Phonons, and its interaction with electrons.

Topic: ionic vibrations.

- Phonons in jellium model.

  ρ_{ion}^{0} : particle density of ion jellium.

  ρ_{el} : fixed (neglected)

  consider small harmonic deviation $\delta\rho_{ion}(\vec{r},t) = \delta\rho_{ion}(\vec{r})e^{-i\Omega t}$

  then:

  $$\rho_{ion}(\vec{r},t) = \rho_{ion}^{0} + \delta\rho_{ion}(\vec{r})e^{-i\Omega t}$$

- particle density $\delta\rho_{ion}$ $\leftrightarrow$ charge density $\underline{Ze}\,\delta\rho_{ion}$

  There exists electric field $\vec{E}$.

  $$\nabla\cdot\vec{E} = \frac{Ze}{\varepsilon_0}\delta\rho_{ion}$$

  $\vec{f} = Ze\rho_{ion}\vec{E}$, force density then $\nabla\cdot\vec{f} = \frac{Z^2 e^2 \rho^0_{ion}}{\varepsilon_0}\,\delta\rho_{ion}$ $\quad(\rho^0_{ion} \approx \rho_{ion})$

Continuity equation

$$\frac{\partial \rho_{ion}}{\partial t} + \nabla\cdot(\rho_{ion}\vec{v}) = 0 \approx \frac{\partial\,\delta\rho_{ion}}{\partial t} + \nabla\cdot(\rho^0_{ion}\vec{v}) = 0$$

Newton's second law $\quad \vec{f} = M\rho_{ion}\partial_t v$

$$\Rightarrow \frac{\partial^2}{\partial t^2}\delta\rho_{ion} + \frac{1}{M}\nabla\cdot\vec{f} = 0.$$

$$\Rightarrow \Omega^2\delta\rho_{ion} = \frac{Z^2 e^2 \rho^0_{ion}}{\varepsilon_0 M}\delta\rho_{ion} \Rightarrow \Omega = \sqrt{\frac{Z^2 e^2 \rho^0_{ion}}{\varepsilon_0}} = \sqrt{\frac{Z^2 e^2 \rho_{ion}}{\varepsilon_0}}.$$

Ω: Ionic plasma frequency, originated from long-range Coulomb potential, ionic oscillation in jellium all have frequency Ω.

Second quantization $\quad H_{ph} = \sum_{\vec{q}} \hbar\Omega\,(b_q^\dagger b_q + \frac{1}{2})$

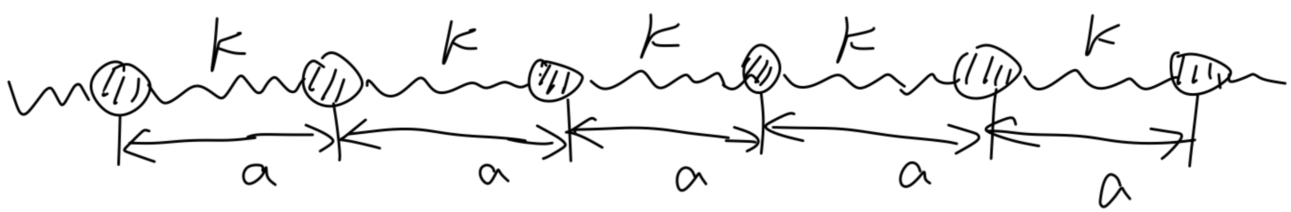
optical/Einstein photons, Einstein 1906.

Adiabatic approximation: electrons move very fast with ions, maintaining charge neutral, lowering Ω.

optical phonons $\rightarrow$ acoustic phonons.

- Lattice vibrations (1D):
  - N ions, mass M, interacting with its 2 neighbors through a spring
  - equilibrium position of jth ion is R_j^0, $a = R_j^0 - R_{j-1}^0$ is constant.

