Transport properties - Boltzmann equation

goal: calculation of conductivity $\quad \vec{j}(\vec{q},\omega) = \sigma(\vec{q},\omega)\vec{E}(\vec{q},\omega)$

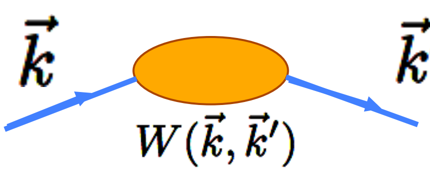
Boltzmann transport theory:

distribution function $\quad f(\vec{k},\vec{r},t)\dfrac{d^3k}{(2\pi)^3}d^3r \quad$ number of particles in infinitesimal phase space volume around $(\vec{k},\vec{r})$

evolution from Boltzmann equation

$$\frac{D}{Dt}f(\vec{k},\vec{r},t) = \left(\frac{\partial}{\partial t} + \dot{\vec{r}}\cdot\vec{\nabla}_{\vec{r}} + \dot{\vec{k}}\cdot\vec{\nabla}_{\vec{k}}\right)f(\vec{k},\vec{r},t) = \left(\frac{\partial f}{\partial t}\right)_{\mathrm{coll}}$$

collision integral for static potential



$$\left(\frac{\partial f}{\partial t}\right)_{\mathrm{coll}} = \int \frac{d^3k'}{(2\pi)^3}W(\vec{k},\vec{k}')[f(\vec{k}',\vec{r},t) - f(\vec{k},\vec{r},t)]$$

relaxation time approximation

$$\left(\frac{\partial f}{\partial t}\right)_{\mathrm{coll}} = \int \frac{d^3k'}{(2\pi)^3} W(\vec{k},\vec{k}')[f(\vec{k}',\vec{r},t) - f(\vec{k},\vec{r},t)]$$

$$\Rightarrow \quad \boxed{\left(\frac{\partial f}{\partial t}\right)_{\mathrm{coll}} = -\frac{f(\vec{k},\vec{r},t) - f_0(\vec{k},\vec{r},t)}{\tau(\epsilon_{\vec{k}})}}$$

relaxation time

equilibrium distribution

$$f_0(\vec{k},\vec{r},t) = \frac{1}{e^{(\epsilon_{\vec{k}}-\mu)/k_BT}+1}$$

small deviations

$$f(\vec{k},\vec{r},t) = f_0(\vec{k},\vec{r},t) + \delta f(\vec{k},\vec{r},t)$$

electrons in oscillating electric field $\vec{E}(t) = \vec{E}(\omega)e^{-i\omega t}$ $\quad \hbar\dot{\vec{k}} = -e\vec{E}$

$$-i\omega\delta f(\vec{k},\omega) - \frac{e\vec{E}(\omega)}{\hbar}\frac{\partial f_0(\vec{k})}{\partial \vec{k}} = -\frac{\delta f(\vec{k},\omega)}{\tau(\epsilon_{\vec{k}})}$$

linearized

$$\delta f \propto E$$

Transport properties - Boltzmann equation

$$\delta f(\vec{k},\omega) = \frac{e\tau\,\vec{E}(\omega)}{\hbar(1-i\omega\tau)}\frac{\partial f_0(\vec{k})}{\partial \vec{k}} = \frac{e\tau\,\vec{E}(\omega)}{\hbar(1-i\omega\tau)}\frac{\partial f_0(\epsilon)}{\partial \epsilon}\frac{\partial \epsilon_{\vec{k}}}{\partial \vec{k}}$$

current density

$$\vec{j}(\omega) = -2e\int\frac{d^3k}{(2\pi)^3}\vec{v}_{\vec{k}}\,f(\vec{k},\omega) = -\frac{e^2}{4\pi^3}\int d^3k\,\frac{\tau(\epsilon_{\vec{k}})[\vec{E}(\omega)\cdot\vec{v}]\,\vec{v}}{1-i\omega\tau(\epsilon_{\vec{k}})}\frac{\partial f_0(\epsilon_{\vec{k}})}{\partial \epsilon_{\vec{k}}}$$

$$\frac{-1}{4k_BT\cosh^2((\epsilon_{\vec{k}}-\mu)/2k_BT)}$$

concentrated at μ

$$j_\alpha(\omega) = \sum_\beta \sigma_{\alpha\beta}(\omega)E_\beta(\omega)$$

conductivity tensor

$$\sigma_{\alpha\beta} = -\frac{e^2}{4\pi^3}\int d\epsilon\,\frac{\partial f_0(\epsilon)}{\partial \epsilon}\,\frac{\tau(\epsilon)}{1-i\omega\tau(\epsilon)}\int d\Omega_{\vec{k}}\,k^2\,\frac{v_{\alpha\vec{k}}\,v_{\beta\vec{k}}}{\hbar|\vec{v}_{\vec{k}}|}$$

