The classical equations of motion for the ions are then

$$M\ddot{\vec{u}}_i = -\frac{\partial U_{ion}}{\partial \vec{u}_i} \Rightarrow M\ddot{u}_{i\alpha} = -\sum_{j\beta} D_{ij}^{\alpha\beta} u_{j\beta}$$

Now by translational invariance of the Bravais lattice $D_{ij}^{\alpha\beta}$ depends only on $\vec{R}_i^0 - \vec{R}_j^0$.

We can define the Fourier transforms

$$\vec{u}_i(t) = \int_{q\in 1^{st}BZ} d^3q \int_{-\infty}^{\infty} d\omega \, e^{i\vec{q}\cdot\vec{R}_i^0} e^{-i\omega t} \vec{u}(\vec{q},\omega)$$

$$D_{ij}^{\alpha\beta} = \int_{q\in 1^{st}BZ} d^3q \, e^{i\vec{q}\cdot(\vec{R}_i^0 - \vec{R}_j^0)} D^{\alpha\beta}(\vec{q})$$

Note: in defining Fourier transform of a function that exists only on the discrete sites of a B.L., the only wavevectors we need to consider are those $\vec{q}$ in the 1^{st} BZ. This is because any wavevector $\vec{k}$ can always be written as $\vec{k} = \vec{q} + \vec{K}$ with $\vec{K}$ a unique R.L. vector and $\vec{q}$ in the 1^{st} BZ. Then the plane wave factor would be

$$e^{i\vec{k}\cdot\vec{R}_i^0} = e^{i(\vec{q}+\vec{K})\cdot\vec{R}_i^0} = e^{i\vec{q}\cdot\vec{R}_i^0} \quad \text{since } e^{i\vec{K}\cdot\vec{R}_i^0} = 1$$

so we still only get oscillations at $\vec{q}$ in 1^{st} BZ substitute these into the equation of motion

$$\int_{q \text{ in } 1^{st} BZ} d^3q \int_{-\infty}^{\infty} d\omega \, e^{i\vec{q}\cdot\vec{R}_i^0} e^{-i\omega t} (-\omega^2) M \, \vec{u}(\vec{q},\omega)$$

$$= -\int_{q \in 1^{st} BZ} d^3q \int_{q' \in 1^{st} BZ} d^3q' \int_{-\infty}^{\infty} d\omega \sum_j e^{i\vec{q}\cdot(\vec{R}_i^0 - \vec{R}_j^0)} e^{i\vec{q}'\cdot\vec{R}_j^0} e^{-i\omega t} \, \overleftrightarrow{D}(q) \cdot \vec{u}(\vec{q}',\omega)$$

matrix product over coordinates

Do the ~~integral~~ summation

$$\sum_j e^{i(\vec{q}'-\vec{q})\cdot\vec{R}_j^0} = \delta(\vec{q}-\vec{q}')$$

Follows since $\{\vec{R}_j^0 + \vec{R}_0^0\} = \{\vec{R}_j^0\}$ since BL is closed under translation by any BL vector $\vec{R}_0^0$

$$\Rightarrow \sum_{R_j^0} e^{i(\vec{q}'-\vec{q})\cdot\vec{R}_j^0} = \sum_{R_j^0} e^{i(\vec{q}'-\vec{q})\cdot(\vec{R}_j^0+\vec{R}_0^0)}$$

$$= e^{-i(\vec{q}'-\vec{q})\cdot\vec{R}_0^0} \sum_{R_j^0} e^{i(\vec{q}'-\vec{q})\cdot\vec{R}_j^0}$$

$$\Rightarrow e^{i(\vec{q}'-\vec{q})\cdot\vec{R}_0^0} = 1 \text{ for any } \vec{R}_0^0 \text{ in } BL$$

$$\Rightarrow \vec{q}'-\vec{q} = \vec{K} \text{ in } R.L.$$

But since $\vec{q}, \vec{q}'$ both in 1^{st} BZ $\Rightarrow \vec{K}=0$
and

$\vec{q} = \vec{q}'$ or the sum must vanish

$$\int_{1^{st} BZ} d^3q \int d\omega\, e^{i(\vec{q}\cdot\vec{R}_i^0 - \omega t)} (-\omega^2) M\, \vec{u}(\vec{q},\omega)$$

$$= -\int_{1^{st} BZ} d^3q\, d\omega\, e^{i(\vec{q}\cdot\vec{R}_i^0 - \omega t)}\, \overleftrightarrow{D}(\vec{q}) \cdot \vec{u}(\vec{q},\omega)$$

equate Fourier amplitudes to get

$$+\omega^2 M\, \vec{u}(\vec{q},\omega) = \overleftrightarrow{D}(\vec{q}) \cdot \vec{u}(\vec{q},\omega)$$