$L = Na$



$$H_{ph} = \sum_{j=1}^{N} \frac{1}{2M} P_j^2 + \frac{1}{2} k (u_j - u_{j-1})^2 .$$

P_j: ion momentum

u_j: displacement.

$$[P_{j_1}, u_{j_2}] = \frac{\hbar}{i} \delta_{j_1 j_2}$$

- Periodic boundary condition : $u_{N+1} = u_1$

FBZ: $\left[-\frac{\pi}{a}+\Delta k,\ -\frac{\pi}{a}+2\Delta k,\ \ldots -\frac{\pi}{a}+N\Delta k\right]$, $\Delta k = \frac{2\pi}{L} = \frac{2\pi}{Na}$

Fourier transform / inverse ... ...

$$P_j = \frac{1}{\sqrt{N}} \sum_{k\in FBZ} P_k e^{ikR_j^0}, \quad u_j = \frac{1}{\sqrt{N}} \sum_{k\in FBZ} u_k e^{ikR_j^0}$$

$$P_k = \frac{1}{\sqrt{N}} \sum_{j\in FBZ} P_j e^{-ikR_j^0}, \quad u_k = \frac{1}{\sqrt{N}} \sum_{j=1}^{N} u_j e^{-ikR_j^0}$$

$$P_k^\dagger = P_{-k}$$

$$u_k^\dagger = u_{-k}$$

$$\delta_{R_j^0,0} = \frac{1}{N}\sum_k e^{ikR_j^0}, \quad \delta_{k,0} = \frac{1}{N}\sum_j e^{-ikR_j^0}$$

Then;
$$\sum_{j=1}^{N} \frac{1}{2M} P_j^2 = \frac{1}{2M} \sum_{k_1,k_2\in FBZ} P_{k_1} P_{k_2} \frac{\sum_j e^{i(k_1+k_2)R_j^0}}{N}$$

$$= \frac{1}{2M} \sum_{k_1,k_2\in FBZ} P_{k_1} P_{k_2}\, \delta_{k_1+k_2,0} = \frac{1}{2M}\sum_k P_k P_{-k}.$$

$$\frac{K}{2}\sum_{j=1}^{N} (u_j-u_{j-1})^2 = K\sum_{j=1}^{N} u_j^2 - K\sum_{j=1}^{N} u_{j-1}u_j. \qquad K\sum_{j=1}^{N} u_j^2 = K\sum_k u_k u_{-k}$$

$$K\sum_{j=1}^{N} u_{j-1}u_j = K\sum_{k_1,k_2} u_{k_1}u_{k_2} \sum_j e^{ik_1R_{j-1}^0 + k_2R_j^0}/N$$

$$= K\sum_{k_1,k_2} u_{k_1}u_{k_2} e^{-ik_1a} \sum_j e^{i(k_1+k_2)R_{j}^0}/N = K\sum_k u_k u_{-k}\, e^{-ika}$$

$$= K\sum_k u_k u_{-k} \cos ka$$

then

$$\frac{K}{2}\sum_{j=1}^{N}(u_j-u_{j-1})^2 = K(1-\cos ka)\sum_k u_k u_{-k}$$
$$= 2K\sin^2\frac{ka}{2}\sum_k u_k u_{-k}$$
$$= \sum_k \frac{M}{2}\omega_k^2 u_k u_{-k} \qquad \omega_k = 2\sqrt{\frac{K}{m}}\left|\sin\frac{ka}{2}\right|$$

therefore:

$$H = \sum_k\left(\frac{1}{2M}p_k p_{-k} + \frac{M}{2}\omega_k^2 u_k u_{-k}\right), \quad \omega_k = 2\sqrt{\frac{K}{m}}\left|\sin\frac{ka}{2}\right|$$

p_k, u_k are not Hermitian, $p_k^\dagger = p_{-k}$, $u_k^\dagger = u_{-k}$

Define:

