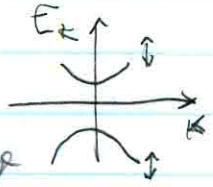
Lecture #19: Electron-phonon interaction



Lattice vibrations can affect electron energy states: They modulate the volume of the unit cell; recall $\varepsilon_F \propto n^{2/3} \propto \frac{1}{V_{cell}^{2/3}}$. Also, lattice vibrations can change the symmetry of the crystal, coupling electrons at different bands. This can lead to interband transitions. Moreover, lattice vibrations can produce internal electric fields that couple to the electrons.

Three different kinds of electron phonon interactions: 1) Deformation potential, 2) Piezoelectric, 3) Fröhlich. At high temperatures one of these will dominate the thermal and electric conductivity.

1) Deformation potential interaction

Under hydrostatic strain the electron energy increases; assuming this is a constant D leads to

$$\mathcal{H}^{DP}_{e\text{-}ph} = D\,\mathrm{Tr}\left(\overleftrightarrow{\varepsilon}\right) = D\,\vec{\nabla}\cdot\vec{u} \qquad \text{since} \quad \varepsilon_{ij} = \frac{1}{2}\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right).$$

Use

$$\vec{u}(\vec{r}) = \sum_{\vec{k},\lambda} \hat{\eta}_{\vec{k},\lambda} \sqrt{\frac{\hbar}{2\rho V \omega_{k\lambda}}} \left(\hat{a}_{\vec{k}\lambda} e^{i\vec{k}\cdot\vec{r}} + a^{\dagger}_{\vec{k}\lambda} e^{-i\vec{k}\cdot\vec{r}}\right)$$

$$\Rightarrow \mathcal{H}^{DP}_{e\text{-}ph} = \sum_{\vec{k},\lambda} D\left(\hat{\eta}_{\vec{k},\lambda}\cdot\vec{k}\right) \sqrt{\frac{\hbar}{2\rho V \omega_{k\lambda}}}\, i\left(\hat{a}_{k\lambda} e^{i\vec{k}\cdot\vec{r}} - a^{\dagger}_{k\lambda} e^{-i\vec{k}\cdot\vec{r}}\right)$$

- $\left(\hat{\eta}_{\vec{k},\lambda}\cdot\vec{k}\right)$: only phonons with longitudinal components contribute!
- $a^{\dagger}_{k\lambda}$: phonon creation
- $e^{-i\vec{k}\cdot\vec{r}}$: electron coordinate

For isotropic material, only $\lambda = L$.

$\mathcal{H}^{DP}_{e\text{-}ph}$ in the 1st quantization form can be used in simple calculations.

Find $\mathcal{H}^{DP}_{e\text{-ph}}$ in 2nd quantization:

$$\mathcal{H}^{DP}_{e\text{-ph}} = \int d^3r\, \hat{\Psi}^\dagger(\vec{r})\, \mathcal{H}^{DP}_{e\text{-ph}}(\vec{r})\, \hat{\Psi}(\vec{r})$$

where

$$\hat{\Psi}(\vec{r}) = \sum_m \sum_{\vec{k}_1} \frac{e^{i\vec{k}_1\cdot\vec{r}}}{\sqrt{V}}\, u_{m\vec{k}_1}(\vec{r})\, \hat{c}_{mk_1}$$

(m: Band index)

$$\Rightarrow \mathcal{H}^{DP}_{e\text{-ph}} = \sum_{\vec{K}} D(\underbrace{\hat{\eta}_{Ki}\vec{K}}_{K}) \sqrt{\frac{\hbar}{2\rho V \omega_{KL}}} \Big\{ i\hat{a}_{\vec{K}L} \int d^3r\, e^{i\vec{K}\cdot\vec{r}} \Big(\sum_{n_2,\vec{k}_2} \frac{e^{-i\vec{k}_2\cdot\vec{r}}}{\sqrt{V}}\, u_{n_2\vec{k}_2}(\vec{r})\, \hat{c}^\dagger_{n_2k_2} \Big) \Big(\sum_{n_1,\vec{k}_1} \frac{e^{i\vec{k}_1\cdot\vec{r}}}{\sqrt{V}}\, u_{n_1\vec{k}_1}(\vec{r})\, \hat{c}_{n_1k_1} \Big)$$

$$+ \text{h.c.} \Big\}$$

$$= \sum_{\vec{K}} DK \sqrt{\frac{\hbar}{2\rho V \omega_{KL}}} \Big\{ \sum_{n_1,n_2} \sum_{\vec{k}_1,\vec{k}_2} \frac{1}{V} \int d^3r\, e^{i(\vec{k}_1-\vec{k}_2+\vec{K})\cdot\vec{r}}\, u_{n_2\vec{k}_2}(\vec{r})\, u_{n_1\vec{k}_1}(\vec{r}) \Big[i\hat{a}_K\, c^\dagger_{n_2k_2} c_{n_1k_1} \Big]$$

$$+ \frac{1}{V} \int d^3r\, e^{i(\vec{k}_1-\vec{k}_2-\vec{K})\cdot\vec{r}}\, u_{n_2k_2}(\vec{r})\, u_{n_1k_1}(\vec{r}) \Big[i\hat{a}^\dagger_K\, c^\dagger_{n_2k_2} c_{n_1k_1} \Big]$$

