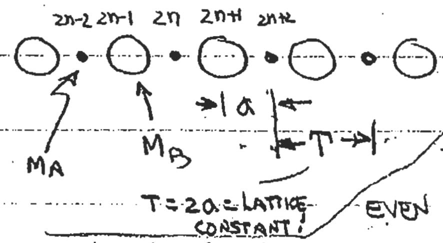
# 3.60 Symmetry, Structure and Tensor Properties of Materials

PROPAGATION OF WAVES ALONG ONE-DIMENSIONAL CRYSTAL WITH TWO KINDS OF ATOMS




CONSIDER A ONE-DIMENSIONAL CRYSTAL WITH 2 KINDS OF ATOMS $M_A$ & $M_B$. NUMBER THE ATOMS ALONG THE CHAINS SUCH THAT A ATOMS ARE EVEN $(2n)$, B ATOMS ODD $(2n+1)$.

ONLY A SINGLE FORCE CONSTANT, $\beta$, REMAINS NECESSARY TO DESCRIBE NEAREST NEIGHBOR INTERACTIONS, AS AN $\underline{A}$ ATOM INTERACTS WITH $\underline{B}$ THE SAME WAY AS $\underline{B}$ WITH AN $\underline{A}$.

IN SETTING UP A FORCE-BALANCE EQUATION WE MUST NOW WRITE A SEPARATE EQUATION FOR THE $\underline{A}$ AND $\underline{B}$ ATOMS — THEIR MASSES ARE DIFFERENT.

$$\begin{cases} M_A \dfrac{\partial^2 u_{2n}}{\partial t^2} = \beta\left(u_{2n+1} - 2u_{2n} + u_{2n-1}\right) \\ M_B \dfrac{\partial^2 u_{2n+1}}{\partial t^2} = \beta\left(u_{2n+2} - 2u_{2n+1} + u_{2n}\right) \end{cases}$$

LOOK FOR TRIAL SOLUTION

$$\begin{cases} u_{2n} = u_A\, e^{i(\omega t - k2na)} \\ u_{2n+1} = u_B\, e^{i[\omega t - k(2n+1)a]} \end{cases}$$

NO REASON TO ASSUME THE SAME AMPLITUDE FOR A & B ATOMS AS THEIR MASSES ARE DIFFERENT

SUBSTITUTING TRIAL SOLUTIONS INTO FORCE EQUATIONS:

$$\begin{cases} -M_A\omega^2 u_A e^{i(\omega t - 2nka)} = \beta\left\{u_B e^{i[\omega t-(2n+1)ka]} - 2u_A e^{i[\omega t - 2nka]} + u_B e^{i[\omega t-(2n-1)ka]}\right\} \\ -M_B\omega^2 u_B e^{i[\omega t-(2n+1)ka]} = \beta\left\{u_A e^{i[\omega t-(2n+2)ka]} - 2u_B e^{i[\omega t-(2n+1)ka]} + u_A e^{i[\omega t - 2nka]}\right\} \end{cases}$$

CANCELING COMMON TERMS

$$\begin{cases} -M_A\omega^2 u_A = \beta\left\{u_B e^{+ika} - 2u_A + u_B e^{-ika}\right\} \\ -M_B\omega^2 u_B = \beta\left\{u_A e^{+ika} - 2u_B + u_A e^{-ika}\right\} \end{cases}$$

NOTE THAT AMPLITUDES REMAIN IN EQS — THINGS ARE NOT QUITE AS TIDY AS BEFORE.

$$\boxed{e^{ix} + e^{-ix} = 2\cos x}$$

$$\begin{cases} -M_A\omega^2 u_A = 2\beta u_B \cos ka - 2\beta u_A \\ -M_B\omega^2 u_B = 2\beta u_A \cos ka - 2\beta u_B \end{cases}$$

REARRANGING TERMS IN $u_A$ & $u_B$

$$\begin{cases} (2\beta - M_A\omega^2)u_A - (2\beta\cos ka)u_B = 0 \\ -(2\beta\cos ka)u_A + (2\beta - M_B\omega^2)u_B = 0 \end{cases}$$

REGARD THE AMPLITUDES $U_A$ & $U_B$ AS UNKNOWNS AND WE HAVE (?: NO! NOT AGAIN!!) A SET of LINEAR HOMOGENEOUS EQUATIONS FOR WHICH A NON-TRIVIAL SOLUTION EXISTS ONLY IF THE DETERMINANT of COEFFICIENTS of THE VARIABLES VANISHES:

$$\begin{vmatrix} (2\beta - M_A\omega^2) & -(2\beta\cos ka) \\ -(2\beta\cos ka) & (2\beta - M_B\omega^2) \end{vmatrix} = 0$$

NOTE — will GIVE VALUES of $\omega$ AS A FUNCTION of $k$ AS EIGENVALUES!

