{p} = \hbar \vec{k}$, THE SPACE
 → CONTAINING ELEMENTS $\vec{k} \in \vec{G}$ IS OFTEN REFERRED TO AS MOMENTUM SPACE

BUT I'M GETTING AHEAD OF MYSELF...

RECIPROCAL
SPACE

THE RECIPROCAL LATTICE AS A BRAVAIS LATTICE

IT TURNS OUT THAT THE COLLECT OF POINTS $\{\vec{G}\}$ IS ITSELF A BRAVAIS LATTICE.

WE CAN PROOVE THIS, DEFINE THE VECTORS $\vec{b}_i$:

$$\vec{b}_1 = 2\pi \frac{\vec{a}_2 \times \vec{a}_3}{\vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3)}$$

$$\vec{b}_2 = 2\pi \frac{\vec{a}_3 \times \vec{a}_1}{\vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3)}$$

$$\vec{b}_3 = 2\pi \frac{\vec{a}_1 \times \vec{a}_2}{\vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3)}$$

WE WILL SEE THAT THESE ARE ^{PRIMITIVE} ~~THESE~~ VECTORS FOR OUR RECIPROCAL LATTICE

TO DEMONSTRATE THIS FACT, FIRST NOTE

$$\vec{a}_1 \cdot \vec{b}_1 = 2\pi \frac{\vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3)}{\vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3)} = 2\pi$$

$$\text{AND } \vec{a}_2 \cdot \vec{b}_1 = 2\pi \frac{\vec{a}_2 \cdot (\vec{a}_2 \times \vec{a}_3)}{\vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3)} = 0$$

SINCE $(\vec{a}_2 \times \vec{a}_3) \perp \vec{a}_2$

IN FACT, ONE CAN CLEARLY SEE

$$\vec{a}_i \cdot \vec{b}_j = 2\pi \delta_{ij}$$

SIDENOTE: IT IS NOT GENERALLY TRUE THAT $\vec{a}_i \parallel \vec{b}_i$, BUT DIRECT AND RECIPROCAL LATTICE VECTORS WILL BE PARALLEL FOR ORTHOGONAL LATTICE VECTORS (e.g. CUBIC LATTICES).

THIS IS BECAUSE $\vec{a}_2 \times \vec{a}_3 \parallel \vec{a}_1$
IN THIS CASE $\rightarrow$ STRONG MOTIVATION FOR USE OF CONVENTIONAL UNIT CELLS

NOW CONSIDER THE WAVEVECTOR

$$\vec{k} = m_1 \vec{b}_1 + m_2 \vec{b}_2 + m_3 \vec{b}_3, \quad m_i \in \mathbb{R}$$

IF $\vec{k} \in \{\vec{G}\}$, THEN

$$e^{i\vec{k} \cdot \vec{R}} = 1 \quad \forall \vec{R}$$

$$\Rightarrow \vec{k} \cdot \vec{R} = 2\pi N \quad N \in \mathbb{Z}$$

$$- (m_1 \vec{b}_1 + m_2 \vec{b}_2 + m_3 \vec{b}_3) \cdot (n_1 \vec{a}_1 + n_2 \vec{a}_2 + n_3 \vec{a}_3) = 2\pi N$$

$$2\pi (m_1 n_1 + m_2 n_2 + m_3 n_3) = 2\pi N \quad \forall n_i \in \mathbb{Z}$$

$$\Rightarrow m_1, m_2, m_3 \text{ MUST BE INTEGERS}$$

THIS MEANS THE $\vec{k} \in \{\vec{G}\}$ FORM A LATTICE AND THIS LATTICE IS A BRAVAIS LATTICE, WITH $\vec{b}_i$ THE PRIMITIVE VECTORS

EXAMPLES :

SIMPLE CUBIC

$$\vec{a}_1 = a\hat{x} \quad a_2 = a\hat{y} \quad a_3 = a\hat{z}$$

$$\vec{b}_1 = \frac{2\pi}{a^3} (a_2 \times a_3) \quad \vec{b}_2 = \frac{2\pi}{a} \hat{y} \quad \vec{b}_3 = \frac{2\pi}{a} \hat{z}$$
$$= \frac{2\pi}{a} \hat{x}$$