annihilation $b_k = \frac{1}{\sqrt{2}}\left(\frac{u_k}{l_k} + i\frac{p_k}{\hbar/l_k}\right)$ $\qquad u_k = l_k\frac{1}{\sqrt{2}}(b_{-k}^\dagger + b_k)$

creation $b_k^\dagger = \frac{1}{\sqrt{2}}\left(\frac{u_{-k}}{l_k} - i\frac{p_{-k}}{\hbar/l_k}\right)$ $\qquad p_k = \frac{\hbar}{l_k}\frac{1}{\sqrt{2}}(b_{-k}^\dagger - b_k)$

$$H = \sum_k \frac{1}{2M}p_k p_{-k} + \frac{M}{2}\omega_k^2 u_k u_{-k}$$
$$= \sum_k \frac{1}{2M}\frac{\hbar^2}{l_k^2}\cdot\frac{-1}{2}\cdot(b_k^\dagger - b_k)^2 + \frac{M}{2}\cdot\omega_k^2\cdot\frac{l_k^2}{2}(b_k^\dagger + b_k)^2.$$
$$= \sum_k\left(\frac{M\omega_k^2}{4}l_k^2 - \frac{\hbar^2}{4Ml_k^2}\right)\left((b_k^\dagger)^2 - b_k^2\right) + \left(\frac{M\omega_k^2 l_k^2}{4} + \frac{\hbar^2}{4Ml_k^2}\right)(b_k^\dagger b_k + b_k b_k^\dagger)$$

let $\frac{M\omega_k^2 l_k^2}{4} = \frac{\hbar^2}{4M l_k^2} \Rightarrow l_k^4 = \frac{4\hbar^2}{4M^2\omega_k^2} \Rightarrow l_k = \sqrt{\frac{\hbar}{M\omega_k}}$

then $H_{ph} = \sum_k \frac{\hbar\omega_k}{2}\left(b_k^\dagger b_k + b_k b_k^\dagger\right)$

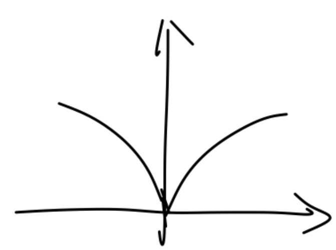
$$= \sum_k \hbar\omega_k\left(b_k^\dagger b_k + \frac{1}{2}\right)$$

phonons

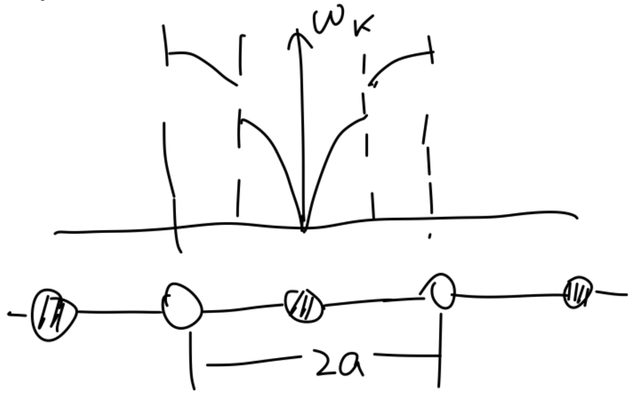
$k \to 0$: $\omega_k = \sqrt{\frac{K}{M}}\, ak$ acoustic phonon

$v_s = \sqrt{\frac{K}{M}}\, a$, sound speed

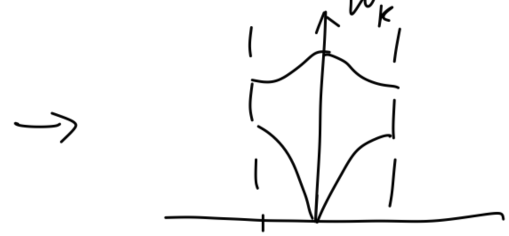
$\omega_k = 2\sqrt{\frac{K}{M}}\left|\sin\left(\frac{ak}{2}\right)\right|$. $k \in FBZ$. $k = -\frac{\pi}{a} + \Delta k, \dots, \frac{\pi}{a}$