EXPANDING

$$(2\beta - M_A\omega^2)(2\beta - M_B\omega^2) - (-2\beta\cos ka)(-2\beta\cos ka) = 0$$

$$4\beta^2 - 2\beta\omega^2(M_A+M_B) + M_AM_B\omega^4 - 4\beta^2\cos^2 ka = 0$$

$$M_AM_B\omega^4 - 2\beta(M_A+M_B)\omega^2 + 4\beta^2\underbrace{(1-\cos^2 ka)}_{=\sin^2 ka} = 0$$

$$\omega^4 - 2\beta\left(\frac{1}{M_A}+\frac{1}{M_B}\right)\omega^2 + \frac{4\beta^2}{M_AM_B}\sin^2 ka = 0$$

SOLVING, USING BINOMIAL THEOREM $\left[ax^2+bx+c=0 \Rightarrow x = \left(-b \pm \sqrt{b^2-4ac}\right)/2a\right]$

$$\omega^2 = \frac{\cancel{2}\beta\left(\frac{1}{M_A}+\frac{1}{M_B}\right) \pm \left\{\cancel{4}\beta^2\left(\frac{1}{M_A}+\frac{1}{M_B}\right)^2 - \cancel{4}\frac{4\beta^2}{M_AM_B}\sin^2 ka\right\}^{\frac{1}{2}}}{\cancel{2}}$$

$$\boxed{\omega^2 = \beta\left(\frac{1}{M_A}+\frac{1}{M_B}\right) \pm \beta\left\{\left(\frac{1}{M_A}+\frac{1}{M_B}\right)^2 - \frac{4}{M_AM_B}\sin^2 ka\right\}^{\frac{1}{2}}}$$

AGAIN WE HAVE THE CONDITION THAT $\omega$ BE A FUNCTION of $k = \frac{2\pi}{\lambda}$ IF OUR PROPOSED SOLUTION IS TO BE ACCEPTABLE (SORRY GANG! THIS IS AS SIMPLE AS WE CAN MAKE IT!)

THERE ARE TWO EIGENVALUES, $\omega^2$, FOR WHICH SOLUTIONS EXIST. EACH, WHEN SUBSTITUTED BACK INTO THE ORIGINAL EQUATION, WOULD PROVIDE EQS FROM WHICH WE COULD SOLVE FOR $U_A$ & $U_B$ — THUS FOR A GIVEN $k$, THERE ARE NOW TWO DIFFERENT WAVES of ANGULAR FREQUENCY $\omega$ WHICH MAY BE PROPAGATED IN THE CRYSTAL

## INTERPRETATION of THE SOLUTIONS

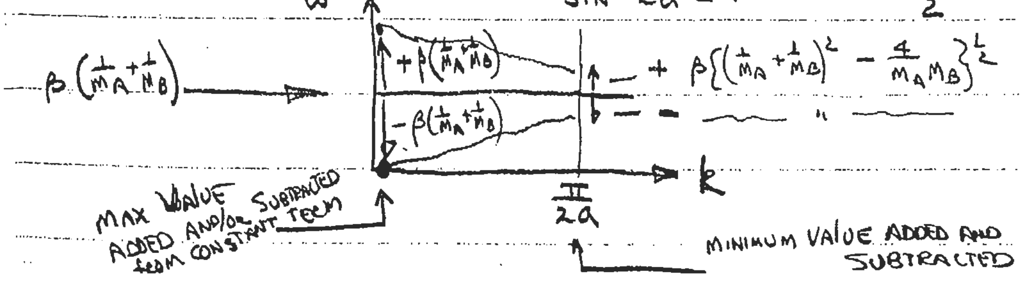
NOTE THAT THE GENERAL FORM of OUR RESULT THAT $\omega^2$ IS A CONSTANT $\left(\beta\frac{1}{M_A}+\beta\frac{1}{M_B}\right)$, TO WHICH WE EITHER ADD OR SUBTRACT A TERM WHICH IS GIVEN BY THE SQUARE ROOT OF A CONSTANT LESS A TERM WHICH IS A FUNCTION OF $k$. ($\sin^2 ka$)