If the eigenvectors and eigenvalues of $\overleftrightarrow{D}(\vec{q})$ are $\vec{\epsilon}_1(\vec{q}), \vec{\epsilon}_2(q), \vec{\epsilon}_3(q)$ and $\lambda_1(\vec{q}), \lambda_2(\vec{q}), \lambda_3(\vec{q})$

Then

$$+\omega_s^2 M = \lambda_s(\vec{q}) \qquad s = 1, 2, 3$$

$$\omega_s = \sqrt{\frac{\lambda_s(\vec{q})}{M}}$$

dispersion relation for elastic vibrations at wave vector $\vec{q}$, polarization $\vec{\epsilon}_s(\vec{q})$

We expect that in the <u>long wave length limit</u> we can expand

$$\overleftrightarrow{D}(q) = \sum_i e^{-i\vec{q}\cdot\vec{R}_i}\, \overleftrightarrow{D}(\vec{R}_i)$$

$$\simeq \sum_i \left\{ 1 - i\vec{q}\cdot\vec{R}_i - \tfrac{1}{2}(\vec{q}\cdot\vec{R}_i) \right\} \overleftrightarrow{D}(\vec{R})$$

$\sum_i \overleftrightarrow{D}(\vec{R}_i) = 0$ because if all $\vec{u}_i = \vec{u}_0$ a uniform displacement, then net force on ion i must vanish

$\sum_i \vec{R}_i \overleftrightarrow{D}(\vec{R}_i) = 0$ by inversion symmetry $\vec{R}_i \to -\vec{R}_i$
$\overleftrightarrow{D}(\vec{R}_i) = \overleftrightarrow{D}(-\vec{R}_i)$

so

$$\overleftrightarrow{D}(\vec{q}) \simeq -\frac{q^2}{2} \sum_{\vec{R}_i} (\hat{q}\cdot\vec{R}_i)^2 \overleftrightarrow{D}(\vec{R})$$

we assume this sum converges

$\Rightarrow \overleftrightarrow{D}(q) \propto q^2$

so $\lambda_s(\vec{q}) \propto q^2$ or $\lambda_s(\vec{q}) = A_s q^2$ for small $\vec{q}$

$\Rightarrow \omega_s = \sqrt{\frac{A_s}{M}}\,|\vec{q}|$ with

$c_s = \sqrt{A_s/M}$ the speed of sound ~~for~~ for polarization s.

$\omega_s = c_s q$ for small $\vec{q}$

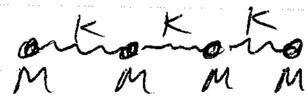
Also at small $\vec{q}$ we expect the spatial orientation of the B.L. to get "averaged over" and so the only directions of $\vec{q}$ and $\perp$ to $\vec{q}$. We then expect the polarization vectors to become as $\vec{q} \to 0$

$\vec{\epsilon}_1(\vec{q}) = \hat{q}$ longitudinal sound mode, speed c_ℓ

$\left.\begin{matrix}\vec{\epsilon}_2(\vec{q})\\ \vec{\epsilon}_3(\vec{q})\end{matrix}\right\} \perp \hat{q}$ transverse sound modes, speed c_{t1}, c_{t2}

Example

1D chain of ions connected by springs



nearest neighbor interaction only
$\frac{1}{2}K(u_i - u_{i+1})^2$

u_i = displacement of ion i

$$M\ddot{u}_i = -K(u_i - u_{i+1}) - K(u_i - u_{i-1})$$

integer n

Assume $u_n(t) = u_0 e^{i(kR_n - \omega t)}$ $\qquad R_n = an$

Substitute in and cancel common factors of $e^{i(kR_n - \omega t)}$

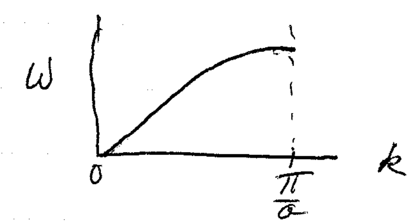
$$-\omega^2 M u_0 = -K(u_0 - u_0 e^{ika}) - K(u_0 - u_0 e^{-ika})$$

