13 ELEKTRÓN - FONÓNOVÁ INTERAKCIA

A) Interakčný hamiltonián

uvažujme kryštál s jednoduchou Bravaisovou mriežkou

$\vec{R}$ = okamžitá poloha iónu $\qquad \vec{R} = \vec{R}^0 + \vec{x}_R$

$\vec{R}^0$ = rovnovážna poloha iónu $\qquad \vec{x}_R$ = výchylka

Zmena potenciálnej energie elektrónu:

$$\delta V(\vec{r}) = \sum_R U(r-R) - \sum_R U(r-R^0) = -\sum_R \frac{\partial U}{\partial \vec{r}}\Big|_{r-R^0} \cdot \vec{x}_R$$

maticový element medzi Blochovými stavmi:

$$\langle k' | \delta V | k \rangle = -\sum_R \vec{x}_R \cdot \int d^3r\, \psi^*_{k'}(r) \frac{\partial U}{\partial \vec{r}}\Big|_{r-R^0} \psi_k(r) \qquad (1)$$

$$\vec{x}_R = \frac{1}{\sqrt{N}} \sum_{q\lambda} \sqrt{\frac{\hbar}{2M\omega_{q\lambda}}} \left(a_{q\lambda} + a^+_{-q\lambda}\right) \vec{e}(q\lambda)\, e^{i\vec{q}\cdot\vec{R}} \qquad (2)$$

$$\psi_k(r) = \frac{1}{\sqrt{\Omega}} e^{ik\cdot r} u_k(r)$$

$$\int d^3r\, \psi^*_{k'}(r) \frac{\partial U}{\partial \vec{r}}\Big|_{r-R^0} \psi_k(r) = \sum_{R'} e^{i(k-k')\cdot R'} \int_{cell} d^3\rho\, \psi^*_{k'}(\rho) \underbrace{\frac{\partial U}{\partial \vec{\rho}}\Big|_{\rho+R'-R}}_{\text{veľké pre } R^{0\prime} = R^0} \psi_k(\rho)$$

$$= e^{i(k-k')\cdot R} \underbrace{N \int_{cell} d^3\rho\, \psi^*_{k'}(\rho) \frac{\partial U}{\partial \vec{\rho}} \psi_k(\rho)}_{\equiv \vec{M}_{k'k}} \qquad (3)$$

$\Omega = N\Omega_0$ ← objem cely

Dosadíme (2),(3) do (1):

$$\langle k' | \delta V | k \rangle = -\frac{1}{\sqrt{N}} \sum_{q\lambda} \sqrt{\frac{\hbar}{2M\omega_{q\lambda}}}\, \vec{M}_{k'k} \cdot \vec{e}(q\lambda) \left(a_{q\lambda} + a^+_{-q\lambda}\right) \cdot \underbrace{\frac{1}{N} \sum_R e^{i(k-k'+q)\cdot R}}$$

$$\boxed{k' = k + q + K}$$

K = vektor inv. mriežky

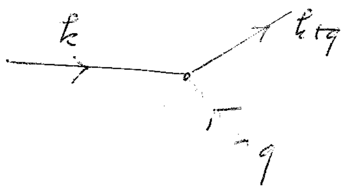
V druhom kvantovaní pre elektróny:

$$\boxed{H_{int} = \frac{1}{\sqrt{N}} \sum_{k\sigma} \sum_{q\lambda} g^{\lambda}_{k,k+q} \left(a_{q\lambda} + a^{+}_{-q\lambda}\right) c^{+}_{k+q\sigma}\, c_{k\sigma}} \qquad (4)$$

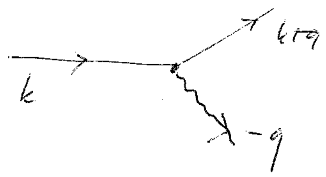
$$\boxed{g^{\lambda}_{k,k+q} = -\sqrt{\frac{\hbar}{2M\omega_{q\lambda}}}\; \vec{e}(q\lambda)\cdot N\int_{cell} d^3\rho\; \psi^{*}_{k'}(\rho)\, \frac{\partial U}{\partial \vec{\rho}}\, \psi_k(\rho)} \qquad (5)$$

$$\psi_k(\rho),\ \vec{e}(q\lambda),\ \omega_{q\lambda} = \text{periodické funkcie } \vec{k}, \vec{q}$$