BCC :

$$\vec{a}_1 = \frac{a}{2} (\hat{y} + \hat{z} - \hat{x})$$

$$\vec{a}_2 = \frac{a}{2} (\hat{z} + \hat{x} - \hat{y})$$

$$\vec{a}_3 = \frac{a}{2} (\hat{x} + \hat{y} - \hat{z})$$

$$\vec{a}_2 \times \vec{a}_3 = \frac{a^2}{4} (\hat{y} - \hat{x} + 0 + 0 + \hat{z} + \hat{y} + \hat{z} + 0 + \hat{x})$$
$$= \frac{a^2}{2} (\hat{y} + \hat{z})$$

$$\vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3) = \frac{a^3}{4} (1+1) = \frac{a^3}{2}$$

$$\Rightarrow \vec{b}_1 = 2\pi \frac{\frac{a^2}{2} (\hat{y} + \hat{z})}{\frac{a^3}{2}} = \frac{2\pi}{a} (\hat{y} + \hat{z})$$

$$\text{AND SIMILARLY } \vec{b}_2 = \frac{2\pi}{a} (\hat{x} + \hat{z})$$

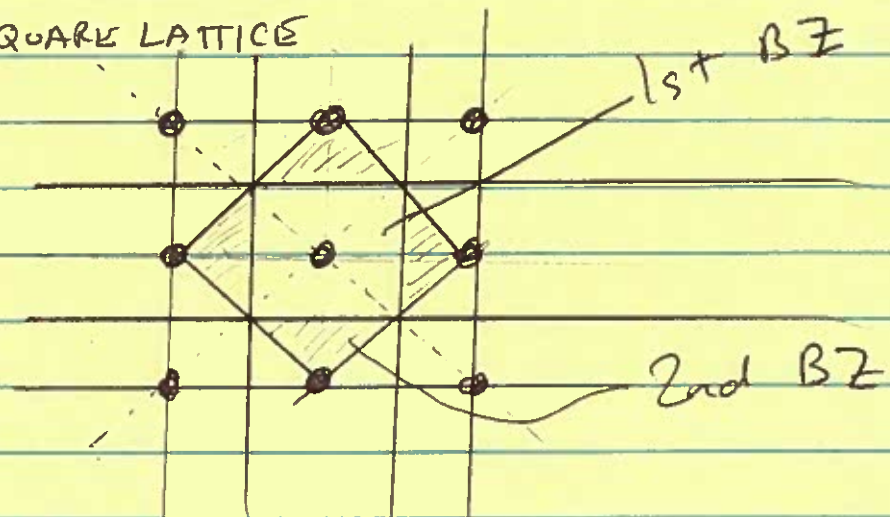
$$\vec{b}_3 = \frac{2\pi}{a} (\hat{y} + \hat{x})$$

→ THE RECIPROCAL LATTICE OF BCC IS FCC!

BRILLOUIN ZONES

SINCE $\vec{G}$ IS A BRAVAIS LATTICE, WE CAN DEFINE A PRIMITIVE UNIT CELL IN THE SAME WAY AS THE DIRECT LATTICE. THE WIGNER-SEITZ CELL OF THE RECIPROCAL LATTICE IS CALLED THE "FIRST BRILLOUIN ZONE", AND YOU FIND IT THE SAME WAY, VIA BISECTORS: (KNOWN AS BOUNDARIES)

e.g. 2D SQUARE LATTICE



THE REGION ACCESSIBLE BY CROSSING ON BOUNDARY IS THE SECOND BZ, 2 BOUNDARIES THE 3RD BZ, etc. THE FIRST ZONE IS THE ONLY SIMPLY CONNECTED ZONE.

THE FIRST BZ IS SIGNIFICANT, AS IT CONTAINS EVERY PHYSICALLY DISTINCT WAVEVECTOR. MUCH LIKE THE DIRECT LATTICE, HIGH ZONES ARE JUST REPETITION.

WE CAN SEE THIS IF WE THINK OF WHERE THIS STARTED (MOTIVATION 2), IN TERMS OF WAVES INSIDE THE PERIODIC STRUCTURE.

$$\psi(\vec{r}) = \psi_0 e^{i\vec{k} \cdot \vec{r}}$$

NOW, LET $\vec{k}$ BE A WAVEVECTOR INSIDE THE FIRST BZ. IF WE GO TO A HIGHER ZONE, AND LOOK AT THE WAVEVECTOR

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

$$\begin{aligned} \Rightarrow \psi(\vec{k}') &= \psi_0 e^{i(\vec{k} + \vec{G}) \cdot \vec{r}} \\ &= \psi_0 e^{i\vec{k} \cdot \vec{r}} e^{i\vec{G} \cdot \vec{r}} \\ &= \psi_0 e^{i\vec{k} \cdot \vec{r}} \end{aligned}$$