For two ions in a unit cell:



the translational invariance is broken.



lower branch : acoustic phonon

higher branch : optical phonon

same wavelength

p ions: 1 acoustic branch

$(p-1)$ optical branches

$$H_{ph} = \sum_{k\lambda} \hbar \omega_{k\lambda} \left(b_{k\lambda}^{\dagger} b_{k\lambda} + \frac{1}{2} \right)$$

λ: index

$$\left[b_{k_1,\lambda_1},\ b_{k_2,\lambda_2}^{\dagger} \right] = \delta_{k_1,k_2} \delta_{\lambda_1,\lambda_2}$$

- Generalizations to 3D:

Ionic equilibrium position $\vec{R}_j^o$, displacement $\vec{u}(\vec{R}_j^o) = (u_1(\vec{R}_j^o), u_2(\vec{R}_j^o), u_3(\vec{R}_j^o))$

$$U(\vec{u}(\vec{R}_1^o), \cdots, u(\vec{R}_N^o))$$

$$U \approx U_0 + \frac{1}{2} \sum_{\vec{R}_i^o, \vec{R}_j^o} \sum_{\alpha,\beta} u_\alpha(\vec{R}_i^o) \frac{\partial^2 U}{\partial u_\alpha(\vec{R}_i^o)\, \partial u_\beta(\vec{R}_j^o)} u_\beta(\vec{R}_j^o)$$

Define $D_{\alpha\beta}(\vec{R}_i^o - \vec{R}_j^o) = \left.\dfrac{\partial^2 U}{\partial u_\alpha(\vec{R}_i^o)\, \partial u_\beta(\vec{R}_j^o)}\right|_{\vec{u}=0,}$

$$D(\vec{R}^o) = (D(\vec{R}^o))^T, \quad D(\vec{R}^o) = D(-\vec{R}^o)$$

$$\sum_{\vec{R}^o} D(\vec{R}^o) = 0.$$

$$D_{\alpha\beta}(\vec{k}) = \sum_{\vec{R}} D_{\alpha\beta}(\vec{R})\, e^{-i\vec{k}\cdot\vec{R}}$$

$$D(\vec{k}) = \sum_{\vec{R}^o} D(\vec{R}^o)\, e^{-ik\cdot\vec{R}^o} = \frac{1}{2}\sum_{\vec{R}^o} D(\vec{R}^o) e^{-i\vec{k}\cdot\vec{R}^o} + D(-\vec{R}^o) e^{+i\vec{k}\vec{R}_o}$$

$$= \frac{1}{2}\sum_{\vec{R}^o} D(\vec{R}^o)\left(e^{i\vec{k}\cdot\vec{R}_o} + e^{-i\vec{k}\cdot\vec{R}_o} - 2\right)$$

$$= -2\sum_{\vec{R}^o} D(\vec{R}^o) \sin^2\left(\tfrac{1}{2}\vec{k}\cdot\vec{R}_o\right)$$

Therefore $D(\vec{k})$ is also real and symmetric, then diagonalizable.

Classical equations of motion:

$$M\ddot{u}_\alpha(\vec{R}_i^o) = \frac{\partial U}{\partial u_\alpha(\vec{R}_i^o)} = \sum_{\vec{R}_j^o} D(\vec{R}_j^o - \vec{R}_i^o)\, u(\vec{R}_j^o)$$