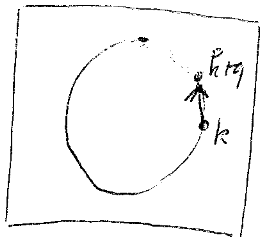
(4) popisuje nasledovné rozptylové procesy:



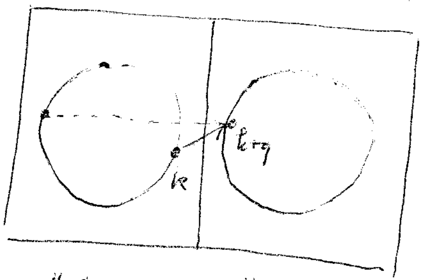
anihilácia fonónu



kreácia fonónu



normálny proces



"Umklapp" proces

Jednoduchý model: $\psi_k = \text{rovinné vlny} = \frac{1}{\sqrt{N\Omega_0}} e^{i\vec{k}\cdot\vec{r}}$

$$g^{\lambda}_{k,k+q} \to g_\lambda(q) = -\sqrt{\frac{\hbar}{2M\omega_{q\lambda}}} \int_{cell} \frac{d^3\rho}{\Omega_0}\, e^{-i\vec{q}\cdot\vec{\rho}}\, \frac{\partial U}{\partial \vec{\rho}}\cdot \vec{e}(q\lambda)$$

$U(\vec{\rho})$ = pomalá funkcia $\to$ v dlhovlnnej limite $(q \to 0)$

$$\boxed{g_\lambda(q) = i\sqrt{\frac{\hbar}{2M\omega_{q\lambda}}} \int_{cell} \frac{d^3\rho}{\Omega_0}\, \vec{q}\cdot\vec{\rho}\, \frac{\partial U}{\partial \vec{\rho}}\cdot \vec{e}(q\lambda)} \qquad (6)$$

akustické módy: $\omega_{q\lambda} = v_\lambda q \to g_\lambda(q) \propto i\, \frac{\vec{q}\cdot\vec{e}_q}{\sqrt{q}}$

nehinené optické módy: $\omega_{q\lambda} \sim \text{konšt} \to g_\lambda(q) \propto i\, \frac{\vec{q}\cdot\vec{e}_q}{q^2}$

Odkiaľ budeme používať

$$\boxed{H_{int} = \frac{1}{\sqrt{N}} \sum_{kq\sigma} g(q)\,(a_q + a^+_{-q})\, c^+_{k+q\sigma} c_{k\sigma}} \quad (7)$$

hamiltonián je hermitovský, ak $g(-q) = g(q)^*$

Pre $g(q) = i f(q)\,(\vec{q}\cdot\vec{e}_q)$ je to splnené, lebo $\vec{e}_{-q}^{\,*} = \vec{e}_q$

B) Poruchová teória

neporušený hamiltonián: $$H_0 = \underbrace{\sum_{k\sigma} \varepsilon_k c^+_{k\sigma} c_{k\sigma}}_{\text{voľné elektróny}} + \underbrace{\sum_q \hbar\omega_q (a_q^+ a_q + \tfrac{1}{2})}_{\text{voľné fonóny}}$$

pri teplote T fonónové stavy obsadené s pravdepodobnosťou $N_q = \dfrac{1}{e^{\frac{\hbar\omega_q}{T}} - 1}$

el. stavy obsadené s pravdepodobnosťou f_k

celková energia $$E(T) = \sum_{k\sigma} \varepsilon_k f_k + \sum_q \hbar\omega_q (N_q + \tfrac{1}{2})$$

$$= \frac{1}{Z} \sum_n E_n e^{-E_n/T} \qquad E_n = \langle n|H_0|n\rangle$$

$|n\rangle$ = stav s dobre definovanými počtami elektrónov a fonónov

korekcia k energii stavu $|n\rangle$:

1. rád: $\delta E_n^{(1)} = \langle n|H_{int}|n\rangle = 0$, lebo $\langle N_q|(a_q + a^+_{-q})|N_q\rangle = 0$

2. rád: $$\delta E_n^{(2)} = \sum_{m\neq n} \frac{\langle n|H_{int}|m\rangle\langle m|H_{int}|n\rangle}{E_n - E_m}$$

Nech $|n\rangle$ obsahuje N_q fonónov.