IT'S THE SAME PHYSICAL STATE. THE 1ST CONTAINS ALL THE INFORMATION

MOREOVER, WE CAN USE THIS INFORMATION TO COUNT THE NUMBER OF MODES IN THE SYSTEM

E.G. SIMPLE CUBIC, WITH N_x UNIT CELLS ALONG $\hat{x}$. THE CONDITION $e^{i\vec{G} \cdot \vec{r}}$ MEANS $k_x = \frac{2\pi}{N_x a} = \frac{2\pi}{L}$ STEPS IN THE $\hat{x}$ DIRECTION. BUT THE FIRST BZ GOES FROM $-\frac{\pi}{a} \leq k_x \leq \frac{\pi}{a}$

$$\# \text{ modes} = \frac{\frac{2\pi}{a}}{\frac{2\pi}{N_x a}} = N_x = \# \text{ DEGREES OF FREEDOM IN } \hat{x}$$

MORE ON THIS LATER!

INVERSE?

THE WORD "RECIPROCAL" INVOKES THE IDEA OF AN INVERSE, ONE MIGHT NATURALLY ASK WHAT THE RECIPROCAL OF THE RECIPROCAL WAS, I.E. WHAT IS THE LATTICE $\vec{H}$ WHICH SATISFIES

$$e^{i\vec{H} \cdot \vec{G}} = 1$$

BUT ONE CAN SEE THAT THIS IS THE SAME EQUATION WE USED TO FIND $\vec{G}$:

$$e^{i\vec{G} \cdot \vec{R}} = 1$$

THUS $\vec{R}$ IS A RECIPROCAL OF $\vec{G}$, HOWEVER IT MUST BE THE ONLY RECIPROCAL LATTICE OF $\vec{G}$. WE CAN PROVE BY CONTRADICTION. CONSIDER $\vec{r} \in \vec{H}$ BUT NOT $\vec{R}$. THEN FOR THAT $\vec{r}$

$$\vec{r} = x_1 \vec{a}_1 + x_2 \vec{a}_2 + x_3 \vec{a}_3$$

for at least one x_i
NOT IN $\mathbb{Z}$

THEN THE DOT PRODUCT

$$\vec{G} \cdot \vec{r} = 2\pi(\text{INTEGER} + x_i m_i)$$

WHICH MEANS IT DOESN'T SATISFY

$$e^{i\vec{G} \cdot \vec{r}} = 1$$

→ NOT RECIPROCAL.

QED

OK, BUT IS IT A FOURIER TRANSFORM?
YES!

CONSIDER ANY FUNCTION WHICH VARIES
WITH THE PERIODICITY OF THE LATTICE, $\vec{R}'$

$$f(\vec{r} + \vec{R}) = f(\vec{r})$$

THEN THE FOURIER TRANSFORM

$$\mathcal{F}[f(\vec{r})] = \int d\vec{r} e^{i\vec{k} \cdot \vec{r}} f(\vec{r})$$

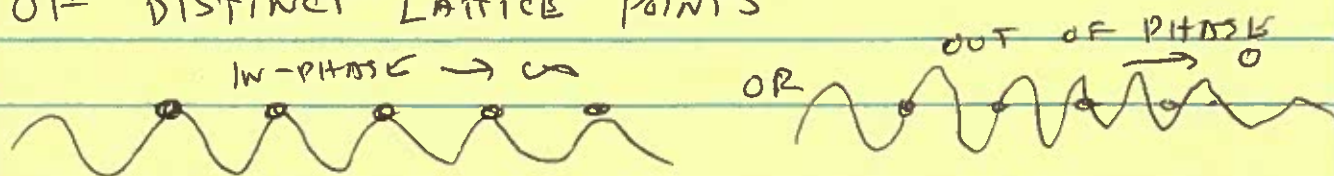
CAN BE BROKEN DOWN INTO ~~REAL~~ LATTICE
AND INTRA-CELL PARTS. LET $\vec{r} = \vec{R} + \vec{x}$

$$\begin{aligned} \rightarrow \mathcal{F}[f(\vec{r})] &= \sum_{\vec{R}} \int_{\text{INTRA CELL}} d\vec{x} e^{i\vec{k} \cdot (\vec{R} + \vec{x})} f(\vec{R} + \vec{x}) \\ &= \left(\sum_{\vec{R}} e^{i\vec{k} \cdot \vec{R}} \right) \left(\int_{\text{Cell}} d\vec{x} e^{i\vec{k} \cdot \vec{x}} f(\vec{x}) \right) \end{aligned}$$

ONE CAN SHOW

$$\sum_{\vec{R}} e^{i\vec{k} \cdot \vec{R}} = \frac{(2\pi)^3}{v} \sum_{\vec{G}} \delta(\vec{k} - \vec{G})$$

