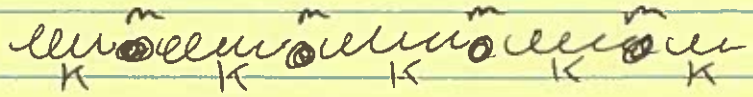
PHYS 460 - LECTURE 8

WHEN WE ENDED LAST LECTURE, WE WERE DISCUSSING THE MONATOMIC HARMONIC CHAIN

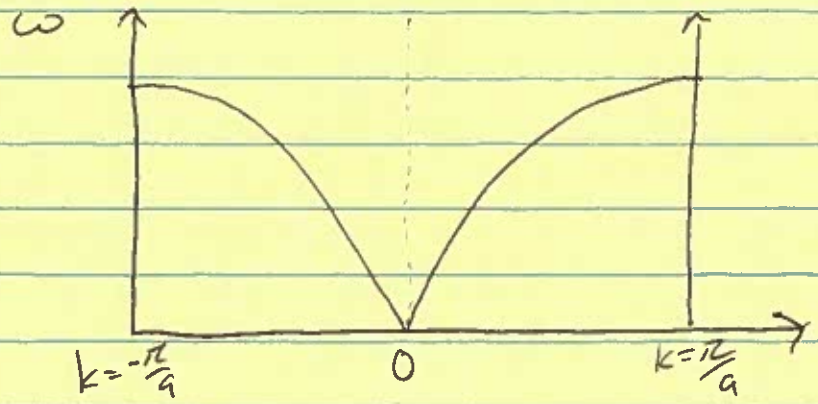


AND SHOWED THAT THE SYSTEM SUPPORTED WAVE-LIKE MOTIONS OF PARTICLES, WHERE THE MOVEMENT OF THE n^{th} PARTICLE WAS DESCRIBED BY

$$\delta x_n \equiv x_n - x_n^{eq} = A e^{i\omega t - ikna}$$

WITH DISPERSION RELATION

$$\omega(k) = 2\sqrt{\frac{K}{m}}\left|\sin\left(\frac{ka}{2}\right)\right|$$



WHICH HAS GENERAL FEATURES

1. LINEAR DISPERSION AS $k \to 0$
2. ZERO GROUP VELOCITY AS $k \to \frac{\pi}{a}$
3. REPEATING PATTER WITH PERIODICITY $\frac{2\pi}{a}$
4. N UNIQUE MODES, FOR THIS SYSTEM WITH N DEGREES OF FREEDOM

So does this help us understand the heat capacity at all (or at least why the Debye model works)?

Well, yes, in fact! Recall, we found

$$U = \sum_{\vec{k}}{}' \hbar\omega(\vec{k})\left(\frac{1}{e^{\frac{\hbar\omega(k)}{k_B T}} - 1} + \frac{1}{2}\right)$$

$$\Rightarrow C_V = \frac{\partial}{\partial T} \sum_{\vec{k}}{}' \left(\frac{\hbar\omega(k)}{e^{\frac{\hbar\omega(k)}{k_B T}} - 1}\right)$$

Check limits

(1) $T \to 0$: Recall Debye model predicted T^3 in this limit by assuming $\omega \propto k$. We see from our full dispersion that ω is indeed proportional to k in the same limit. $\therefore$ full dispersion has same form.

(2) $T \to \infty$: In this limit, we note that the Bose factor $n_B = (e^{\frac{\hbar\omega}{k_B T}} - 1) \to e^{-\frac{\hbar\omega}{k_B T}}$ just becomes a Boltzmann factor. Thus in this limit, heat capacity is given by the equipation theorem

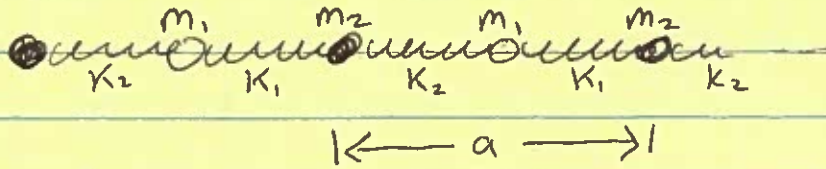
$$C_V = 3 k_B T N \quad \text{for } N \text{ degrees of freedom}$$

Debye assumed it, but we derived this factor of from boundary conditions!