Simple harmonic solution:

$$\vec{u}(\vec{R}^0, t) \propto \vec{\epsilon} \cdot e^{i(\vec{k}\cdot\vec{R}^0 - \omega t)} \Rightarrow M\omega^2 \vec{\epsilon} = D(\vec{k})\vec{\epsilon}$$

eigenvalue problem. $D(\vec{k})\,\epsilon_{\vec{k}\lambda} = K_{\vec{k}\lambda}\,\epsilon_{\vec{k}\lambda}$, $\epsilon_{\vec{k}\lambda}\cdot\epsilon_{\vec{k}\lambda'} = \delta_{\lambda\lambda'}$, $\lambda = 1, 2, 3, \cdots$

$$\Rightarrow u_{\vec{k}\lambda}(\vec{R}^0, t) = \epsilon_{\vec{k}\lambda}\, e^{i(\vec{k}\cdot\vec{R}^0 - \omega_{\vec{k}\lambda} t)}, \quad \omega_{\vec{k}\lambda} = \sqrt{\frac{K_{\vec{k}\lambda}}{M}}.$$

Then define $\vec{u}_{k\lambda} = l_{k\lambda}\frac{1}{\sqrt{2}}(b^\dagger_{k\lambda} + b_{\vec{k}\lambda})\epsilon_{\vec{k}\lambda}$, $l_{\vec{k}\lambda} = \sqrt{\frac{\hbar}{M\omega_{\vec{k}\lambda}}}$

$$H_{ph} = \sum_{\vec{k},\lambda} \hbar\omega_{\vec{k}\lambda}\left(b^\dagger_{\vec{k}\lambda} b_{k\lambda} + \frac{1}{2}\right) \qquad [b_{\vec{k}\lambda}, b^\dagger_{\vec{k}'\lambda'}] = \delta_{\vec{k}\vec{k}'}\,\delta_{\lambda\lambda'}$$

For 3p modes: 3 acoustic

3(p-1) optical.

· Electron-phonon interaction

$$V_{el-Ion} = \int dr\,(-e)\,\rho_{el}(\vec{r}) \sum_{j=1}^{N} V_{ion}(\vec{r} - \vec{R}_j)$$

$$= \underbrace{\int dr\,(-e)\,\rho_{el}(\vec{r}) \sum_{j=1}^{N} V_{ion}(\vec{r} - \vec{R}_j^0)}_{\text{part of } H_{Bloch}} - \underbrace{\int dr\,(-e)\,\rho_{el}(\vec{r}) \sum_{j=1}^{N} \nabla_{\vec{r}} V_{ion}(\vec{r} - \vec{R}_j^0)\cdot\vec{u}_j}_{\text{electron-phonon.}}$$

$$V_{el\text{-}phonon} = \int d\vec{r}\, \rho_{el}(\vec{r}) \left(\sum_j e\vec{u}_j \cdot \nabla_r V_{ion}(\vec{r}-\vec{R}_j^0) \right)$$

Define $V_{ion}(\vec{r}) = \frac{1}{V} \sum_{\vec{p}} V_p e^{i\vec{p}\cdot\vec{r}}$, $\vec{p} = \vec{q}+\vec{G}$, $q \in FBZ$, $\vec{G} \in RL$.

$$\nabla_r V_{ion}(\vec{r}-\vec{R}_j^0) = \frac{1}{V} \sum_{q\in FBZ} \sum_{G\in RL} i(q+G) V_{q+G}\, e^{i(\vec{q}+\vec{G})(\vec{r}-\vec{R}_j^0)}$$

$$\vec{u}_j = \frac{1}{\sqrt{N}} \sum_{k\in FBZ} \sum_\lambda \frac{l_{\vec{k}\lambda}}{\sqrt{2}} \left(b_{\vec{k}\lambda} + b^\dagger_{-\vec{k}\lambda} \right) \epsilon_{\vec{k}\lambda}\, e^{i\vec{k}\cdot\vec{R}_j^0}$$

$$\Rightarrow \sum_j e\vec{u}_j \cdot \nabla_r V_{ion}(\vec{r}-\vec{R}_j^0) = \frac{1}{V}\frac{1}{\sqrt{N}} \sum_{q,G,\vec{k}} \sum_\lambda \frac{l_{\vec{k}\lambda}}{\sqrt{2}} (b_{\vec{k}\lambda} + b^\dagger_{-\vec{k}\lambda})\, i(q+G) V_{q+G}\, \epsilon_{\vec{k}\lambda}\, e^{i(\vec{q}+\vec{G})\cdot r} \underbrace{\sum_j e^{i(k-q-G)R_j^0}}_{N\delta_{k,q}}$$

