EE236
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Interaction of light in semiconductors.

Most active optoelectronic devices use semiconductor media. This is because semiconductors allow direct control of their electronic states by injection of holes & electrons, gain can be very high, and the devices compact & inexpensive (relative to other types of lasers)

To understand solid-state electronic devices we will first need to cover some semiconductor physics background.

The states which photons interact with in a semiconductor are: vibrational modes (phonons)
distributed electron states (electrons & holes)

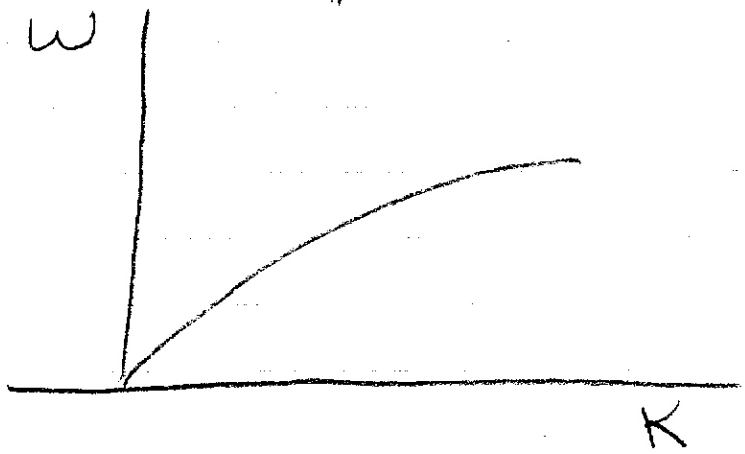
both of these are best viewed as <u>pseudo particles</u>, moving through the crystal as waves.

phonons are sound waves, but they travel at high velocities because the materials are quite strong.

A crystal with a phonon propagating might look something like this:

For low frequency phonons, the velocity is the speed of sound in the material, so we have

$$\frac{\omega_{phonon}}{K_{phonon}} = v_{sound}$$



where the displacement of the atoms is given by

$$\vec{R} = \vec{R}_0 e^{i(\omega t - K \cdot z)}$$

The atoms can be displaced along the direction of $\vec{K}$ (acoustic longitudinal phonons) or transverse to the direction of $\vec{K}$ (transverse acoustic phonons)

In the crystals which are of interest to us, there are two kinds of atoms in the lattice. This gives rise to a different kind of phonons called the optical phonon (the name is not intuitive)

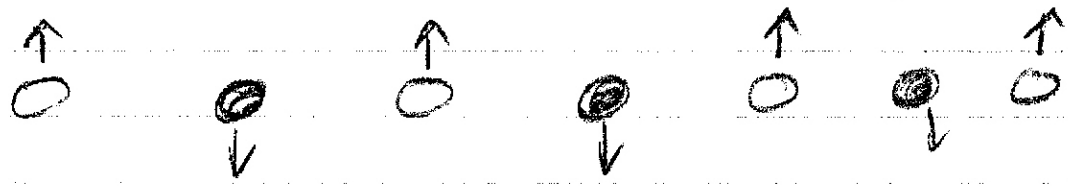
Notice in the above plane wave, $\vec{R}$ is only defined for z on a lattice point. If there are more than one types of atoms, each will have its

own displacement vector,

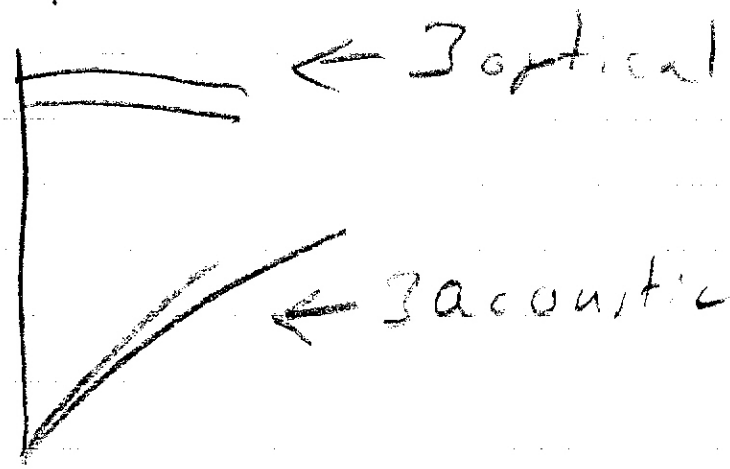
$$R_g = \vec{R}_{0g}\, e^{i(\omega t - kz)}$$