THE MAXIMUM VALUE of THE TERM WHICH WE ADD-OR-SUBTRACT OCCURS WHEN THE TERM WHICH IS A fn of $k$ IS A MINIMUM — NAMELY

$$\sin^2 ka = 0 \qquad ka = 0 \qquad k = 0$$

THE MINIMUM VALUE of THE TERM WHICH WE ADD-OR-SUBTRACT OCCURS WHEN THE TERM WHICH IS A fn of $k$ IS A MAXIMUM — NAMELY

$$\sin^2 ka = 1 \qquad ka = \frac{\pi}{2} \qquad k = \frac{\pi}{2a}$$



## (A) Solutions for small $k$

Solution with $\oplus$ sign: AT $k=0$

$$\omega^2 = \beta\left(\frac{1}{M_A}+\frac{1}{M_B}\right) \oplus \beta\left[\left(\frac{1}{M_A}+\frac{1}{M_B}\right)^2 - \underbrace{\frac{4}{M_AM_B}\sin^2 ka}_{\to 0}\right]^{\frac{1}{2}}$$

$$\omega^2 = 2\beta\left(\frac{1}{M_A}+\frac{1}{M_B}\right)$$

DECREASES from this maximum with increasing $k$, as size of term ADDED becomes smaller.

Solution with $\ominus$ sign: AT $k=0$

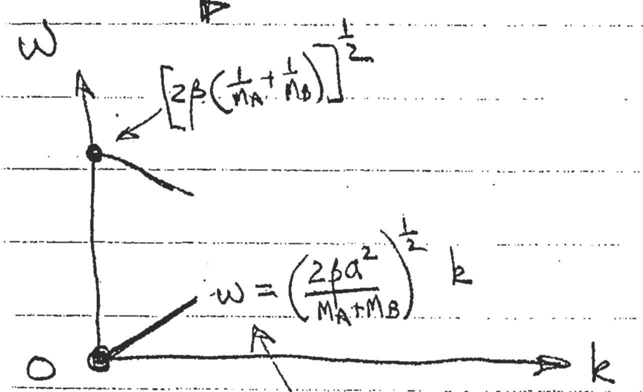
$$\omega^2 = \beta\left(\frac{1}{M_A}+\frac{1}{M_B}\right) \ominus \beta\left[\left(\frac{1}{M_A}+\frac{1}{M_B}\right)^2 - \underbrace{\frac{4}{M_AM_B}\sin^2 ka}_{\to 0}\right]^{\frac{1}{2}} = 0$$

NEAR $k=0$

$$\omega^2 = \beta\left(\frac{1}{M_A}+\frac{1}{M_B}\right) \ominus \beta\left[\left(\frac{1}{M_A}+\frac{1}{M_B}\right)^2 - \frac{4}{M_AM_B}k^2a^2\right]^{\frac{1}{2}}$$

$\sin x \approx x$ for small $x$

If $k$ is small and this approximation is valid, a term in $k^4$ would be absolutely miniscule so we could add it to this expression without any effect.




$$\omega^2 = \beta\left(\frac{1}{M_A}+\frac{1}{M_B}\right) \ominus \beta\left[\left(\frac{M_A+M_B}{M_AM_B}\right)^2 - \frac{4}{M_AM_B}(ka)^2 + \text{"}\frac{4a^4k^4}{M_A+M_B}\text{"}\right]^{\frac{1}{2}}$$

Term in $k^4$ too small to quibble about

$$\approx \beta\left(\frac{1}{M_A}+\frac{1}{M_B}\right) \ominus \beta\left\{\left[\frac{M_A+M_B}{M_AM_B} - \frac{2a^2k^2}{M_A+M_B}\right]^2\right\}^{\frac{1}{2}}$$

$$\approx \cancel{\beta\left(\frac{M_B+M_A}{M_AM_B}\right)} \ominus \cancel{\beta\left(\frac{M_A+M_B}{M_AM_B}\right)} + \beta\,\frac{2a^2k^2}{M_A+M_B}$$