NOW LET'S ADD ANOTHER (VERY COMMON) COMPLICATING FACTOR, AND SEE WHAT HAPPENS: A MULTI-ATOM BASIS!

THE DIATOMIC CHAIN

AGAIN RESTRICTING OUR ATTENTION TO 1D, LET'S CONSIDER WHAT HAPPENS WHEN WE ADD 2 ATOMS, INSTEAD OF JUST ONE



NOW THE LATTICE PARAMETER, a, SEPARATES THE REPEATING UNIT, NOT THE INDIVIDUAL ATOMS, AND THE EQUILIBRIUM POSITIONS OF THE TWO ATOMS (SAY x : y) ARE GIVEN BY

$$x_n^{eq} = na + x_0$$
$$y_n^{eq} = na + y_0$$

FOR x_0 AND y_0 THE "BASIS VECTORS" OF THE ATOMS WITHIN THE UNIT CELL.

NOW THE EQUATIONS OF MOTION ARE

$$m_1 \delta\ddot{x}_n = K_2(\delta y_n - \delta x_n) + K_1(\delta y_{n-1} - \delta x_n)$$

AND $$m_2 \delta\ddot{y}_n = K_1(\delta x_{n+1} - \delta y_n) + K_2(\delta x_n - \delta y_n)$$

AGAIN, LET'S LOOK FOR SOLUTIONS OF THE FORM

$$\delta x_n = A_x e^{i\omega t - ikna}$$
$$\delta y_n = A_y e^{i\omega t - ikna}$$

WHERE A_x/A_y MIGHT BE COMPLEX

FOR SIMPLICITY, LET'S CONSIDER THE SPECIAL CASE $m_1 = m_2 \equiv m$, AND PLUG IN THE ABOVE FUNCTIONS INTO THE EQUATIONS OF MOTION

$$-\omega^2 m A_x = K_2 A_y + K_1 A_y e^{ika} - (K_1+K_2)A_x$$

AND $$-\omega^2 m A_y = K_1 A_x e^{-ika} + K_2 A_x - (K_1+K_2)A_y$$

THESE ARE TWO COUPLED LINEAR EQUATIONS $\rightarrow$ MATRIX EQUATION

$$m\omega^2 \begin{pmatrix} A_x \\ A_y \end{pmatrix} = \begin{pmatrix} K_1+K_2 & -K_2 - K_1 e^{ika} \\ -K_2 - K_1 e^{-ika} & K_1+K_2 \end{pmatrix} \begin{pmatrix} A_x \\ A_y \end{pmatrix}$$

THUS, SOLUTIONS SATISFY

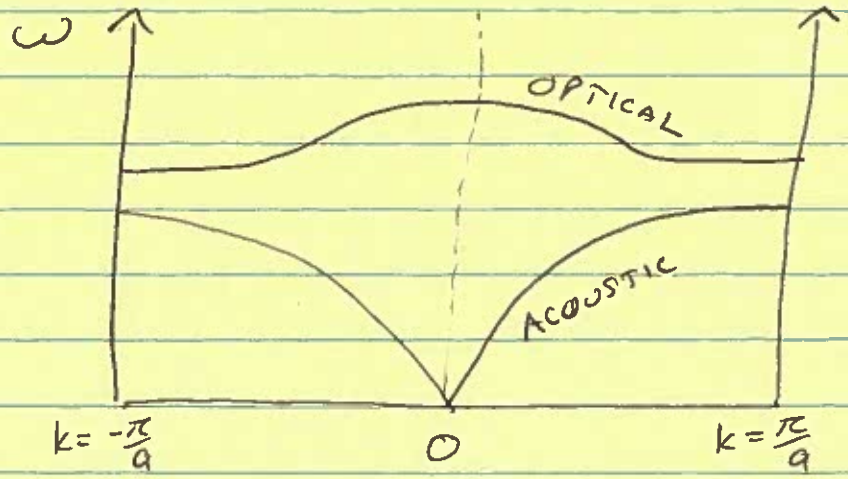
$$0 = (K_1+K_2 - m\omega^2)^2 - |K_2 + K_1 e^{ika}|^2$$