Transport properties - Drude form

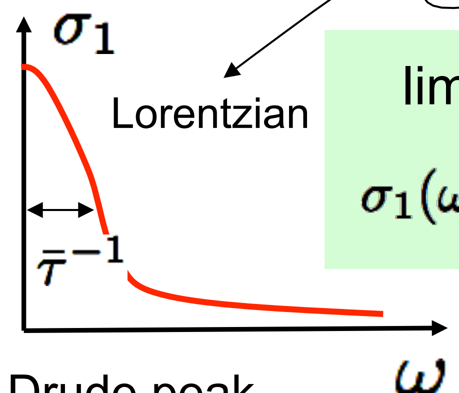
isotropic uniform $$\sigma_{\alpha\beta} = \delta_{\alpha\beta}\sigma$$

dc-conductivity
$\omega = 0$

$$\sigma = -\frac{e^2 n}{m}\int d\epsilon \frac{\partial f_0}{\partial \epsilon}\tau(\epsilon) = \frac{e^2 n\bar{\tau}}{m} = \frac{\omega_p^2\bar{\tau}}{4\pi}$$

ac-conductivity

$$\sigma(\omega) = \frac{\omega_p^2}{4\pi}\frac{\bar{\tau}}{1-i\omega\bar{\tau}} = \frac{\omega_p^2}{4\pi}\left(\frac{\bar{\tau}}{1+\omega^2\bar{\tau}^2} + \frac{i\bar{\tau}^2\omega}{1+\omega^2\bar{\tau}^2}\right) = \sigma_1 + i\sigma_2$$



Drude peak

limit $\bar{\tau} \to \infty$

$$\sigma_1(\omega) = \frac{\omega_p^2}{4}\delta(\omega)$$

f-sum rule

$$\int_0^\infty d\omega\, \sigma_1(\omega) = \int_0^\infty d\omega\, \frac{\omega_p^2}{4\pi}\frac{\bar{\tau}}{1+\omega^2\bar{\tau}^2} = \frac{\omega_p^2}{8}$$

Electron-phonon interaction

real space

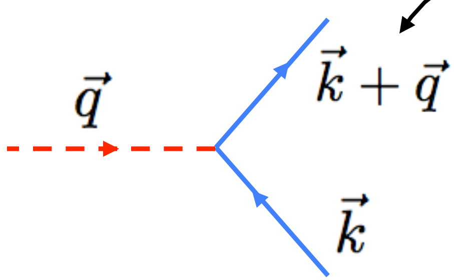
$$\hat{V}_{ep} = -e^2 \sum_s \int d^3r\, d^3r' \underbrace{\vec{\nabla}\cdot\hat{\vec{u}}(\vec{r})}_{\text{ion lattice density fluctuation}} \overset{\text{screened Coulomb potential}}{V(\vec{r}-\vec{r}')} \underbrace{\hat{\Psi}_s^\dagger(\vec{r}')\hat{\Psi}_s(\vec{r}')}_{\text{electron density}}$$

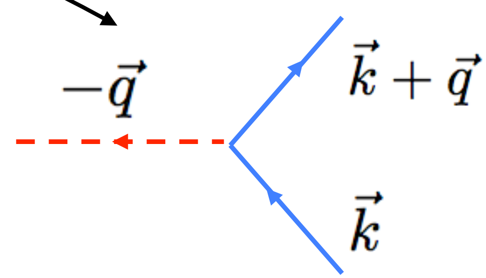
k-space

$$\hat{V}_{\mathrm{ep}} = i \sum_{\vec{k},\vec{q},s} \tilde{V}_{\vec{q}}\, \vec{q}\cdot\left\{ \hat{\vec{u}}_{\vec{q}}\, \hat{c}^\dagger_{\vec{k}+\vec{q},s}\, \hat{c}_{\vec{k},s} - \hat{\vec{u}}^\dagger_{-\vec{q}}\, \hat{c}^\dagger_{\vec{k},s}\, \hat{c}_{\vec{k}+\vec{q},s} \right\}$$

phonon operators

$$= 2i \sum_{\vec{k},\vec{q},s} \tilde{V}_{\vec{q}} \sqrt{\frac{\hbar}{2\rho_0\omega_{\vec{q}}}}\, |\vec{q}|\,(\hat{b}_{\vec{q}} - \hat{b}^\dagger_{-\vec{q}})\, \hat{c}^\dagger_{\vec{k}+\vec{q},s}\, \hat{c}_{\vec{k}s}$$





