Example

1D chain of cons connected by springs

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

$$u_i = \text{displacement of con } i$$

Assume $$u_i(t) = u_0 e^{i(kr_n - wt)}$$

Substitute in and cancel common factors of $$e^{i(kr_n - wt)}$$

$$-\omega^2 M \dot{u}_0 = -K(u_0 - u_0 e^{ika}) - K(u_0 - u_0 e^{-ika})$$

$$\Rightarrow -\omega^2 M u_0 = -K(1-e^{ika} + 1-e^{-ika})$$

$$= -2K(1-\cos ka)$$

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

$$\omega = \sqrt{\frac{K}{M} 2\sin^2(\frac{ka}{2})}$$

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

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

$$c = \sqrt{\frac{K}{M}} a$$
Previous discussion assumed monatomic BL. When there BL with basis, the dynamic matrix must acquire an additional index that labels the \( n \) atoms in the basis at any BL site \( \mathbf{R}_i \).

\[ \Rightarrow \text{3 modes for each atom in primitive cell of BL} \]

\[ \Rightarrow \text{3n elastic modes} \]

Of these, 3 are acoustic modes as before - one longitudinal, two transverse - with

\[ w_s \propto C_s q \quad \text{as } q \to 0. \]

The \( 2(n-1) \) remaining modes are "optical" modes where \( w_s(q) \to \text{const as } q \to 0. \)

\[ \frac{q}{\alpha} \]

optical modes correspond to 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.

"internal"

\[ \text{see A&M Clpt 22} \]

\[ \text{Problem 41 on Problem Set 6} \]
When we treat the elastic vibrations of the solid quantum mechanically, these "normal modes" of elastic vibration, i.e., the independent modes of harmonic oscillation, get quantized just like harmonic oscillators. Each degree of excitation of a given mode of oscillation is called a "phonon".

For example, if the vibration at wave vector \( \vec{q} \) polarized \( \vec{s} \) has energy

\[
\hbar \omega_s (\vec{q}) (n + \frac{1}{2})
\]

We say there are \( n \) phonons of wave vector \( \vec{q} \) polarized \( \vec{s} \).

As with excitations of any harmonic oscillator, phonons behave as bosons, and their number is not conserved (chemical potential \( \mu_{\text{phonon}} = 0 \)).

Electrons can scatter by absorbing or emitting phonons, while conserving energy and crystal momentum, i.e., for absorption

\[
E(\vec{k}_f) = E(\vec{k}_i) + \hbar \omega_s (\vec{q})
\]

\[
\vec{k}_f = \vec{k}_i + \vec{q} + \vec{K}
\]

Initial electron crystal momentum \( \vec{k}_i \)

Initial electron crystal momentum

Final electron crystal momentum

Final electron crystal momentum
But if we consider the conduction electrons as frozen, and the ion-ion interaction to be Coulomb.

In our discussion of plasma oscillations we saw that the only longitudinal mode of oscillation of a Coulomb-interacting set of charges \( q_i \), as \( q \to 0 \), at the plasma frequency, for ions of mass \( M \) and density \( n_{\text{ion}} \), this would be

\[
\Omega_p = \sqrt{\frac{4\pi n_{\text{ion}} q_{\text{ion}}^2}{M}}
\]

\( q_{\text{ion}} = \text{charge of ion} \)

This does not agree with the expectation above that the frequency of oscillation for a longitudinally polarized elastic vibration should be \( \omega = c q \), vanishing as \( q \to 0 \)!

Why? Because if interaction between ions \( i \) have Coulomb, then the sum \( \sum (\delta, R_i) \delta^2 (R_i) \) does not converge as we \( \delta \) had assumed in the previous discussion!

But we know from experiment and experience that longitudinal (acoustic) sound mode do exist with \( \omega = c q \) linear dispersion relation! What is the resolution of this paradox?
The answer is screening! We make the adiabatic approximation 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 $\sum_i (\mathbf{q} \cdot \mathbf{R}_i)^2 \mathbf{D}(\mathbf{R}_i)$ now converges and we get the longitudinal elastic modes with $\omega_0 = \frac{q}{c_s}$. Moreover we can use this argument to estimate the speed of sound $c_s$.