$$m\omega^2 = (K_1+K_2) \pm |K_1 + K_2 e^{ika}|$$

$$\Rightarrow \quad \omega_{\pm} = \sqrt{\frac{K_1 + K_2}{m} \pm \frac{1}{m}\sqrt{K_1^2 + K_2^2 + 2K_1K_2\cos(ka)}}$$

$$= \sqrt{\frac{K_1 + K_2}{m} \pm \frac{1}{m}\sqrt{(K_1 + K_2)^2 - 4K_1K_2\sin^2\left(\frac{ka}{2}\right)}}$$

LOOKS COMPLICATED, BUT FOR ALL VALUES OF K_1, K_2, m THE CURVES LOOK LIKE THIS



NOTICE

(1) THERE ARE NOW TWO SOLUTIONS AT EVERY VALUE OF k. THIS IS ALWAYS THE CASE. THE BOTTOM MODE IS ALWAYS CALLED THE "ACOUSTIC" MODE. THE TOP MODE IS THE "OPTICAL" MODE.

BOUNDARY CONDITIONS AGAIN TELL US THERE ARE N UNIQUE VALUES OF k, WHERE N = # OF CELLS IN THE CHAIN. WITH 2 BRANCHES → 2N UNIQUE MODES

(2) IN LIMIT $ka \ll 1$

$$\omega_\pm \approx \sqrt{\frac{K_1+K_2}{m} \pm \frac{K_1+K_2}{m}\sqrt{1 - 4\frac{K_1K_2}{(K_1+K_2)}\frac{k^2a^2}{4}}}$$

$$= \sqrt{\frac{K_1+K_2}{m}}\left(1 \pm 1 \mp \frac{K_1K_2}{2(K_1+K_2)}k^2a^2\right)^{\frac{1}{2}}$$

$$\Rightarrow \omega_- \approx \sqrt{\frac{K_1K_2}{2m}}\,ka \quad \propto k$$

$\rightarrow$ LINEAR DISPERSION

$$\omega_+ \approx \sqrt{\frac{K_1+K_2}{m}}\left(2 - \frac{K_1K_2}{2(K_1+K_2)}k^2a^2\right)^{\frac{1}{2}}$$

$$\approx \sqrt{\frac{2(K_1+K_2)}{m}}\left(1 - \frac{K_1K_2}{8(K_1+K_2)}k^2a^2\right)$$

$\frac{d\omega_+}{dk} \rightarrow 0$ AS $k \rightarrow 0$

ZERO GROUP VELOCITY

AS $k \rightarrow 0$ EXACTLY, OUR MATRIX EQUATION BECOMES

$$\omega^2\begin{pmatrix} A_x \\ A_y \end{pmatrix} = \frac{K_1+K_2}{2}\begin{pmatrix} 1 & -1 \\ -1 & 1 \end{pmatrix}\begin{pmatrix} A_x \\ A_y \end{pmatrix}$$

PLUGGING IN $\omega_- = 0$ TELLS US

$$A_x = A_z$$

⇒ ATOMS ARE MOVING IN SAME DIRECTION

WHEREAS FOR $\omega_+ = \sqrt{\frac{2(K_1+K_2)}{m}}$

$$2(K_1+K_2)\begin{pmatrix} A_x \\ A_z \end{pmatrix} = \begin{pmatrix} (K_1+K_2) & -(K_1+K_2) \\ -(K_1+K_2) & (K_1+K_2) \end{pmatrix}\begin{pmatrix} A_x \\ A_z \end{pmatrix}$$

$$\begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix}\begin{pmatrix} A_x \\ A_z \end{pmatrix} = 0$$

$$A_x = -A_z$$

⇒ ATOMS MOVING OPPOSITELY

→ EXPLAINS HIGHER ENERGY

(3) LIMIT $k \to \frac{\pi}{a}$

$$\omega_\pm = \sqrt{\frac{K_1+K_2}{m} \pm \frac{1}{m}\sqrt{K_1^2 + K_2^2 - 2K_1K_2\left(\frac{\pi}{2} - ka\right)^2}}$$