$$\omega \approx \left(\frac{2\beta a^2}{M_A+M_B}\right)^{\frac{1}{2}} k$$

### Values of Amplitudes

**Solution with $\oplus$ sign at $k=0$**

$$\left.\begin{aligned}(2\beta - M_A\omega^2)u_A - (2\beta\cos ka)u_B &= 0\\ -(2\beta\cos ka)u_A + (2\beta - M_B\omega^2)u_B &= 0\end{aligned}\right\} \Rightarrow \left[\begin{aligned}&\left\{2\beta - M_A\left[2\beta\left(\frac{1}{M_A}+\frac{1}{M_B}\right)\right]\right\}u_A - 2\beta\underbrace{\cos ka}_{=1}\,u_B = 0\\ &-2\beta\underbrace{\cos ka}_{1 \text{ for } k=0}\,u_A + \left\{2\beta - M_B\left[2\beta\left(\frac{1}{M_A}+\frac{1}{M_B}\right)\right]\right\}u_B = 0\end{aligned}\right.$$

$$\therefore \left\{\begin{aligned}\cancel{2\beta}\left[1 - M_A\left(\frac{M_A+M_B}{M_AM_B}\right)\right]u_A - \cancel{2\beta}\,u_B &= 0\\ -\cancel{2\beta}\,u_A + \cancel{2\beta}\left[1 - M_B\left(\frac{M_A+M_B}{M_AM_B}\right)\right]u_B &= 0\end{aligned}\right\} \Rightarrow \left\{\begin{aligned}-\frac{M_A}{M_B}u_A - u_B &= 0\\ -u_A - \frac{M_B}{M_A}u_B &= 0\end{aligned}\right.$$

This is a motion in which the amplitudes of A & B are inversely proportional to the mass of the atoms and opposite in sign.

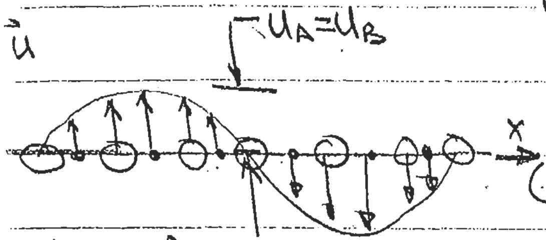
$$\boxed{\frac{u_A}{u_B} = -\frac{M_B}{M_A}} \qquad u_A \sim \frac{1}{M_A} \qquad u_B \sim \frac{1}{M_B}$$

THE CENTER of MASS of THE UNIT CELL STAYS FIXED

**Solution with ⊖ sign at $k=0$**

$$\left.\begin{aligned}(2\beta - \underbrace{M_A\omega^2}_{0})u_A - 2\beta \underbrace{\cos ka}_{1}\, u_B &= 0\\ (-2\beta \underbrace{\cos ka}_{1})u_A + (2\beta - \underbrace{M_B\omega^2}_{0})u_B &= 0\end{aligned}\right\} \Rightarrow \begin{aligned}2\beta u_A - 2\beta u_B &= 0\\ -2\beta u_A + 2\beta u_B &= 0\end{aligned}$$

$$\therefore \boxed{u_A = u_B}$$




Acoustic Branch
($k \to 0$)

This was the situation for a normal elastic wave — a volume element (and all atoms in it) has a certain amplitude.

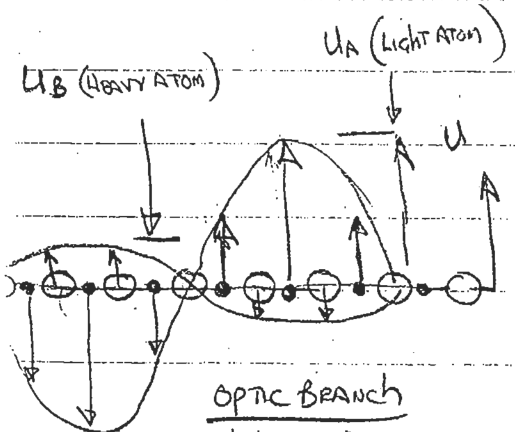
We obtained, above the result (for small $k$)

That $\omega \approx \left(\frac{2\beta a^3}{M_A + M_B}\right)k$

i.e., the velocity of the wave $V = \left(\frac{2\beta a^2}{M_A + M_B}\right)^{\frac{1}{2}}$