The phonon freq for polarization $\mathbf{E}$, wave vector $\mathbf{q}$ was determined by

$$\omega^2 M \mathbf{E}_0 = \mathbf{D}(\mathbf{q}) \cdot \mathbf{E}_0$$

If we let $\mathbf{D}(\mathbf{q})$ be the dynamical matrix due to bare Coulombic ion-ion interactions, the we expect for the longitudinal mode that $\omega_0 = \frac{q}{c_s}$, i.e.

$$\omega^2 M \mathbf{E}_0 = \mathbf{D}^0(\mathbf{q}) \cdot \mathbf{E}_0$$
Now a longitudinal sonic 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 \( \frac{1}{\varepsilon(\vec{q})} \) where \( \varepsilon(\vec{q}) \) is the electron dielectric function.

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

\[
\bar{D}(\vec{q}) = \frac{\bar{D}^0(\vec{q})}{\varepsilon(\vec{q})}
\]

Hence we expect that

\[
\frac{\Omega_p^2}{M} \bar{\vec{e}}_e = \bar{D}(\vec{q}) \cdot \bar{\vec{e}}_e \quad \Rightarrow \quad \frac{\Omega_p^2}{M} \bar{\vec{e}}_e = \frac{\bar{D}(\vec{q})}{\varepsilon(\vec{q})} \cdot \bar{\vec{e}}_e
\]

\[
\Rightarrow \quad \frac{\Omega_p^2}{\varepsilon(\vec{q})} M \bar{\vec{e}}_e = \bar{D}(\vec{q}) \cdot \bar{\vec{e}}_e
\]

So the freq of oscillation \( \omega \) now

\[
\omega^2(\vec{q}) = \frac{\Omega_p^2}{\varepsilon(\vec{q})}
\]
For small $q$ we can use the Thomas-Fermi approx

$$
E(q) = 1 + \frac{k_0^2}{q^2} \quad \text{where} \quad k_0 = \frac{4\pi e^2 q}{\varepsilon_F}
$$

So

$$
W_e(q) = \frac{\Sigma^2_p}{1 + \frac{k_0^2}{q^2}} \approx \frac{\Sigma^2_p}{k_0^2} \frac{q^2}{k_0^2 + q^2} \approx \frac{\Sigma^2_p}{k_0^2} q^2
$$

for small $q \ll k_0$

$$
W_e(q) = \left(\frac{\Sigma^2_p}{k_0^2}\right) q^2 \quad \Rightarrow \quad \text{speed of sound} \quad c_e = \frac{\Sigma^2_p}{k_0}
$$

$$
\Rightarrow \quad c_e^2 = \frac{4\pi N_{\text{ion}} Q_{\text{ion}}^2}{M} \frac{1}{4\pi e^2 q(\varepsilon_F)}
$$

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

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

$$
C_e^2 = \frac{nZ}{M g(\varepsilon_F)}
$$

in the free electron approx $g(\varepsilon_F) = \frac{3}{2} \frac{M}{e^2}\varepsilon_F$

$$
S_0 \quad C_e^2 = \frac{nZ}{M(\frac{3}{2} \frac{n}{\varepsilon_F})} = \frac{2Z\varepsilon_F}{3M} = \frac{2}{3} \frac{Ze}{M} \frac{1}{2} m v_F^2
$$

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

$$
C_e = \sqrt{\frac{\frac{2}{3} \frac{m}{M}}{}} v_F
$$
For CMS (\(e^+m_{\text{electron}} \sim \frac{1}{2000}\)) we expect

\[
\frac{c_e}{u_F} = \sqrt{\frac{2}{3} \frac{m}{M}} \sim 0.01
\]

Our result that \(c_e \approx 0.01 u_F\) is consistent with the adiabatic approx that electrons move with speeds \(u_F\) much greater than the CMS \(c_e\).

The above result is known as the Bohm–Stoner relation.

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

\[u_F \sim 10^8 \text{ cm/sec}\]

\[c_e \sim 10^6 \text{ cm/sec}\]