$$\frac{d\omega_\pm}{dk} = \frac{-a\sin(ka)\,2K_1K_2}{\sqrt{\quad}} \to 0$$

FOR BOTH BRANCHES

$$\omega_\pm = \sqrt{\frac{K_1+K_2}{m} \pm \frac{(K_2-K_1)}{m}}$$

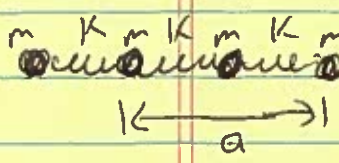
$$\Rightarrow \omega_-\left(k=\frac{\pi}{a}\right) = \sqrt{\frac{2K_1}{m}}, \quad \omega_+\left(k=\frac{\pi}{a}\right) = \sqrt{\frac{2K_2}{m}}$$

DON'T TOUCH UNLESS $K_1 = K_2$

(4) LIMIT $K_1 = K_2 \equiv K$

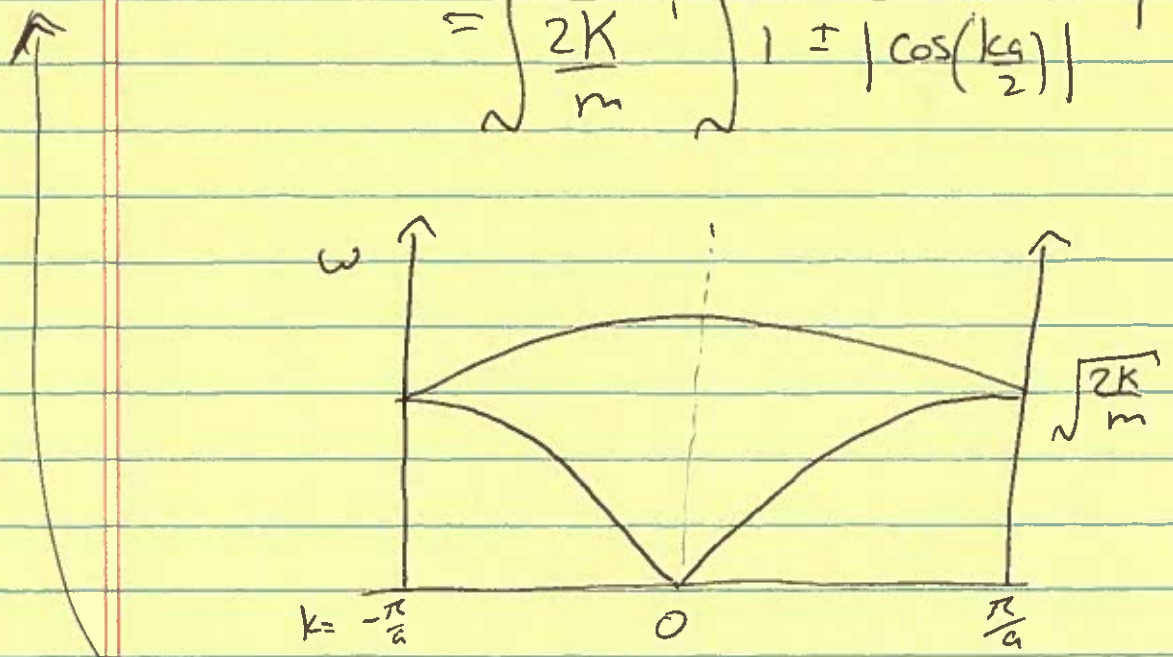
IN THIS SPECIAL CASE, THE TWO BANDS DO TOUCH

$$\omega_\pm = \sqrt{\frac{2K}{m} \pm \frac{1}{m}\sqrt{(2K)^2 - 4K^2 \sin^2\left(\frac{ka}{2}\right)}}$$