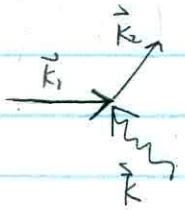
Assuming $K(V_{cell})^{\frac{1}{3}} \ll 1$ ($u_{n\vec{k}}(\vec{r})$ approximately constant over a wavelength) and $u_{n\vec{k}}(\vec{r}) \approx u_{n0}(\vec{r})$:

$$\frac{1}{V} \int d^3r\, e^{i(\vec{k}_2-\vec{k}_1+\vec{K})\cdot\vec{r}}\, u^*_{n_2 0}(\vec{r})\, u_{n_1 0}(\vec{r}) = \frac{1}{N} \sum_{\vec{R}} e^{i(\vec{k}_2-\vec{k}_1+\vec{K})\cdot\vec{R}} \underbrace{\frac{1}{V_{cell}} \int_{V_{cell}} d^3r\, u^*_{n_2 0}(\vec{r})\, u_{n_1 0}(\vec{r})}_{\delta_{n_1,n_2}}$$

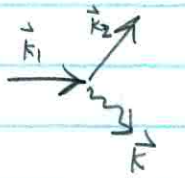
$$= \delta_{k_2,\, \vec{k}_1+\vec{K}}\, \delta_{n_1,n_2}$$

Therefore:

$$\mathcal{H}_{epph}^{DP} = \sum_{\vec{k}} D k \sqrt{\frac{\hbar}{2\rho V \omega_{kL}}} \left\{ \sum_{\substack{\vec{k}_1, m_1 \\ \vec{k}_2, m_2}} \delta_{m_1, m_2} \left[i \hat{a}_k c^{+}_{m_2 \vec{k}_2} c_{m_1 \vec{k}_1} \delta_{\vec{k}_2, \vec{k}_1 + \vec{k}} \delta_{m_1, m_2} \right. \right.$$



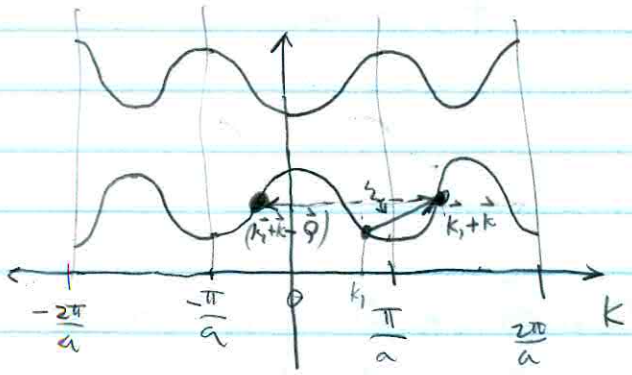
$$\left. \left. - i a^{+}_k c^{+}_{m_2 \vec{k}_2} c_{m_1, \vec{k}_1} \delta_{\vec{k}_2, \vec{k}_1 - \vec{k}} \right] \right\}$$



Hydrostatic DP

$$\mathcal{H}_{e\text{-}ph} = \sum_{\vec{k}, \vec{k}_1, m_1} D k \sqrt{\frac{\hbar}{2\rho V \omega_{kL}}} \, i \left(\hat{a}_k c^{+}_{m_1 (\vec{k}_1 + \vec{k})} c_{m_1 \vec{k}_1} - a^{\dagger}_k c^{+}_{m_1 \vec{k}_1} c_{m_1, \vec{k}_1 - \vec{k}} \right)$$

what if $(\vec{k}_1 + \vec{k})$ is outside the Brillouin zone? Umklapp! Electron goes to $(\vec{k}_1 + \vec{k} - \vec{Q})$, where $\vec{Q}$ is reciprocal lattice vector.



