Phonons in Band Metal and Insulators

Jinyuan Wu

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The general theory of phonons can be found in this solid state physics note. In this note we just discuss some phenomenon induced by phonons. We have **longitude acoustic (LA) phonons**, **transverse acoustic (TA) phonons**, **longitude optical (LO) phonons**, and **transverse optical (TO) phonons**.

1 Self-energy correction of LA phonons and the Bohm-Staver formula

Phonons are usually derived by considering the displacement of each atom in the lattice as a bosonic field and then doing canonical quantization. This approach is based on effective potentials between atoms, which takes the effective interaction induced by electrons into account. In this section, we consider the case of alkali metals and show how can we derive the spectrum of phonons from just Coulomb interaction.

Ions in a alkali metal can be thought as point charges with charge $+|e|$, and they repulse each other. If we view the electrons in the metal as a uniform jellium, we can just apply (**??**) in this noteto *atoms*, and find that

$$\ddot{Q}_{\boldsymbol{q}} + \Omega_{\boldsymbol{q}}^2 Q_{\boldsymbol{q}} = 0, \quad \Omega_{\boldsymbol{q}}^2 = \frac{4\pi n e^2}{M}, \tag{1}$$

where n is the density of number of electron and M is the mass of an atom. This phonon branch is a longitude mode, since it is related to density fluctuations and therefore we must have $\boldsymbol{\nabla} \cdot \boldsymbol{u} \sim \boldsymbol{k} \cdot \boldsymbol{u} \neq 0$. It is also acoustic, since in a plasmon mode, all particles vibrate synchronously, so we can see a long range density fluctuation. Note that $\Omega_{\boldsymbol{q}}$ has nothing to do with $\boldsymbol{q}$, and we do not see the regular linear dispersion.

Note

Note that since we have a lattice structure, there are collective modes other than long-range density fluctuations, and that is how TA phonons come into existence. For an ideal *fluid*, with just longitude interaction between particles (here the longitude interaction force is the Coulomb force), it is impossible to have transverse modes, but in a crystal it is possible. Suppose that the interaction potential is

$$V(r) = \frac{1}{2} k r^2,$$

and therefore the force is

$$\boldsymbol{F} = k\boldsymbol{r}, \quad \boldsymbol{\nabla} \times \boldsymbol{F} = 0.$$

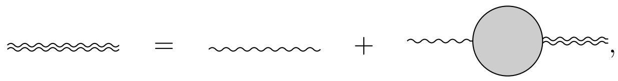
Now the EOM of an atom is

$$m\ddot{\boldsymbol{u}}_{\boldsymbol{i}} = k(\boldsymbol{u}_{\boldsymbol{i}+\hat{\boldsymbol{x}}} + \boldsymbol{u}_{\boldsymbol{i}-\hat{\boldsymbol{x}}} + \boldsymbol{u}_{\boldsymbol{i}+\hat{\boldsymbol{y}}} + \boldsymbol{u}_{\boldsymbol{i}-\hat{\boldsymbol{y}}} + \boldsymbol{u}_{\boldsymbol{i}+\hat{\boldsymbol{z}}} + \boldsymbol{u}_{\boldsymbol{i}-\hat{\boldsymbol{z}}} - 6\boldsymbol{u}_{\boldsymbol{i}}),$$

and we find that the spectrum of phonon modes is independent of the amplitude – and therefore, the polarization – of the modes.

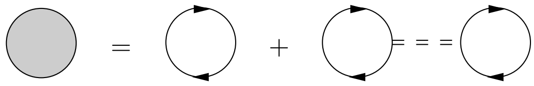
In this section things are a little bit more complicated, since the interaction force is the Coulomb force and not linear to $\boldsymbol{k}$. By invoking the jellium model, what we are doing here is to find the longitude (and therefore concerning density fluctuations) collective modes of the atom lattice with Coulomb repulsion in an easier way. It does not mean that it is the *only* way to have atomic collective modes.