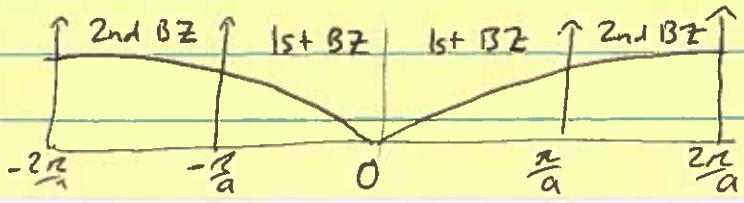


$$= \sqrt{\frac{2K}{m}}\sqrt{1 \pm \sqrt{1 - \sin^2\left(\frac{ka}{2}\right)}}$$

$$= \sqrt{\frac{2K}{m}}\sqrt{1 \pm \left|\cos\left(\frac{ka}{2}\right)\right|}$$



BUT NOTE THAT THIS IS NOW JUST THE MONATOMIC HARMONIC CHAIN WITH a NOW THE 2-ATOM DISTANCES. WHY DOES IT LOOK DIFFERENT? JUST A PLOTTING CHOICE (i.e A "FOLDED" SCHEME). WE COULD HAVE JUST AS EASILY PLOTTED USING AN "EXTENDED" SCHEME:



PHONONS IN HIGHER DIMENSIONS

CONCEPTUALLY, THE CALCULATION OF PHONON DISPERSIONS IS NO DIFFERENT IN HIGHER DIMENSIONS, BUT THE MATH IS SLIGHTLY MORE COMPLICATED. INSTEAD OF A SINGLE POSITION VARIABLE, ONE NEEDS TO KEEP TRACK OF ATOMIC POSITIONS VIA VECTORS; $\vec{r} = \vec{R} + \delta\vec{r}$, AND ONE NEEDS TO USE GRADIENT OPERATORS AND THE 3D VERSION OF THE TAYLOR EXPANSION

$$f(\vec{r}+\delta\vec{r}) = f(\vec{r}) + \delta\vec{r}\cdot\vec{\nabla}f(\vec{r}) + \frac{1}{2!}(\delta\vec{r}\cdot\vec{\nabla})^2 f(\vec{r}) + \frac{1}{3!}(\delta\vec{r}\cdot\vec{\nabla})^3 f(\vec{r}) + \cdots$$

SIMILAR TO THE DERIVATION IN 1D, ONE CAN ASSUME THAT N ATOMS ARE AT THE EQUILIBRIUM POSITIONS OF A BRAVAIS LATTICE, $\vec{R}$, TAYLOR EXPAND AND TRUNCATE AFTER THE QUADRATIC TERM (LINEAR TERM IS ZERO). DOING THIS (SEE ASHCROFT, CHAPTER 22) LEADS TO THE EXPRESSION

$$\mathcal{U}_{TOTAL} = \frac{1}{2}\sum_{\substack{\vec{R}\vec{R}'\\ \mu\nu}} u_\mu(\vec{R})\, D_{\mu\nu}(\vec{R}-\vec{R}')\, u_\nu(\vec{R}')$$

WHERE $D_{\mu\nu}(\vec{R}-\vec{R}') \equiv \delta_{R,R'}\sum_{\vec{R}''} V_{\mu\nu}(\vec{R}-\vec{R}'') - \frac{\partial^2 V(\vec{R}-\vec{R}')}{\partial r_\mu \partial r_\nu}$

AND I HAVE USED $u_\mu(\vec{R})$ INSTEAD OF $\delta r_\mu(\vec{R})$ TO AVOID CONFUSION

USUALLY THIS IS REWRITTEN IN VECTOR/MATRIX NOTATION

$$\mathcal{U}_{TOT} = \frac{1}{2} \sum_{\vec{R},\vec{R}'}{}' \vec{u}(\vec{R}) \hat{D}(\vec{R}-\vec{R}') \vec{u}(\vec{R}')$$

$$\rightarrow m \ddot{\vec{u}}(\vec{R}) = -\sum_{\vec{R}'}{}' D(\vec{R}-\vec{R}') \vec{u}(\vec{R}')$$

LOOKING FOR SOLUTIONS OF THE FORM

$$\vec{u}(\vec{R},t) = \vec{\epsilon}\, e^{i(\vec{k}\cdot\vec{R} - \omega t)}$$

($\vec{\epsilon}$: "POLARIZATION VECTOR")