If $M_A = M_B = M$ this reduces to $V = \left(\frac{\beta a^3}{M}\right)^{\frac{1}{2}}$,

the same as previously obtained for a continuum or for a crystal containing only one type atom. This is a normal elastic wave of the sort which would be present in propagation of sound. The solution with the ⊖ sign is accordingly called the Acoustic Branch




Optic Branch
($k \to 0$)

The solution with ⊕ sign (for which $\omega \neq 0$ at $k=0$) for which the center of mass of the cell remains fixed has amplitudes of vibration for the two atoms which are opposite in sign. This sort of wave (totally unaccounted for in the continuum model!!) might well be excited if an electromagnetic field we incident on a ionic crystal — ions of opposite charge would be pulled in opposing directions. The solution with the ⊕ sign is accordingly called the Optic Branch

## (B) Solutions for $k = k_{max}$

Other extreme in solutions occurs when $\sin^2 ka$ reaches maximum value — namely:

$\sin ka = 1 \qquad ka = \frac{\pi}{2} \qquad \boxed{k_{max} = \frac{\pi}{2a}}$

Note that for a 1-D xl with one kind of atom we had earlier obtained $k_{max} = \frac{\pi}{a}$. The present result looks different until we realize that

$T = a$ = lattice constant with 1 kind of atom
$T = 2a$ = lattice constant with 2 kinds of atom

$\therefore \boxed{k_{max} = \frac{\pi}{T}}$ in both

$$\omega^2 = \beta\left(\frac{1}{M_A} + \frac{1}{M_B}\right) \pm \beta\left\{\left(\frac{1}{M_A} + \frac{1}{M_B}\right)^2 - \frac{4}{M_A M_B}\sin^2 ka\right\}^{\frac{1}{2}}$$

As $k \to k_{max}$

$$\omega^2 = \beta\left(\frac{1}{M_A} + \frac{1}{M_B}\right) \pm \beta\left\{\left(\frac{1}{M_A^2} + \frac{1}{M_B^2} + \frac{2}{M_A M_B}\right) - \frac{4}{M_A M_B}\right\}^{\frac{1}{2}}$$

$$= \beta\left(\frac{1}{M_A} + \frac{1}{M_B}\right) \pm \beta\left\{\frac{1}{M_A^2} + \frac{1}{M_B^2} - \frac{2}{M_A M_B}\right\}^{\frac{1}{2}} = \beta\left(\frac{1}{M_A} + \frac{1}{M_B}\right) \pm \beta\left\{\left(\frac{1}{M_A} - \frac{1}{M_B}\right)^2\right\}^{\frac{1}{2}}$$

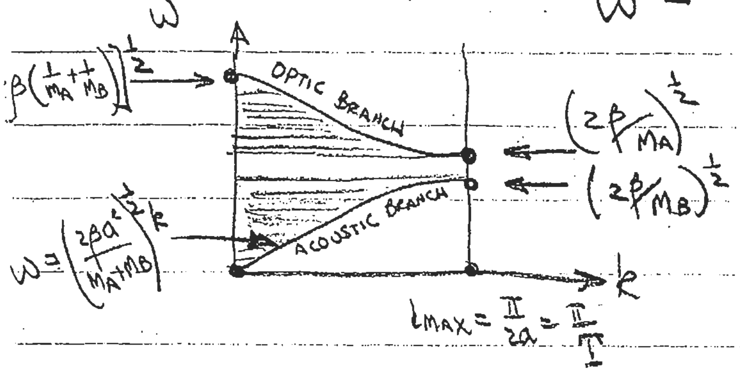
OR $$W^2 = \beta\left(\frac{1}{M_A}+\frac{1}{M_B}\right) \pm \beta\left(\frac{1}{M_A}-\frac{1}{M_B}\right)$$

POSITIVE BRANCH (OPTIC BRANCH)

$$W^2 = \frac{2\beta}{M_A}$$

NEGATIVE SOLUTION (ACOUSTIC BRANCH)

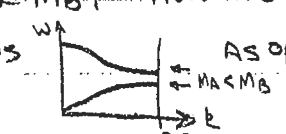
$$W^2 = \frac{2\beta}{M_B}$$



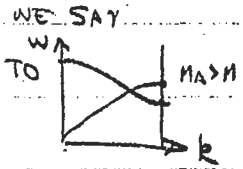

A first UNEXPECTED RESULT of this PROBLEM WAS THE PRESENCE OF THE OPTIC BRANCH (which would be UNANTICIPATED IN THE CONTINUUM APPROACH) WE NOW SEE A SECOND UNEXPECTED FEATURE — NAMELY, THE PRESENCE OF A BAND of FORBIDDEN INTERMEDIATE FREQUENCIES