$$R_a = \vec{R}_{0a}\, e^{i(\omega t - kz)}$$

when these are substituted into the equations of motion, we get ω & k the same, but $\vec{R}_{0g}$ & $\vec{R}_{0a}$ can be different. For example



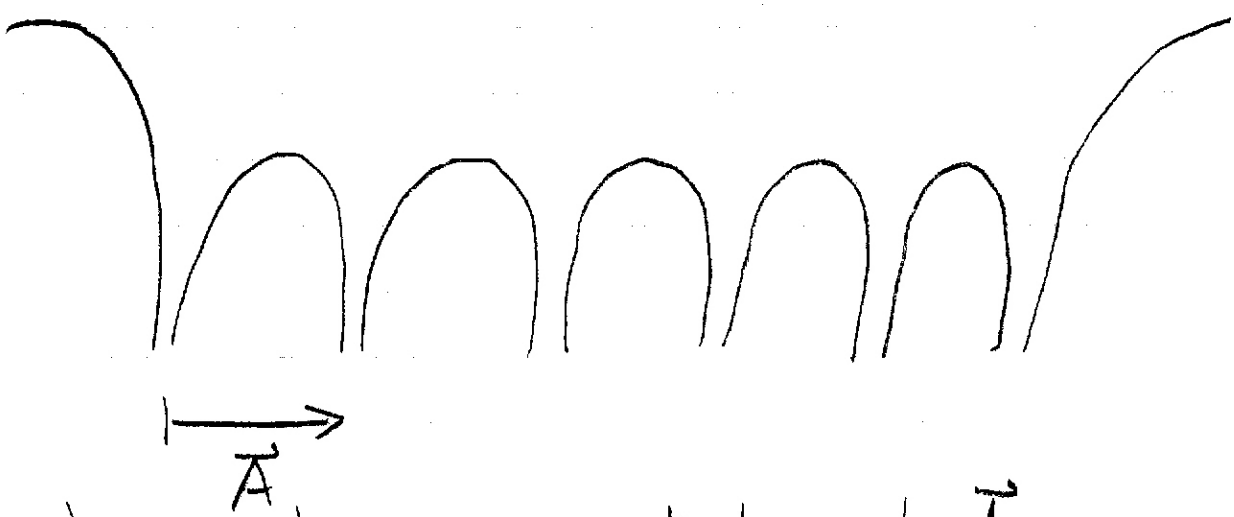
the phase change from one lattice point to another is 0, so $k = 0$, but obviously ω is not zero, this gives the optical branch of the phonons



Each of these mechanical modes can be quantized as a harmonic oscillator, giving us the <u>phonons</u>. (just as we did for E+M fields)

The electron states are perhaps more intuitive being particles in a box, but we need to deal with many at once, and the potential is periodic across the crystal

We have a potential something like



which repeats over a displacement $\vec{A}$

to understand how that will affect our electronic states, let's do it in 1-D first
First, we will show the Bloch theorem
Schrodinger's equation is a linear differential equation of the form

$$\frac{d^2\psi}{dx^2} + f(x)\psi(x) = 0$$

where $f(x)$ contains the eigenvalue and the potential $V(x)$, so $f(x)$ is periodic, $f(x+a) = f(x)$