ONE GETS THE EIGENVALUE PROBLEM

$$\boxed{M\omega^2 \vec{\epsilon} = \hat{D}(\vec{k})\hat{\epsilon}}$$

WHERE

$$\hat{D}(\vec{k}) = \sum_{\vec{R}} \hat{D}(\vec{R}) e^{-i\vec{k}\cdot\vec{R}}$$

IS THE "DYNAMICAL MATRIX"

WITHOUT GOING INTO DETAIL, HERE ARE MAIN NEW PIECES OF INFORMATION

(1) THE POLARIZATION VECTOR NOW GIVES NATURAL 3D DIRECTIONS OF ATOMIC MOTION (NOT JUST BACK AND FORTH)

(2) MODES NOW SEPARATE INTO "LONGITUDINAL" MODES, WHERE $\hat{\epsilon} \parallel \vec{k}$ AND "TRANSVERSE" MODES WITH $\hat{\epsilon} \perp \vec{k}$

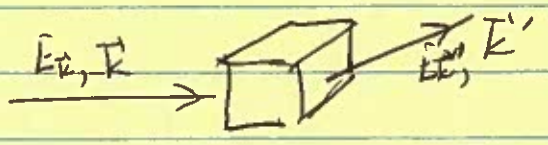
(3) FOR d DIMENSIONS, THERE WILL NOW BE d ACOUSTIC MODES, REGARDLESS OF THE NUMBER OF ATOMS. 1 WILL BE LONGITUDINAL.

(4) FOR N ATOMS IN A BASIS, THERE WILL BE $dN-d$ OPTICAL MODES.

MEASURING PHONONS

THE EXISTENCE OF PHONONS SHOWS UP IN A NUMBER OF EXPERIMENTAL RESULTS, BUT THE MOST DIRECT AND STANDARD MEANS OF MEASURING PHONON DISPERSIONS IS VIA INELASTIC NEUTRON SCATTERING

JUST LIKE WITH DIFFRACTION, THIS EXPERIMENT INVOLVES BOUNCING A STREAM OF NEUTRONS OFF A CRYSTAL AND OBSERVING THE FINAL SCATTERING ANGLE



BUT NOW WE ALLOW FOR THE POSSIBILITY THAT THE NEUTRON MIGHT DONATE OR RECEIVE ENERGY FROM THE CRYSTAL

IN THIS CASE, THE NEUTRON IS CHANGING THE VIBRATIONAL ENERGY MODE OF THE CRYSTAL, OR EQUIVALENTLY ADDING OR DESTROYING PHONONS. WE LEARN ABOUT THESE PHONONS BY MEASURING THE CHANGE IN NEUTRON ENERGY $E_{k'} - E_k$ FOR A GIVEN CHANGE IN NEUTRON MOMENTUM $\hbar\vec{k}' - \hbar\vec{k}$. WE USE CONSERVATION LAWS

ENERGY	CRYSTAL MOMENTUM
$E' - E = -\sum_{\vec{k}'} \hbar\omega_{\vec{k}'} \Delta n_{\vec{k}'}$	$\hbar\vec{k}' - \hbar\vec{k} = -\sum_{\vec{k}'} \hbar\vec{k}' \Delta n_{\vec{k}'} + \hbar\vec{G}$

($\Delta n_{\vec{k}'}$: occupation of crystal modes)

NOTICE THAT PHONON MOMENTUM IS ONLY CONSERVED MODULO A FACTOR OF RECIPROCAL LATTICE. THIS IS A DIRECT RESULT OF THE DISCRETE TRANSLATIONAL SYMMETRY OF THE LATTICE.

THESE FORMULAS ARE VERY GENERAL, AND ONE MAY EXCITE ANY NUMBER OF PHONON MODES WITH A NEUTRON. IN PRACTICE, ONE CHOOSES EXPERIMENTAL CONFIGURATIONS TO ONLY OBSERVE SPECIAL CASES:

(I) ZERO PHONON SCATTERING $(\Delta n_{\vec{k}} = 0)$

$\Rightarrow E' = E$, $\vec{k}' - \vec{k} = \vec{G}$

$\rightarrow$ LAUE CONDITION

(II) ONE PHONON SCATTERING $(\Delta n_{\vec{k}} = 1)$

$$E' = E + \hbar\omega_{\vec{k}}$$

$$\vec{p}' - \vec{p} = \pm\hbar\vec{k}' + \hbar\vec{G}$$

FOR ABSORPTION

$$\rightarrow \frac{p'^2}{2m_n} - \frac{p^2}{2m_n} = \hbar\omega\left(\frac{\vec{p}'-\vec{p}}{\hbar}\right)$$