Now we introduce the self-energy correction of phonons.



$$\tag{2}$$

where under the RPA, we have



$$\begin{aligned} &= \mathrm{i}M_{\boldsymbol{q}}\mathrm{i}\Pi^0_q\mathrm{i}M_{-\boldsymbol{q}} + \mathrm{i}M_{\boldsymbol{q}}\mathrm{i}\Pi^0_q(-\mathrm{i}V^{\text{eff}}_q)\mathrm{i}\Pi^0_q\mathrm{i}M_{-\boldsymbol{q}} \\ &= -\mathrm{i}\Pi^0_q|M_{\boldsymbol{q}}|^2 - \mathrm{i}|M_{\boldsymbol{q}}|^2(\Pi^0_q)^2V^{\text{eff}}_q, \end{aligned} \tag{3}$$

where $M_{\boldsymbol{q}}$ is the phonon-electron interaction vertex and Π^0_q is defined in (**??**) in this note. The propagator of the phonon is

$$\mathrm{i}D^0_q = \mathrm{i}\frac{2\Omega_{\boldsymbol{q}}}{(q^0)^2 - \Omega^2_{\boldsymbol{q}} + \mathrm{i}0^+}, \tag{4}$$

and we have

$$\begin{aligned} \mathrm{i}D_q &= \frac{\mathrm{i}D^0_q}{1 - \mathrm{i}D^0_q \times \text{normal self-energy}} \\ &= \frac{\mathrm{i}2\Omega_{\boldsymbol{q}}}{\omega^2 - \Omega^2_{\boldsymbol{q}} + \mathrm{i}0^+ - \mathrm{i}2\Omega_{\boldsymbol{q}} \times (-\mathrm{i}\Pi^0_q|M_{\boldsymbol{q}}|^2 - \mathrm{i}|M_{\boldsymbol{q}}|^2(\Pi^0_q)^2V^{\text{eff}}_q)} \\ &= \mathrm{i}\frac{2\Omega_{\boldsymbol{q}}}{\omega^2 - \Omega^2_{\boldsymbol{q}} - 2\Omega_{\boldsymbol{q}}|M_{\boldsymbol{q}}|^2\Pi^0_q(1 + \Pi^0_qV^{\text{eff}}_q)}. \end{aligned}$$

The corrected pole is no longer $\omega = \pm\Omega_{\boldsymbol{q}}$, but

$$\omega^2 = \Omega^2_{\boldsymbol{q}} + 2\Omega_{\boldsymbol{q}}|M_{\boldsymbol{q}}|^2\Pi^0_q(1 + \Pi^0_qV^{\text{eff}}_q).$$

Since

$$V^{\text{eff}}_q = \frac{V_q}{1 - V_q\Pi^0_q},$$

we have

$$\omega^2 = \Omega^2_{\boldsymbol{q}} + 2\Omega_{\boldsymbol{q}}|M_{\boldsymbol{q}}|^2\frac{\Pi^0_q}{1 - \Pi^0_qV_q}. \tag{5}$$

In this simple case we are able to find $M_{\boldsymbol{q}}$. We have

$$\begin{aligned} V_{\text{e-i}} &= -\sum_\sigma \int \mathrm{d}^3\boldsymbol{r} \sum_{\boldsymbol{i}} \frac{e^2\psi^\dagger_\sigma(\boldsymbol{r})\psi_\sigma(\boldsymbol{r})}{|\boldsymbol{r} - \boldsymbol{R}^0_{\boldsymbol{i}} - \boldsymbol{X}_{\boldsymbol{i}}|} \\ &\approx -\sum_\sigma \int \mathrm{d}^3\boldsymbol{r} \sum_{\boldsymbol{i}} \boldsymbol{X}_{\boldsymbol{i}} \cdot \boldsymbol{\nabla}_{\boldsymbol{X}_i} \frac{e^2\psi^\dagger_\sigma(\boldsymbol{r})\psi_\sigma(\boldsymbol{r})}{|\boldsymbol{r} - \boldsymbol{R}^0_{\boldsymbol{i}} - \boldsymbol{X}_{\boldsymbol{i}}|} \\ &= \sum_\sigma \int \mathrm{d}^3\boldsymbol{r} \sum_{\boldsymbol{i}} \boldsymbol{X}_{\boldsymbol{i}} \cdot \boldsymbol{\nabla}_{\boldsymbol{r}} \frac{e^2\psi^\dagger_\sigma(\boldsymbol{r})\psi_\sigma(\boldsymbol{r})}{|\boldsymbol{r} - \boldsymbol{R}^0_{\boldsymbol{i}}|}, \end{aligned}$$