NOT 15

To account for shear deformations that change the crystal symmetry, we must generalize D to be a matrix in the band space:

$$D \rightarrow \hat{D} = \sum_{n, n'} D_{nn'} |n\rangle\langle n'|$$

(4)

Since $\hat{\Psi}(\vec{r}) = \sum_n \hat{\Psi}_n(\vec{r})$:

$$\mathcal{H}^{DP}_{e-ph} = \int d^3r\, \hat{\Psi}^\dagger(\vec{r})\, \mathcal{H}(\vec{r})\, \hat{\Psi}(\vec{r}) = \sum_{n,n'} \mathcal{H}_{nn'}$$

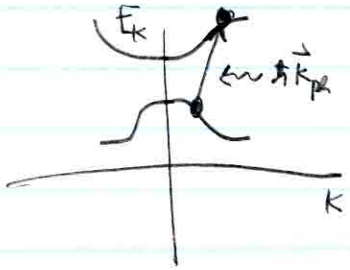
$$\mathcal{H}_{nn'} = \int d^3r\, \hat{\Psi}^\dagger_n(\vec{r})\, \mathcal{H}\, \hat{\Psi}_{n'}(\vec{r})$$

The integral over Bloch states will become:

$$\frac{1}{V_{cell}} \int d^3r\, u^*_{n0}(\vec{r})\, \hat{D}\, u_{n'0}(\vec{r}) = \langle n | \hat{D} | n' \rangle = D_{nn'}$$

$$\Rightarrow \mathcal{H}_{nn'} = \sum_{\vec{k}_2, \vec{k}_1} \langle n | \hat{D} | n' \rangle (\vec{k}_1, \hat{\eta}_{\vec{k}_2}) \sqrt{\frac{\hbar}{2\rho V \omega_k}}\, i \left(\hat{a}_{k_2} \hat{c}^\dagger_{n, k_1+k}\, \hat{c}_{n', k_1} - \hat{a}^\dagger_{k_2} c^\dagger_{n, k_1-k}\, c_{k_1} \right)$$

$\Rightarrow$ Intraband transitions!



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2) Piezoelectric interaction

A piezoelectric material has the property: Strain generate electric field, should couple strongly to electrons!

$$D_i = \sum_{jl} e_{jli}\, \varepsilon_{jl} \quad \text{assuming } \vec{\epsilon} \text{ is diagonal (isotropic material)} \Rightarrow E_i = \frac{1}{\epsilon} \sum_{jl} e_{jli}\, \underbrace{\varepsilon_{jl}}_{\frac{1}{2}\left(\frac{\partial u_j}{\partial x_l} + \frac{\partial u_l}{\partial x_j}\right)}$$

Assume symmetric piezoelectric tensor:

$$e_{jli} = e_{lji} \Rightarrow E_i = \frac{1}{\varepsilon} \sum_{jl} e_{jli}\, \frac{\partial u_l}{\partial x_j}$$

From $\vec{u}(\vec{r}) = \sum_{\vec{k},\lambda} \hat{\eta}_{k\lambda} \sqrt{\frac{\hbar}{2\rho V \omega_{k\lambda}}} \left(\hat{a}_{k\lambda} e^{i\vec{k}\cdot\vec{r}} + \hat{a}^{\dagger}_{k\lambda} e^{-i\vec{k}\cdot\vec{r}} \right)$

$$\frac{\partial u_\ell}{\partial x_j} = \sum_{k,\lambda} (\hat{\eta}_{k\lambda} \cdot \hat{e}_\ell) \sqrt{\frac{\hbar}{2\rho V \omega_{k\lambda}}}\, i k_j \left(\hat{a}_{k\lambda} e^{i\vec{k}\cdot\vec{r}} - \hat{a}^{\dagger}_{k\lambda} e^{-i\vec{k}\cdot\vec{r}} \right)$$

$$\Rightarrow E_i = \frac{1}{\varepsilon} \sum_{\vec{k},\lambda} \sum_{j,\ell} e_{j\ell i} (k_j \hat{\eta}_{k\lambda} \cdot \hat{e}_\ell) \sqrt{\frac{\hbar}{2\rho V \omega_{k\lambda}}}\, i \Big(\underbrace{\hat{a}_{k\lambda} e^{i\vec{k}\cdot\vec{r}}}_{E_+} - \underbrace{\hat{a}^{\dagger}_{k\lambda} e^{-i\vec{k}\cdot\vec{r}}}_{E_-} \Big)$$

Electric field generated by piezophonons is a plane wave with longitudinal component!

What is the electrostatic potential that gives rise to this $\vec{E}$?

If $\vec{E} = \vec{E}_+ e^{i\vec{k}\cdot\vec{r}}$ then we must have $\phi = \phi_+ e^{i\vec{k}\cdot\vec{r}}$, where

$$\vec{E} = -\vec{\nabla}\phi \Rightarrow \vec{\nabla}\cdot\vec{E} = -\nabla^2\phi \Rightarrow i\vec{k}\cdot\vec{E}_+ = +k^2\phi_+$$

$$\Rightarrow \phi_+ = -\frac{\vec{k}\cdot\vec{E}_+}{ik^2} \Rightarrow \boxed{\phi = -\frac{\vec{k}\cdot\vec{E}_+}{ik^2} + \frac{\vec{k}\cdot\vec{E}_-}{ik^2}}$$

Note: Also, need $\vec{A} \neq 0$ to account for transverse components of $\vec{E}$. But these contribute only a small magnetostatic energy for the electron since kinetic energy will become $\frac{(\vec{p} - e\vec{A})^2}{2m}$. This can be shown to be quite small.