$$= \frac{\sqrt{N}}{V} \sum_{\substack{q\in FBZ\\ G\in RL}} \frac{l_{\vec{q}\lambda}}{\sqrt{2}} (b_{\vec{q}\lambda} + b^\dagger_{-\vec{q}\lambda})\, i(q+G) V_{q+G}\, \epsilon_{\vec{q}\lambda}\, e^{i(\vec{q}+\vec{G})\cdot r}$$

$$= \frac{1}{V} \sum_{\substack{q\in FBZ\\ G\in RL}} g_{\vec{q},\vec{G},\lambda} (b_{\vec{q},\lambda} + b^\dagger_{-\vec{q},\lambda})\, e^{i(\vec{q}+\vec{G})\cdot\vec{r}}$$

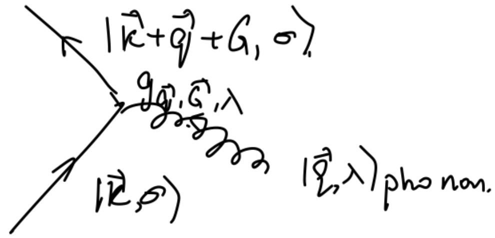
with $\rho_{el}(\vec{r}) = \frac{1}{V} \sum_{k,\vec{p},\sigma} e^{-i\vec{p}\cdot\vec{r}} c^\dagger_{\vec{k}+\vec{p}\sigma} c_{\vec{k}\sigma}$.

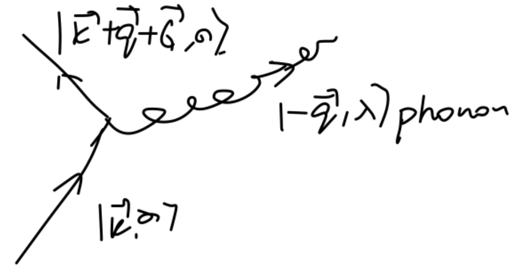
$$V_{el\text{-}ph} = \frac{1}{V} \sum_{\vec{k}\sigma} \sum_{\vec{q}\lambda} \sum_{\vec{G}} g_{\vec{q},\vec{G},\lambda}\, c^\dagger_{\vec{k}+\vec{q}+\vec{G},\sigma} c_{\vec{k}\sigma} (b_{\vec{q},\lambda} + b^\dagger_{-\vec{q},\lambda})$$

Physical intepretation: $|\vec{k},\sigma\rangle_{electron} \xrightarrow[b^\dagger_{-q,\lambda}]{b_{q,\lambda}} |\vec{k}+\vec{q}+\vec{G},\sigma\rangle$

lattice freedom

Graphical:





normal processes: neglect when $G \neq 0$.

istropical: $\epsilon_{\vec{q},\lambda} \cdot \vec{q}$ is only nonzero for longitudinally polarized phonons

$$V^{IN}_{el-ph} = \frac{1}{V} \sum_{\vec{k},\sigma} \sum_{q,\lambda_l} g_{\vec{q},\lambda_l} C^{\dagger}_{\vec{k}+\vec{q},\sigma} C_{\vec{k}\sigma} \left(b_{\vec{q},\lambda_l} + b^{\dagger}_{-\vec{q},\lambda_l} \right)$$

Only considering acoustic phonons.

$$V^{INA}_{el-ph} = \frac{1}{V} \sum_{\vec{k},\sigma} \sum_{\vec{q}} g_{\vec{q}} C^{\dagger}_{\vec{k}+\vec{q}} C_{\vec{k}\sigma} \left(b_{q} + b^{\dagger}_{-q} \right)$$