and by Fourier transformation, we have

$$\begin{aligned} V_{\text{e-i}} &= \sum_\sigma \int \mathrm{d}^3\boldsymbol{r} \sum_{\boldsymbol{i}} \sum_{\boldsymbol{k},\boldsymbol{k}'} \frac{1}{\sqrt{V}}\mathrm{e}^{-\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{r}}c^\dagger_{\boldsymbol{k}\sigma}\frac{1}{\sqrt{V}}\mathrm{e}^{\mathrm{i}\boldsymbol{k}'\cdot\boldsymbol{r}}c_{\boldsymbol{k}'\sigma}\boldsymbol{X}_{\boldsymbol{i}} \cdot \boldsymbol{\nabla}_{\boldsymbol{r}}\frac{e^2}{|\boldsymbol{r} - \boldsymbol{R}^0_{\boldsymbol{i}}|} \\ &= \frac{1}{V}\sum_\sigma \sum_{\boldsymbol{i}} \sum_{\boldsymbol{k},\boldsymbol{k}'} c^\dagger_{\boldsymbol{k}\sigma}c_{\boldsymbol{k}'\sigma} \int \mathrm{d}^3\boldsymbol{r}\, \boldsymbol{X}_{\boldsymbol{i}} \cdot \boldsymbol{\nabla}_{\boldsymbol{r}}\frac{e^2}{|\boldsymbol{r} - \boldsymbol{R}^0_{\boldsymbol{i}}|}\mathrm{e}^{\mathrm{i}(\boldsymbol{k}'-\boldsymbol{k})\cdot\boldsymbol{r}} \\ &= -\frac{1}{V}\sum_\sigma \sum_{\boldsymbol{i}} \sum_{\boldsymbol{k},\boldsymbol{k}'} c^\dagger_{\boldsymbol{k}\sigma}c_{\boldsymbol{k}'\sigma} \int \mathrm{d}^3\boldsymbol{r}\, \boldsymbol{X}_{\boldsymbol{i}} \cdot \frac{e^2}{|\boldsymbol{r} - \boldsymbol{R}^0_{\boldsymbol{i}}|}\boldsymbol{\nabla}_{\boldsymbol{r}}\mathrm{e}^{\mathrm{i}(\boldsymbol{k}'-\boldsymbol{k})\cdot(\boldsymbol{r}-\boldsymbol{R}^0_i)}\mathrm{e}^{\mathrm{i}(\boldsymbol{k}'-\boldsymbol{k})\cdot\boldsymbol{R}^0_i} \\ &= -\frac{1}{V}\sum_\sigma \sum_{\boldsymbol{i}} \sum_{\boldsymbol{k},\boldsymbol{k}'} c^\dagger_{\boldsymbol{k}\sigma}c_{\boldsymbol{k}'\sigma}\boldsymbol{X}_{\boldsymbol{i}} \cdot \mathrm{i}(\boldsymbol{k}' - \boldsymbol{k})\mathrm{e}^{\mathrm{i}(\boldsymbol{k}'-\boldsymbol{k})\cdot\boldsymbol{R}^0_i} \int \mathrm{d}^3\boldsymbol{r}\, \frac{e^2}{|\boldsymbol{r} - \boldsymbol{R}^0_{\boldsymbol{i}}|}\mathrm{e}^{\mathrm{i}(\boldsymbol{k}'-\boldsymbol{k})\cdot(\boldsymbol{r}-\boldsymbol{R}^0_i)} \\ &= \frac{1}{V}\sum_\sigma \sum_{\boldsymbol{i}} \sum_{\boldsymbol{k},\boldsymbol{k}'} c^\dagger_{\boldsymbol{k}\sigma}c_{\boldsymbol{k}'\sigma}\boldsymbol{X}_{\boldsymbol{i}} \cdot \mathrm{i}(\boldsymbol{k} - \boldsymbol{k}')\mathrm{e}^{\mathrm{i}(\boldsymbol{k}'-\boldsymbol{k})\cdot\boldsymbol{R}^0_i}\frac{4\pi e^2}{|\boldsymbol{k} - \boldsymbol{k}'|}. \end{aligned}$$