Electron-phonon interaction

matrix elements of scattering processes

$$\langle \vec{k}+\vec{q}; N_{\vec{q}\,'} | (\hat{b}_{\vec{q}} - \hat{b}^\dagger_{-\vec{q}}) \hat{c}^\dagger_{\vec{k}+\vec{q},s} \hat{c}_{\vec{k}\,s} | \vec{k}; N'_{\vec{q}\,'} \rangle$$

$$= \langle \vec{k}+\vec{q} | \hat{c}^\dagger_{\vec{k}+\vec{q},s} \hat{c}_{\vec{k}\,s} | \vec{k} \rangle \left\{ \sqrt{N'_{\vec{q}\,'}}\, \delta_{N_{\vec{q}\,'},N'_{\vec{q}\,'}-1}\, \delta_{\vec{q},\vec{q}\,'} - \sqrt{N'_{\vec{q}\,'}+1}\, \delta_{N_{\vec{q}\,'},N'_{\vec{q}\,'}+1}\, \delta_{\vec{q},-\vec{q}\,'} \right\}.$$

collision integral

spontaneous emission

$$\left(\frac{\partial f}{\partial t}\right)_{\text{coll}} = -\frac{2\pi}{\hbar} \sum_{\vec{q}} |g(\vec{q})|^2 \Big[\Big\{ f(\vec{k}) \left(1 - f(\vec{k}+\vec{q})\right) (1 + N_{-\vec{q}})$$

$$- f(\vec{k}+\vec{q}) \left(1 - f(\vec{k})\right) N_{-\vec{q}} \Big\} \delta(\epsilon_{\vec{k}+\vec{q}} - \epsilon_{\vec{k}} + \hbar\omega_{-\vec{q}})$$

$$- \Big\{ f(\vec{k}+\vec{q}) \left(1 - f(\vec{k})\right) (1 + N_{\vec{q}})$$

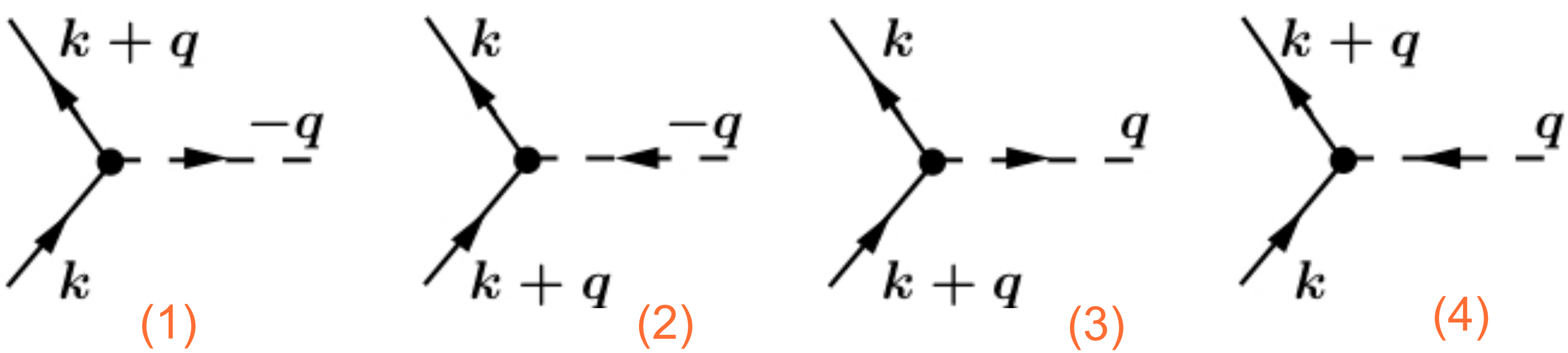
$$- f(\vec{k}) \left(1 - f(\vec{k}+\vec{q})\right) N_{\vec{q}} \Big\} \delta(\epsilon_{\vec{k}+\vec{q}} - \epsilon_{\vec{k}} - \hbar\omega_{\vec{q}}) \Big]$$

e-p-coupling

$$g(\vec{q}) = \tilde{V}_{\vec{q}} |\vec{q}| \sqrt{\frac{2\hbar}{\rho_0 \omega_{\vec{q}}}}$$