The electron-piezophonon interaction is just

$$H^{pz}_{e\text{-}ph} = e\phi = e\left(\frac{-\vec{k}\cdot\vec{E}_+}{ik^2} + \frac{\vec{k}\cdot\vec{E}_-}{ik^2} \right) = -\frac{e}{\varepsilon} \sum_{\vec{k},\lambda} \sum_{i,j,\ell} e_{j\ell i} \frac{k_i k_j (\hat{\eta}_{k\lambda}\cdot\hat{e}_\ell)}{k^2} \sqrt{\frac{\hbar}{2\rho V \omega_{k\lambda}}} \times$$

$$\times \left(\hat{a}_{k\lambda} e^{i\vec{k}\cdot\vec{r}} + \hat{a}^{\dagger}_{k\lambda} e^{-i\vec{k}\cdot\vec{r}} \right)$$

use $\omega_{k\lambda} = v_\lambda k$ and

Note: $\mathcal{H}^{PZ}_{e\text{-}ph} \propto \frac{1}{\sqrt{k}}$!

For long wavelengths (at low T) PZ is much more important than deformation potential.

e.g. in GaAs or any other III-V semiconductor.

3) Fröhlich interaction (optical phonons)

optical phonon mode:
Each unit cell will have a strong electric dipole moment!

$$\vec{E} = -F\vec{u} \qquad \left(\text{remember, electric field due to a dipole is } \vec{E} = \frac{\vec{p} - (\vec{p}\cdot\hat{n})\hat{n}}{4\pi\varepsilon_0 r^3} = \overleftrightarrow{F}\cdot\vec{p}\right)$$

Note the difference from Deformation potential and piezophonons: there $\mathcal{H} \propto \frac{\partial u}{\partial x}$, instead of $\mathcal{H} \propto u$!

$$\Rightarrow \mathcal{H}^{Fröhlich}_{e\text{-}ph} = e\phi = e\left(\frac{-\vec{k}\cdot\vec{E}_+ + k\cdot\vec{E}_-}{ik^2}\right)$$

For optical phonons, use $\vec{u}(\vec{r}) = \sum_{\vec{k},\lambda} \hat{\eta}_{\vec{k}\lambda} \sqrt{\frac{\hbar}{2\underbrace{m_r N}_{\rho} \omega_{LO}}} \left(\hat{a}_{k\lambda} e^{i\vec{k}\cdot\vec{r}} + \hat{a}^+_{k\lambda} e^{-i\vec{k}\cdot\vec{r}}\right)$

because $\rho = \frac{m_r}{V_{cell}}$, $V = N V_{cell}$

m_r = reduced mass $= \frac{M_1 M_2}{M_1 + M_2}$.

Two optical phonons also determine ϵ (they are a pole in ϵ, as seen in AMW A3, problem 4).

We can show that:

$$F = \omega_{LO}\sqrt{\frac{m_r}{V_{cell}}}\left(\frac{1}{\epsilon(\omega=\infty)} - \frac{1}{\epsilon(\omega=0)}\right)^{1/2}$$

$$\Rightarrow \mathcal{H}^{F}_{e\text{-}ph} = eF\frac{\vec{k}\cdot(\vec{u}_+ - \vec{u}_-)}{ik^2} = e\left(\frac{1}{\epsilon(\infty)} - \frac{1}{\epsilon(0)}\right)^{1/2}\sum_{k,\lambda}\sum_{\vec{k}_1}\frac{(\vec{k}\cdot\hat{\eta}_{k\lambda})}{k^2}\sqrt{\frac{\hbar\omega_{LO}}{2V}}\left(\frac{1}{i}\right)\left(\hat{a}_{k\lambda}\, b^{\dagger}_{m,\vec{k}_1+\vec{k}}\, b_{m,\vec{k}_1} - \hat{a}^{\dagger}_{k\lambda}\, b^{\dagger}_{m,\vec{k}_1-\vec{k}}\, b_{m,\vec{k}_1}\right)$$

ω_{LO} is independent of $\vec{k}$:

$$\mathcal{H}^{F}_{e\text{-}ph} \propto \frac{1}{k}\ !$$

At low T, there are no LO phonons thermally excited. However, because $\mathcal{H}^{F}_{e\text{-}ph}$ is so strong, each electron will spontaneously create and destroy LO phonons.

"Polaron": An electron surrounded by a phonon cloud.