Now we use the expansion (3.11) in this solid state physics note, and we have

$$\begin{aligned}
V_{\text{e-i}} &= \frac{1}{V}\sum_{\sigma}\sum_{\boldsymbol{i}}\sum_{\boldsymbol{k},\boldsymbol{k}'}\sum_{\boldsymbol{q},\lambda} c^\dagger_{\boldsymbol{k}\sigma}c_{\boldsymbol{k}'\sigma}\frac{1}{\sqrt{2MN\Omega_{\boldsymbol{q}\lambda}}}(\boldsymbol{\lambda}b_{\boldsymbol{q}\lambda}\mathrm{e}^{\mathrm{i}\boldsymbol{q}\cdot\boldsymbol{R}_i^0}+\text{h.c.})\cdot\mathrm{i}(\boldsymbol{k}-\boldsymbol{k}')\mathrm{e}^{\mathrm{i}(\boldsymbol{k}'-\boldsymbol{k})\cdot\boldsymbol{R}_i^0}\frac{4\pi e^2}{|\boldsymbol{k}-\boldsymbol{k}'|} \\
&= \frac{N}{V}\sum_{\sigma}\sum_{\boldsymbol{k},\boldsymbol{k}'}\sum_{\boldsymbol{q},\lambda} c^\dagger_{\boldsymbol{k}\sigma}c_{\boldsymbol{k}'\sigma}\frac{1}{\sqrt{2MN\Omega_{\boldsymbol{q}\lambda}}}\mathrm{i}(\boldsymbol{k}-\boldsymbol{k}')\cdot\boldsymbol{\lambda}(b_{\boldsymbol{q}\lambda}\delta_{\boldsymbol{q}+\boldsymbol{k}',\boldsymbol{k}}+b^\dagger_{\boldsymbol{q}\lambda}\delta_{-\boldsymbol{q}+\boldsymbol{k}',\boldsymbol{k}}))\frac{4\pi e^2}{|\boldsymbol{k}-\boldsymbol{k}'|} \\
&= \frac{1}{V}\sum_{\sigma}\sum_{\boldsymbol{k},\boldsymbol{k}'}\sum_{\boldsymbol{q},\lambda} c^\dagger_{\boldsymbol{k}\sigma}c_{\boldsymbol{k}'\sigma}\sqrt{\frac{N}{2M\Omega_{\boldsymbol{q}\lambda}}}(\mathrm{i}\boldsymbol{q}\cdot\boldsymbol{\lambda}b_{\boldsymbol{q}\lambda}\delta_{\boldsymbol{q}+\boldsymbol{k}',\boldsymbol{k}}-\mathrm{i}\boldsymbol{q}\cdot\boldsymbol{\lambda}b^\dagger_{\boldsymbol{q}\lambda}\delta_{-\boldsymbol{q}+\boldsymbol{k}',\boldsymbol{k}}))\frac{4\pi e^2}{\boldsymbol{q}^2}.
\end{aligned}$$

Note that this interaction channel only involves longitude phonons, which is expected, since it comes from Coulomb interaction. From symmetry analysis, we have

$$V_{\text{e-i}} = \frac{1}{V}\sum_{\boldsymbol{k},\boldsymbol{q},\sigma,\lambda} M_{\boldsymbol{q}}a^\dagger_{\boldsymbol{k}\sigma}a_{\boldsymbol{k}-\boldsymbol{q},\sigma}b_{\boldsymbol{q}\lambda}+\text{h.c.},$$

and therefore we have

$$M_{\boldsymbol{q}} = \mathrm{i}\boldsymbol{q}\cdot\boldsymbol{\lambda}\sqrt{\frac{N}{2M\Omega_{\boldsymbol{q}\lambda}}}\frac{4\pi e^2}{\boldsymbol{q}^2} = \frac{\mathrm{i}4\pi e^2}{|\boldsymbol{q}|}\sqrt{\frac{N}{2M\Omega_{\boldsymbol{q}\lambda}}}. \tag{6}$$