WHICH IS A RELATION KNOWN AS THE POISSON RESUMMATION
FORMULA. QUALITATIVELY, ONE CAN UNDERSTAND IT
IN TERMS OF WAVES SUMMED OVER A SERIES
OF DISTINCT LATTICE POINTS



$$\Rightarrow \boxed{f[\vec{r}] = (2\pi)^3 \sum_{\vec{G}} \delta(\vec{k} - \vec{G}) S(\vec{x})}$$

WHERE $S(\vec{x}) = \int_{\text{cell}} d\vec{x} f(\vec{x}) e^{i\vec{k} \cdot \vec{x}}$

IS A FUNCTION WE CALL THE
"STRUCTURE FACTOR"

STILL NOT CLEAR? CONSIDER THE PARTICULAR
CASE WHERE $f(\vec{r}) = \sum_{\vec{r}} \delta(\vec{r} - \vec{r})$

THE ATOM DENSITY, THEN, $S(\vec{x}) = 1$ AND

$$f[\vec{r}] = (2\pi)^3 \sum_{\vec{G}} \delta(\vec{k} - \vec{G})$$

THE RECIPROCAL LATTICE POINT
DENSITY

→ THE RECIPROCAL LATTICE IS THE
FOURIER TRANSFORM!

MOREOVER, IT CAN BE USED TO
CALCULATE THE FOURIER TRANSFORM (VIA
THE STRUCTURE FACTOR) OF ANY FUNCTION
THAT REPEATS WITH SAME PERIODICITY AS
THE LATTICE.

INDEXING LATTICE PLANES

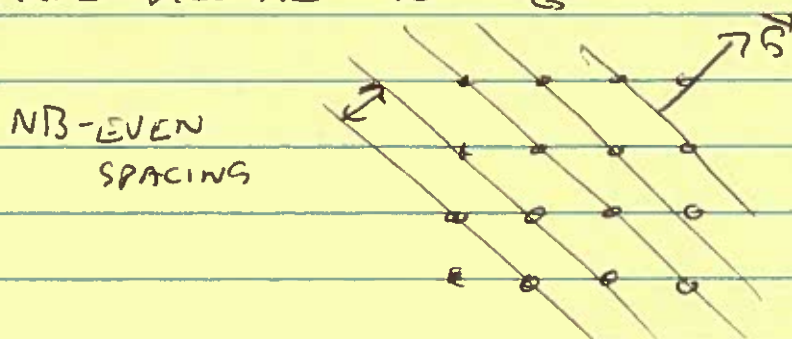
ANOTHER WAY TO THINK ABOUT THE RECIPROCAL LATTICE IS AS A LIST OF ALL THE FAMILIES OF PARALLEL PLANES INSIDE A CRYSTAL STRUCTURE

THIS COMES FROM THE OBSERVATION THAT

$$\vec{G} \cdot \vec{r} = 2\pi m \quad m \in \mathbb{Z}$$

FOR $\vec{r} \in \vec{R}$

BUT SINCE $\vec{G} \cdot (\vec{r} - \vec{r}_0) = 0$ IS AN EQUATION FOR A PLANE, THIS MEANS ALL $\vec{r}$ IN $\vec{R}$ BELONG TO SOME PLANE PERPENDICULAR TO $\vec{G}$



WHICH PLANE IS DETERMINED BY THE INTEGER m FOR ANY GIVEN DIRECTION $\vec{G}$

MOREOVER, IF YOU CONSIDER ANY TWO ATOMS IN ADJACENT PLANES, $\vec{r}_1, \vec{r}_2$

$$\begin{aligned} \text{THEN } \vec{G} \cdot (\vec{r}_1 - \vec{r}_2) &= 2\pi(m+1 - m) = 2\pi \\ \Rightarrow |\vec{r}_1 - \vec{r}_2|_{\text{parallel}} &= \frac{2\pi}{|\vec{G}|} \equiv d \end{aligned}$$

$\vec{G}$ DETERMINES DIRECTION AND SPACING!

THUS, IT IS VERY COMMON TO REFER TO A GIVEN FAMILY OF PLANES IN TERMS OF THEIR "MILLER INDICES", WHICH ARE SIMPLY THE INTEGER COEFFICIENTS OF THE PRIMITIVE VECTORS OF $\vec{G}$

$$\vec{G}_{(h,k,l)} = h\vec{b}_1 + k\vec{b}_2 + l\vec{b}_3$$

WHERE $\vec{G} \perp$ PLANE OF INTEREST AND $d = \frac{2\pi}{|\vec{G}_{hkl}|}$ IS THE DISTANCE BETWEEN PLANES

NOTES: (1) MILLER WAS A MINERALOGIST, WHO INVENTED THESE INDICES TO DESCRIBE DIRECTIONS IN WHICH CRYSTALS NATURALLY "CLEAVE". THE MATH PREDATES THE ATOMIC MODEL.