$$\Rightarrow -\omega^2 M = -K(1 - e^{ika} + 1 - e^{-ika})$$
$$= -2K(1 - \cos ka)$$

$$\omega = \sqrt{\frac{2K}{M}(1 - \cos ka)}$$

use $\frac{1 - \cos ka}{2} = \sin^2\left(\frac{ka}{2}\right)$

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



at small $ka \ll 1$, $\sin ka \simeq ka$

$$\omega \simeq \sqrt{\frac{K}{M}}\, ka \Rightarrow \text{speed of sound}$$

$$c = \sqrt{\frac{K}{M}}\, a$$

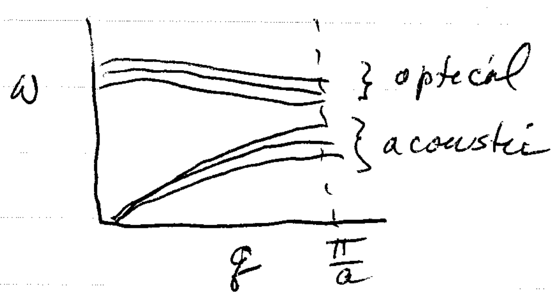
Previous discussion assumed monatomic B.L.
When have BL with basis, the dynamic matrix must acquire an additional index that labels the n atoms in the basis at any BL site R_i

$\Rightarrow$ 3 modes for each atom in primitive cell of BL

$\Rightarrow$ 3n elastic modes

of these, 3 are acoustic modes as before – one longitudinal, two transverse – with $\omega_s \simeq c_s q$ as $q \to 0$.

The $3(n-1)$ remaining modes are "optical" modes where $\omega_s(q) \to$ const as $q \to 0$.



see A+M chpt 22 and problem #1 on Problem Set 6

optical modes correspond to "internal" vibrations of the atoms within a primitive cell of the BL ~~with respect to each other~~
acoustic modes correspond to motions of the primitive cell as a whole.

But: Suppose we consider the conduction electrons as frozen and uniform, and the ion-ion interaction therefore is Coulomb.

In our discussion of plasma oscillations we saw that the only longitudinal mode of oscillation of a Coulomb interacting set of charges is, as $\vec{q}\to 0$, at the plasma frequency. For ions of mass M and density n_{ion}, this would be

$$\Omega_p = \sqrt{\frac{4\pi n_{ion} Q_{ion}^2}{M}} \qquad Q_{ion} = \text{Charge of ion}$$

This does not agree with the expectation above that the frequency of oscillation for a longitudinally polarized elastic vibration should be, $\omega_\ell = c_\ell q$, vanishing as $q\to 0$!

Why? Because if interaction between ions is bare Coulomb, then the sum $\sum_{R_i} (\hat{q}\cdot\vec{R}_i)^2 \overleftrightarrow{\mathbb{D}}(\vec{R}_i)$ does not converge, as we had assumed in the previous discussion!

But we know from experiment and experience that longitudinal (acoustic) sound modes do exist with $\omega_\ell = c_\ell q$ linear dispersion relation! What is the resolution of this paradox?

also called Born-Oppenheimer approx

The answer is screening! We make the <u>adiabatic approximation</u> and assume that conduction electrons move so much faster than ions that they always relax to their minimum energy configuration corresponding to the instantaneous positions of the ions, as the ions move. The electrons will then screen the Coulombic ion-ion interaction and make it short ranged. The sum $\sum_i (\hat{q}\cdot\vec{R}_i)^2 \overleftrightarrow{\mathbb{D}}(R_i)$ now converges and we get the longitudinal elastic modes with $\omega_\ell = c_\ell q$. Moreover we can use this argument to estimate the speed of sound c_ℓ.