Now we can evaluate (5) explicitly. The renormalized pole of the phonon propagator is

$$\begin{aligned}
\omega^2 &= \Omega_{\boldsymbol{q}}^2 + 2\Omega_{\boldsymbol{q}}|M_{\boldsymbol{q}}|^2\frac{\Pi_q^0}{1-\Pi_q^0V_q} \\
&= \Omega_{\boldsymbol{q}}^2 + 2\Omega_{\boldsymbol{q}}\frac{4\pi e^2N}{2M\Omega_{\boldsymbol{q}\lambda}}\frac{4\pi e^2}{\boldsymbol{q}^2}\frac{\Pi_q^0}{1-\Pi_q^0V_q} \\
&= \Omega_{\boldsymbol{q}}^2 + \Omega_{\boldsymbol{q}}^2V_q\frac{\Pi_q^0}{1-\Pi_q^0V_q} = \frac{\Omega_{\boldsymbol{q}}^2}{1-\Pi_q^0V_q},
\end{aligned}$$

and therefore we get the renormalized LA phonon spectrum:

$$\omega_{\boldsymbol{q}}^2 = \frac{\Omega_{\boldsymbol{q}}^2}{\epsilon(\omega_{\boldsymbol{q}},\boldsymbol{q})}, \tag{7}$$

or in the language of atom motion,

$$\ddot{Q}_{\boldsymbol{q}} + \frac{\Omega_{\boldsymbol{q}}^2}{\epsilon(\boldsymbol{q})}Q_{\boldsymbol{q}} = 0. \tag{8}$$

Since usually LA phonon frequencies are much lower than the characteristic frequency of electrons, we can take the Thomas-Fermi approximation (see (14) in this note, and here $\epsilon_0 = 1/4\pi$)

$$\epsilon(\omega=0,\boldsymbol{q}) = 1+\frac{k_{\text{TF}}^2}{\boldsymbol{q}^2}, \quad k_{\text{TF}}^2 = \frac{6\pi e^2 n}{\epsilon_{\text{F}}}, \tag{9}$$

and the dispersion relation of the LA phonon is

$$\omega^2 \approx \frac{\Omega_{\boldsymbol{q}}^2}{1+\frac{k_{\text{TF}}^2}{\boldsymbol{q}^2}} = \frac{\Omega_{\boldsymbol{q}}^2}{\boldsymbol{q}^2+k_{\text{TF}}^2}\boldsymbol{q}^2,$$

and in the long wave length approximation, i.e. $\boldsymbol{q}\to 0$, we have

$$\omega_{\boldsymbol{q}}^2 \approx \frac{\Omega_{\boldsymbol{q}}^2}{k_{\text{TF}}^2}\boldsymbol{q}^2 = \frac{2\epsilon_{\text{F}}}{3M}\boldsymbol{q}^2 = \frac{m}{3M}v_{\text{F}}^2\boldsymbol{q}^2, \quad \omega_{\boldsymbol{q}} = \sqrt{\frac{m}{3M}}v_{\text{F}}|\boldsymbol{q}|. \tag{10}$$

This is called the **Bohm-Staver formula** of sound speed.

The above derivation can be simplified if we notice the fact that what electrons do is to screen the Coulomb interaction between ions in the metal, which is just Coulomb repulsion exactly the same as the mutual interaction between electrons, and the screening is therefore the same as (**??**) and (**??**) in this note. With this insight, since $\Omega_{\boldsymbol{q}}^2$ is just proportion to the Coulomb repulsion force, we can directly write down (8).

Zhengzhong Li Sec. 5.3