$\left(2\beta/M_B\right)^{\frac{1}{2}} < \omega < \left(\frac{2\beta}{M_A}\right)^{\frac{1}{2}}$ for which NO ACCEPTABLE SOLUTION $\omega = f(k)$ IS DEFINED, AND which THEREFORE ARE MODES which CANNOT BE PROPAGATED IN THE CRYSTAL. [STIR ANY PRIMORDIAL RECOLLECTIONS of forbidden ENERGIES for ELECTRONS MOVING IN CRYSTALS ????]

DIGRESSION. NOW HOLD ON A SEC, THE DISCRIMINATING STUDENT will EXPOSTULATE! If THE PRECEDING PAGES ARE EXAMINED, WE HAVE NOWHERE SPECIFIED which IS THE GREATER ATOMIC MASS, $M_A$ OR $M_B$! HOW THEN CAN WE SAY THAT $\omega$ AS A function of $k$ DOES this




AS OPPOSED TO




IS IT THEREFORE NECESSARY THAT A GAP IN $\omega$ EXIST ??

WELL NOW, DISCRIMINATING STUDENT: If THE TWO BRANCHES ARE TO CROSS AS IN THE SECOND SKETCH, THERE MUST BE SOME $k$ for which THE BRANCHES CROSS. THAT IS, LOOKING AT $\omega$ AS A fn of $k$:

$$\omega^2 = \beta\left(\frac{1}{M_A}+\frac{1}{M_B}\right) \pm \beta\Big\{\underbrace{\left(\frac{1}{M_A}+\frac{1}{M_B}\right)^2 - \frac{4}{M_A M_B}\sin^2 ka}_{\text{THIS TERM MUST, for SOME } k, \text{ BE ZERO IF BRANCHES CROSS.}}\Big\}^{\frac{1}{2}}$$

CAN WE PROVE

$$\left(\frac{1}{M_A}+\frac{1}{M_B}\right)^2 - \frac{4}{M_A M_B}\underbrace{\sin^2 ka}_{\text{MAX VALUE for SECOND TERM IS when this } = 1} \geq 0 \ ??$$

$$\left(\frac{1}{M_A}+\frac{1}{M_B}\right)^2 - \frac{4}{M_A M_B} \geq 0 \ ?$$

$$\frac{1}{M_A^2}+\frac{1}{M_B^2}+\frac{2}{M_A M_B}-\frac{4}{M_A M_B} \geq 0 \ ?$$

$$\frac{1}{M_A^2}+\frac{1}{M_B^2}-\frac{2}{M_A M_B} = \left(\frac{1}{M_A}-\frac{1}{M_B}\right)^2 \geq 0 \ ?$$

YES! ALWAYS TRUE! QED THERE IS A GAP IN $\omega$.

[ NOTE THAT THE REASON FOR THE PARADOX, RESOLVED ABOVE, IS THAT $\left(\frac{1}{M_A} - \frac{1}{M_B}\right)^2 = \left(\frac{1}{M_B} - \frac{1}{M_A}\right)^2$. THE EXPRESSION WE ELECT TO USE AT THE BOTTOM OF Pg 4 DETERMINES WHETHER $\frac{1}{M_A}$ OR $\frac{1}{M_B}$ APPEARS AT $k_{MAX}$ IN EACH BRANCH ]

## DISPLACEMENTS AT $k_{MAX}$

$$\begin{cases} (2\beta - M_A\omega^2)u_A - (2\beta\cos ka)u_B = 0 \\ -2\beta\cos ka\, u_A + (2\beta - M_B\omega^2)u_B = 0 \end{cases}$$