SHARP PEAKS AT SINGLE $\vec{p}'$ AT A GIVEN ΔE

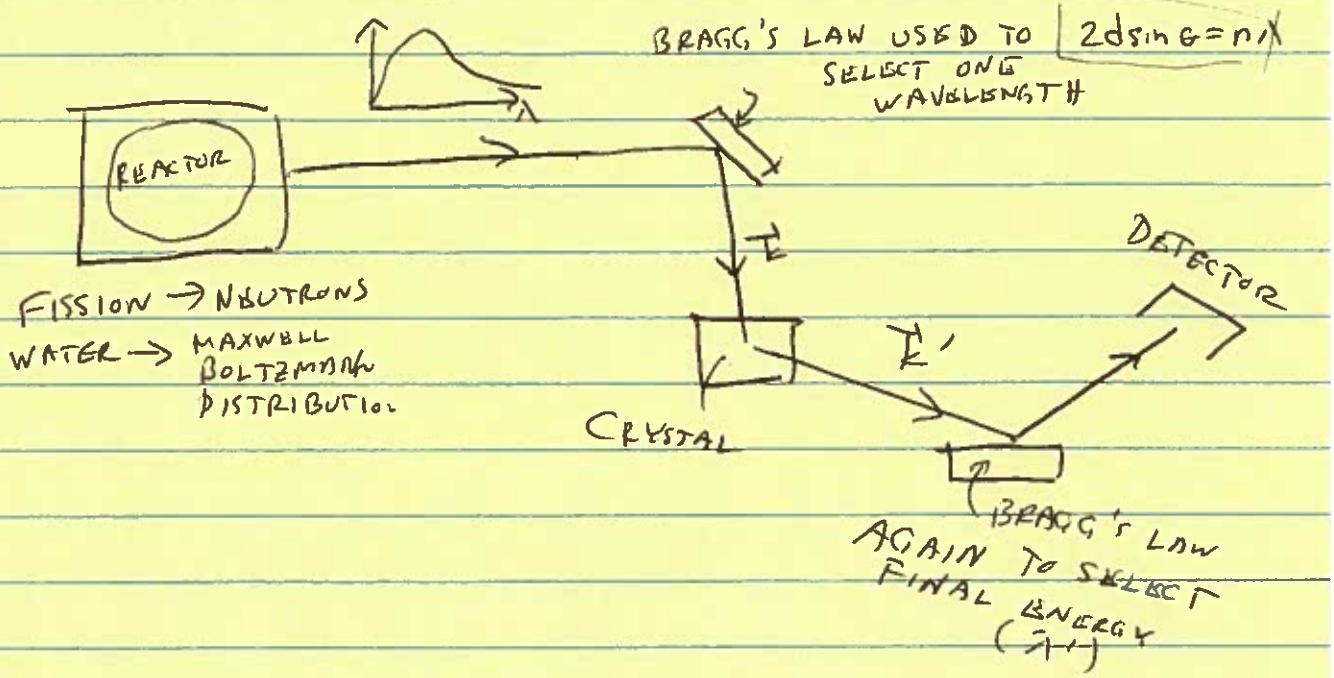
(III) TWO OR MORE PHONONS

$\longrightarrow$ DIFFUSE BG SCATTERING

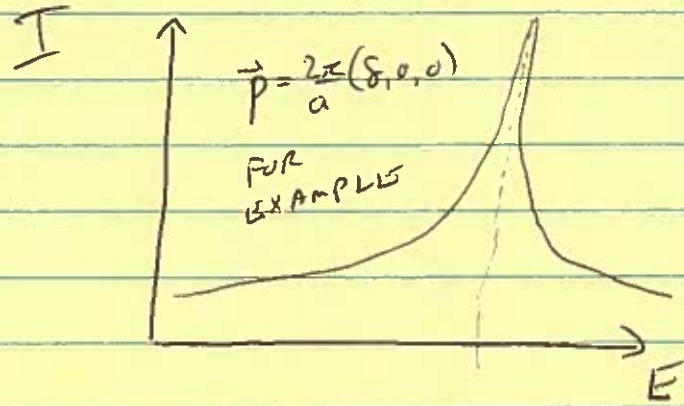
(MULTIPLE WAYS OF SATISFYING CONSERVATION LAWS)