The phonon freq for polarization s, wavevector $\vec{q}$ was determined by

$$\omega^2 M \vec{\epsilon}_s = \overleftrightarrow{\mathbb{D}}(\vec{q})\cdot\vec{\epsilon}_s$$

If we let $\overleftrightarrow{\mathbb{D}}^0(q)$ be the dynamical matrix due to bare Coulombic ion-ion interactions, the we expect for the longitudinal mode that $\omega_\ell = \Omega_p$, ie

$$\Omega_p^2 M \vec{\epsilon}_\ell = \overleftrightarrow{\mathbb{D}}^0(q)\cdot\vec{\epsilon}_\ell$$

Now a longitudinal ionic vibration of wave vector $\vec{q}$ sets up a charge density of wave vector $\vec{q}$, which sets up an electric field of wave vector $\vec{q}$. The electrons screen this field by a factor $\frac{1}{\varepsilon(q)}$ where $\varepsilon(q)$ is the electron dielectric function.

Since $\overleftrightarrow{D}(q)$, the dynamical matrix, is $\propto$ to the ion-ion forces (effective ion-ion spring constant in the harmonic approx) we expect that these forces will get screened by the electrons and so the screened dynamical matrix $\overleftrightarrow{D}$ is related to the bare $\overleftrightarrow{D}^0$ by

$$\overleftrightarrow{D}(\vec{q}) = \frac{\overleftrightarrow{D}^0(\vec{q})}{\varepsilon(\vec{q})}$$

Hence we expect that

$$\Omega_p^2 M \vec{\epsilon}_\ell = \overleftrightarrow{D}^0(\vec{q})\cdot\vec{\epsilon}_\ell \Rightarrow \frac{\Omega_p^2}{\varepsilon(q)} M \vec{\epsilon}_\ell = \frac{\overleftrightarrow{D}^0(q)}{\varepsilon(q)}\cdot\vec{\epsilon}_\ell$$

$$\Rightarrow \frac{\Omega_p^2}{\varepsilon(q)} M \vec{\epsilon}_\ell = \overleftrightarrow{D}(q)\cdot\vec{\epsilon}_\ell$$

so the freq of oscillation is now

$$\boxed{\omega_\ell^2(\vec{q}) = \frac{\Omega_p^2}{\varepsilon(q)}}$$

For small $\vec{q}$ we can use the Thomas-Fermi approx

$$\varepsilon(q) \simeq 1 + k_0^2/q^2 \quad \text{where } k_0^2 = 4\pi e^2 g(\varepsilon_F)$$

So

$$\omega_\ell^2(q) = \frac{\Omega_p^2}{1 + k_0^2/q^2} = \frac{\Omega_p^2 q^2}{k_0^2 + q^2} \simeq \frac{\Omega_p^2}{k_0^2} q^2$$

for small $q \ll k_0$

$$\omega_\ell(q) = \left(\frac{\Omega_p}{k_0}\right) q \Rightarrow \text{speed of sound is}$$

$$\boxed{c_\ell = \frac{\Omega_p}{k_0}}$$

$$\Rightarrow c_\ell^2 = \frac{4\pi n_{ion} Q_{ion}^2}{M} \frac{1}{4\pi e^2 g(\varepsilon_F)}$$

if n is conduction electron density and Z the valence number of conduction electrons, then

$$n_{ion} = \frac{n}{Z}, \quad Q_{ion} = Ze$$

$$\boxed{c_\ell^2 = \frac{nZ}{M\, g(\varepsilon_F)}}$$

In the free electron approx, $g(\varepsilon_F) = \frac{3}{2} \frac{n}{\varepsilon_F}$

So

$$c_\ell^2 = \frac{nZ}{M\left(\frac{3}{2}\frac{n}{\varepsilon_F}\right)} = \frac{2Z\varepsilon_F}{3M} = \frac{2Z}{3M} \frac{1}{2} m v_F^2$$

$$c_\ell^2 = \frac{Zm}{3M} v_F^2$$

$$\boxed{c_\ell = \sqrt{\frac{Z}{3}\frac{m}{M}}\, v_F}$$

For ions $\left(\frac{m_{elec}}{M_{proton}} \sim \frac{1}{2000} \right)$ we expect

$$\frac{c_\ell}{v_F} = \sqrt{\frac{Z}{3}\frac{m}{M}} \sim 0.01$$

Our result that $c_\ell \simeq 0.01 v_F$ is consistent with the adiabatic approx that electrons move with speeds (v_F) much greater than the ions (c_ℓ)

The above result is known as the Bohm–Staver relation

It gives results in correct order of magnitude agreement with experiment. For typical metals

$$v_F \sim 10^8 \text{ cm/sec}$$

$$c_\ell \sim 10^6 \text{ cm/sec}$$