This 1-D linear D.E. of second order must have exactly two independent solutions, so

$$\psi(x) = A\,g(x) + B\,h(x)$$

Since any solution must be a linear sum of $g(x)$ + $h(x)$, we have

$$g(x+a) = \alpha_1 g(x) + \alpha_2 h(x)$$
$$h(x+a) = \beta_1 g(x) + \beta_2 h(x)$$

where a is the lattice spacing and α_1 α_2 β_1 β_2 are constants

and

$$\psi(x+a) = A\,g(x+a) + B\,h(x+a)$$

$$= (\alpha_1 A + \beta_1 B)\,g(x)$$

$$+ (\alpha_2 A + \beta_2 B)\,h(x)$$

Now lets try to find solutions of the form:

$$\psi(x+a) = \lambda\,\psi(x)$$

(since a displaced solution is also a solution, we should be able to diagonalize the displacement operator at the same time)

plugging in, we have

$$(\alpha_1 - \lambda)\,A + \beta_1 B = 0$$

$$\alpha_2 A + (\beta_2 - \lambda)\,B = 0$$

(since $g(x)$ & $h(x)$ are linearly independent)

to have A & B not both zero, the determinant of this set of equations must be zero

$$\begin{vmatrix} \alpha_1 - \lambda & \beta_1 \\ \alpha_2 & \beta_2 - \lambda \end{vmatrix} = 0$$

$$\lambda^2 - (\alpha_1 + \beta_2)\lambda + (\alpha_1 \beta_2 - \alpha_2 \beta_1) = 0$$

the two roots of this equation give the values of λ for which

$$\psi_1(x+a) = \lambda_1 \psi_1(x) \qquad \psi_2(x+a) = \lambda_2 \psi(x+a)$$

$$\lambda = \frac{\alpha_1 + \beta_2 \pm \sqrt{(\alpha_1 + \beta_2)^2 - 4(\alpha_1 \beta_2 - \alpha_2 \beta_1)}}{2}$$

now define $\lambda_1 = e^{ik_1 a}$

$$\lambda_2 = e^{ik_2 a}$$

and define $u_{k_1}(x) = e^{-ik_1 x}\, \psi(x)$

$$u_{k_2}(x) = e^{-ik_2 x}\, \psi(x)$$

plugging in,

$$u_{k_1}(x+a) = e^{-ik_1(x+a)}\psi(x+a)$$

$$= e^{-ik_1(x+a)}\lambda_1\psi(x)$$

$$= e^{-ik_1(x+a)}e^{ik_1a}\psi(x)$$

$$= e^{-ik_1x}\psi(x)$$

$$= u_{k_1}(x)$$

$\Rightarrow$ so $u_{k_1}(x) = u_{k_1}(x+a) \Rightarrow$
u is periodic with a period $\underline{a}$

So we can write, always,

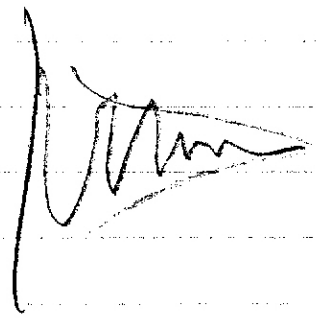
$$\psi_k(x) = e^{ikx}u_k(x)$$

where $u_k(x)$ is periodic over the lattice

In 3-D this becomes

$$\psi_k(r) = e^{i\vec{k}\cdot\vec{r}}u_k(r)$$

if K turns out to be real for a particular energy $E = \hbar\omega$, then this state extends uniformly across the crystal. If it does not, then the state is a edge state



In 1-d, there are two solutions to K for every $E = \hbar\omega$

We call a group of states with similar $u_{\nu K}$ a band of states.

In general, ω, $u_{\nu K}$ K will be smoothly related.

For periodic B.C., we will get only the states for K real

So each electron in a crystal can be expanded over a set of eigenstates which are of this form

the value of $\vec{K}$ is the wave vector, and represents the change of phase with distance from one lattice point to the next, the periodic function $U_k(r)$ is the behavior of the wavefunction <u>within</u> the cell.

If we impose a boundary condition on the crystal as a whole, for example

$$\psi(x+Na) = \psi(x)$$

$$e^{iKNa} = 1$$

we get a finite set of allowed K such that

$$K_n = \frac{2\pi n}{Na}$$ the same as

the density of states in K-space for E+M modes.