(2) MILLER INDICES ARE STRONGLY RELATED TO THE METHOD FOR DESCRIBING PLANES Laid OUT IN THE LAST LECTURE - BY LOOKING AT INVERSES OF INTERCEPTS

$$\frac{1}{x_1} : \frac{1}{x_2} : \frac{1}{x_3} = h : k : l$$

for INTERCEPTS x_1, x_2, x_3

(3) CLEARLY THESE INDICES ARE TREMENDOUSLY RELEVANT TO OUR FIRST MOTIVATING EXAMPLE: X-RAY DIFFRACTION

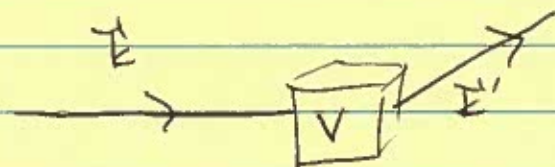
X-RAY DIFFRACTION - A BEGINNER'S GUIDE

THE SCATTERING OF WAVES BY A PERIODIC POTENTIAL IS ACTUALLY AN ADVANCED AND SUBTLE QUANTUM MECHANICAL CALCULATION, BUT IT REDUCES TO SOME FAMILIAR CONCEPTS (PLANES, RECIPROCAL LATTICES...), SO ONE CAN EASILY OBTAIN A PRACTICAL WORKING KNOWLEDGE OF THE TECHNIQUE.

THE SCATTERING OF ANY WAVE IN MOMENTUM STATE, $\vec{k}$, TO MOMENTUM STATE, $\vec{k}'$, IS DESCRIBED BY "FERMI'S GOLDEN RULE"

$$\Gamma(\vec{k}', \vec{k}) = \frac{2\pi}{\hbar} |\langle \vec{k}' | V | \vec{k} \rangle|^2 \delta(E_{\vec{k}'} - E_{\vec{k}})$$

WHERE Γ IS THE TRANSITION RATE, AND THE δ FUNCTION ENSURES CONSERVATION OF ENERGY



HERE, THE MATRIX ELEMENT

$$\begin{aligned} \langle \vec{k}' | V | \vec{k} \rangle &= \int d\vec{r} \frac{e^{-i\vec{k}' \cdot \vec{r}}}{\sqrt{L^3}} V(\vec{r}) \frac{e^{i\vec{k} \cdot \vec{r}}}{\sqrt{L^3}} \\ &= \frac{1}{L^3} \int d\vec{r} e^{-i(\vec{k}' - \vec{k}) \cdot \vec{r}} V(\vec{r}) \end{aligned}$$

LOOK FAMILIAR? THIS IS VERY SIMILAR
TO OUR FOURIER TRANSFORM CALCULATION
IF $V(\vec{r})$ IS PERIODIC ON LATTICE $\vec{R}$,
AND WE LET $\vec{r} = \vec{R} + \vec{x}$

$$\Rightarrow \langle \vec{k}' | V | \vec{k} \rangle = \frac{1}{L^3} \sum_{\vec{R}} \int_{\text{cell}} d\vec{x} e^{-i(\vec{k}' - \vec{k}) \cdot (\vec{x} + \vec{R})} V(\vec{x} + \vec{R})$$

$$= \frac{1}{L^3} \left[\sum_{\vec{R}} e^{-i(\vec{k}' - \vec{k}) \cdot \vec{R}} \right] \left[\int_{\text{cell}} d\vec{x} e^{-i(\vec{k}' - \vec{k}) \cdot \vec{x}} V(\vec{x}) \right]$$

AS WE SAW BEFORE, THE FIRST TERM~~2~~
IS ZERO UNLESS

$$\vec{k}' - \vec{k} = \vec{G}, \quad \text{A RECIPROCAL LATTICE VECTOR}$$

•• THE INTENSITY OF A SCATTERED X-RAY
BEAM IS

$$I(\vec{k}' - \vec{k}) \propto \delta(\vec{k}' - \vec{k} - \vec{G}) |S(\vec{k}' - \vec{k})|^2$$

OR FOR A GIVEN $\vec{k}$, JUST A DIRECT
IMAGE OF THE RECIPROCAL LATTICE!

(TIMES SOME STRUCTURE FACTOR)
THAT REFLECTS HOW ELECTRON DENSITY
IS DISTRIBUTED IN THE
CELL