INSTRUMENTS - 2 MAIN METHODS, DEPENDING ON HOW NEUTRONS ARE PRODUCED

(1) REACTOR SOURCE → TRIPLE AXIS SPECTROMETER

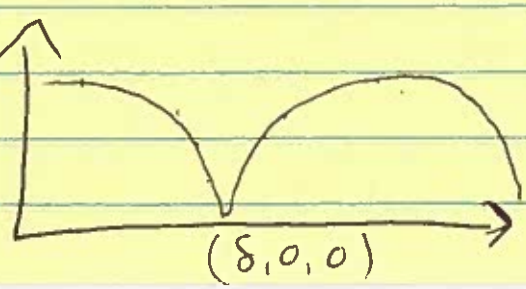


USUALLY FIX E', AND SCAN E FOR A NUMBER OF DIFFERENT $\vec{k}' - \vec{k} \equiv \vec{P}$



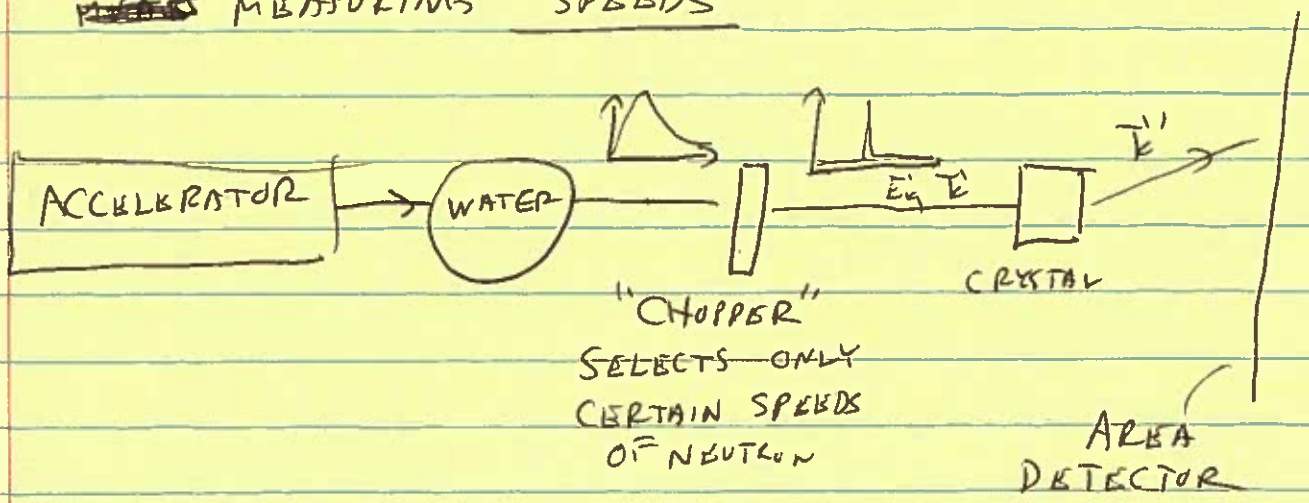
$E = \hbar\omega$

$\Rightarrow$



(2) ACCELERATOR SOURCES → TIME-OF-FLIGHT SPECTROMETER

THESE METHODS USE THE FINITE MASS OF THE NEUTRON TO EXTRACT ENERGIES FROM MEASURING SPEEDS



NOW E IS FIXED, AND MULTIPLE VALUES OF $\vec{p} = \vec{k}' - \vec{k}$ ARE & MEASURED SIMULTANEOUSLY USING AREA DETECTORS. DETECTION EVENTS ARE TIMED, AND KNOWING DISTANCES WELL ALLOWS ONE TO ASSOCIATE EACH TIME t_f WITH A FINAL ENERY, E'