Electron-phonon interaction

$$
\begin{aligned}
\left(\frac{\partial f}{\partial t}\right)_{\text{coll}} = -\frac{2\pi}{\hbar}\sum_{\vec{q}} |g(\vec{q})|^2 \Big[\Big\{ & f(\vec{k})\left(1-f(\vec{k}+\vec{q})\right)(1+N_{-\vec{q}}) && \text{(1)} \\
& -f(\vec{k}+\vec{q})\left(1-f(\vec{k})\right)N_{-\vec{q}}\Big\}\delta(\epsilon_{\vec{k}+\vec{q}}-\epsilon_{\vec{k}}+\hbar\omega_{-\vec{q}}) && \text{(2)} \\
-\Big\{ & f(\vec{k}+\vec{q})\left(1-f(\vec{k})\right)(1+N_{\vec{q}}) && \text{(3)} \\
& -f(\vec{k})\left(1-f(\vec{k}+\vec{q})\right)N_{\vec{q}}\Big\}\delta(\epsilon_{\vec{k}+\vec{q}}-\epsilon_{\vec{k}}-\hbar\omega_{\vec{q}})\Big] && \text{(4)}
\end{aligned}
$$



Electron-phonon interaction

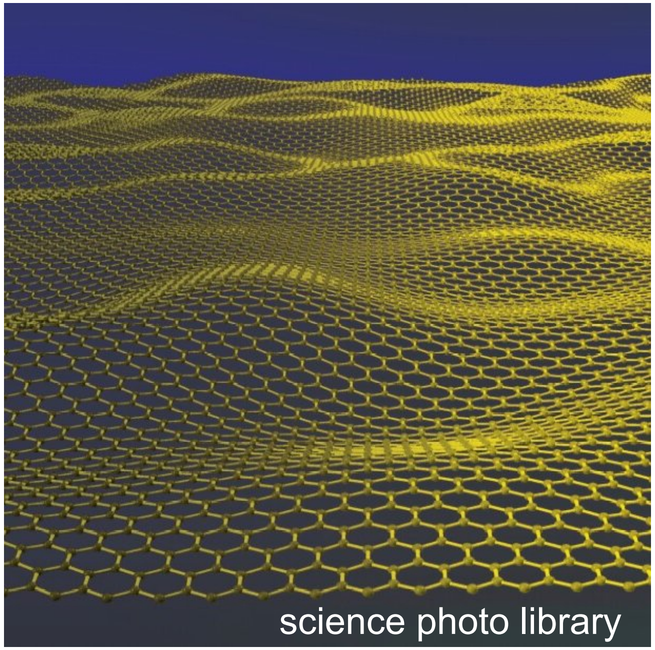
approximation: static potential limit (Born-Oppenheimer)

$$\left(\frac{\partial f}{\partial t}\right)_{\text{coll}} = \frac{2\pi}{\hbar}\sum_{\vec{q}} |g(\vec{q})|^2 2N(\omega_{\vec{q}})[f(\vec{k}+\vec{q}) - f(\vec{k})]\delta(\epsilon_{\vec{k}+\vec{q}} - \epsilon_{\vec{k}})$$

real space view

$$\hat{V}_{ep} = -e^2 \sum_s \int d^3r d^3r' \vec{\nabla}\cdot\hat{\vec{u}}(\vec{r}) V(\vec{r}-\vec{r}\,')\hat{\Psi}_s^\dagger(\vec{r}\,')\hat{\Psi}_s(\vec{r}\,')$$

$$= \sum_s \int d^3r'\, U(\vec{r}\,') \sum_s \hat{\Psi}_s^\dagger(\vec{r}\,')\hat{\Psi}_s(\vec{r}\,')$$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potential due to quasi-static deformation

$$U(\vec{r}\,') = -e^2 \int d^3r\, \langle \vec{\nabla}\cdot\hat{\vec{u}}(\vec{r})\rangle V(\vec{r}-\vec{r}\,')$$