AT $k = k_{MAX}$ $\quad \omega^2_{optic} = \left(\frac{2\beta}{M_A}\right)^{\frac{1}{2}}$ $\quad \omega^2_{acoustic} = \left(\frac{2\beta}{M_B}\right)^{\frac{1}{2}}$ $\quad$ WHERE $M_B > M_A$, $\quad k = \frac{\pi}{2a}$

$$\begin{cases} \left(2\beta - M_A\frac{2\beta}{M_A}\right)u_A - (2\beta\cos ka)u_B = 0 \\ -2\beta\cos ka\, u_A + 2\beta - M_B\cdot\frac{2\beta}{M_A}u_B = 0 \end{cases} \qquad k = \frac{\pi}{2a},\ \cos ka \to 0$$

$$\begin{cases} (2\beta - 2\beta)u_A - 0\,u_B = 0 \\ -0\,u_A + \left(2\beta - 2\beta\frac{M_B}{M_A}\right)u_B = 0 \end{cases}$$

$$\begin{cases} 0\,u_A - 0\,u_B = 0 \\ 0\,u_A + 2\beta\left(1 - \frac{M_B}{M_A}\right)u_B = 0 \end{cases}$$

$\Rightarrow u_B = 0$

for OPTIC MODE AT $k_{MAX}$

HEAVY ATOM STAYS MOTIONLESS, $u_A$ for LIGHT ATOM IS ANY VALUE.

$$\begin{cases} \left(2\beta - M_A\frac{2\beta}{M_B}\right)u_A - \left(2\beta\cos\frac{\pi}{2a}\cdot a\right)u_B = 0 \\ \left(-2\beta\cos\frac{\pi}{2a}\cdot a\right)u_A + \left(2\beta - M_B\frac{2\beta}{M_B}\right)u_B = 0 \end{cases}$$

$$\begin{cases} 2\beta(1 - M_A/M_B)\,u_A - 0\,u_B = 0 \\ 0\,u_A + 0\,u_B = 0 \end{cases}$$

$\Rightarrow u_A = 0 \quad u_B =$ ANYTHING

for ACOUSTIC MODE AT $k_{MAX}$

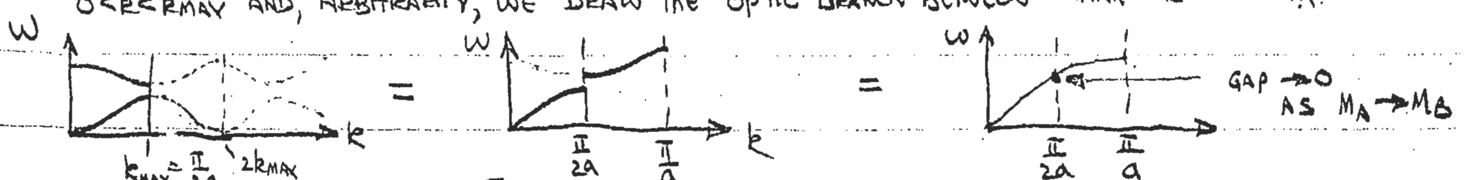
LIGHT ATOM STAYS MOTIONLESS.

## CORRESPONDENCE TO THE IDENTICAL-ATOM PROBLEM

OUR SOLUTION TO THE TWO-ATOM-PER-CELL PROBLEM LOOKS VERY DIFFERENT FROM OUR EARLIER RESULT FOR A ONE-DIMENSIONAL CRYSTAL WITH ONE KIND OF ATOM — NAMELY WE HAVE FOUND THE PRESENCE OF A SECOND CLASS OF MODES — THE OPTIC BRANCH.

SUPPOSE, NOW, THAT $M_B \to M_A$. THE PROBLEM THEN IS INDISTINGUISHABLE FROM THE 1-D XL / ONE KIND OF ATOM PROBLEM. HOW DOES THE OPTIC BRANCH KNOW IT HAS TO DISAPPEAR WHEN $M_A = M_B$ ??

RECALL THAT ALL PHYSICALLY MEANINGFUL MODES EXIST FOR RANGES OF $k$ WITHIN THE FIRST BRILLOUIN ZONE; LARGER VALUES OF $k$ MAY BE SHIFTED TO WITHIN THE ZONE BY SUBTRACTING A $\Delta k$ WHICH DOES NOT ALTER PHASE BETWEEN NEIGHBORING ATOMS. LET US REDRAW $\omega(k)$ SUCH THAT THE ACOUSTIC BRANCH IS DRAWN BETWEEN $0 < k < k_{MAX}$ AND, ARBITRARILY, WE DRAW THE OPTIC BRANCH BETWEEN $k_{MAX} < k < 2k_{MAX}$.




[DOES THIS REMIND YOU OF E(k) FOR ELECTRONS ??]