Príspevok absorbčnej časti H_{int}:

= obsadzovacie čísla pre stav $|n\rangle$ hodnoty: 0, 1 (preto nebudeme písať stredné hodnoty)

$$\delta E_n^{(2)\,abs} = \frac{1}{N} \sum_{kq\sigma} |g_q|^2 \frac{n_{k\sigma}(1 - n_{k+q\sigma})}{\varepsilon_k - \varepsilon_{k+q} + \hbar\omega_q} \underbrace{|\langle N_q - 1|a_q|N_q\rangle|^2}_{= N_q}$$

Príspevok emisnej časti

$$\delta E_n^{(2)\,\mathrm{emis}} = \frac{1}{N}\sum_{kq\sigma} |g_q|^2 \frac{n_{k\sigma}(1-n_{k-q\sigma})}{\varepsilon_k-\varepsilon_{k-q}-\hbar\omega_q} \underbrace{|\langle N_q+1|a_q^\dagger|N_q\rangle|^2}_{(N_q+1)}$$

celková energia:

$$\delta E^{(2)} = \frac{1}{Z}\sum_n e^{-E_n/T}\left[\delta E_n^{(2)\,\mathrm{abs}} + \delta E_n^{(2)\,\mathrm{emis}}\right]$$

tepelné stredovanie: nahradiť $n_{k\sigma}$ Fermiho funkcia f_k, $N_q \to$ Bose dostaneme

$$\boxed{\delta E^{(2)} = \cancel{2}\frac{1}{N}\sum_{kq\sigma}|g_q|^2 \left[\frac{f_{k\sigma}(1-f_{k+q\sigma})N_q}{\varepsilon_k-\varepsilon_{k+q}+\hbar\omega_q} + \frac{f_{k\sigma}(1-f_{k-q\sigma})(N_q+1)}{\varepsilon_k-\varepsilon_{k-q}-\hbar\omega_q}\right]} \quad (8)$$

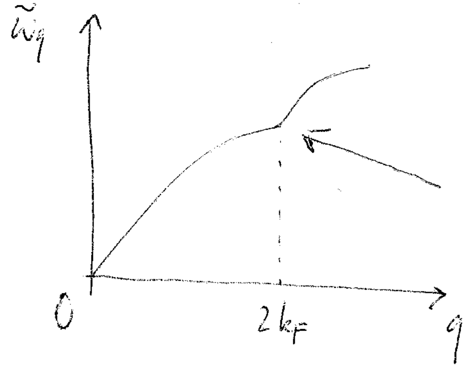
c) Kohnove anomálie (vplyv elektrónov na fonóny)

fonónová energia: $\hbar\tilde{\omega}_q = \frac{\partial E}{\partial N_q} = \frac{\partial E^{(0)}}{\partial N_q} + \frac{\partial E^{(2)}}{\partial N_q}$

$$\hbar\tilde{\omega}_q = \hbar\omega_q + 2|g_q|^2\frac{1}{N}\sum_k\left[\frac{f_k(1-f_{k+q})}{\varepsilon_k-\varepsilon_{k+q}+\hbar\omega_q} + \underbrace{\frac{f_k(1-f_{k-q})}{\varepsilon_k-\varepsilon_{k-q}-\hbar\omega_q}}_{}\right]$$

zámena $k \to k+q$
$k-q \to k$

$$\boxed{\hbar\tilde{\omega}_q = \hbar\omega_q - \frac{2|g_q|^2}{N}\sum_k \frac{f_{k-q}-f_k}{\varepsilon_k-\varepsilon_{k-q}-\hbar\omega_q}}$$



Kohnova anomália

(spôsobená singularitou funkcie $\chi(q) = \frac{1}{N}\sum_k \frac{f_{k-q}-f_k}{\varepsilon_k-\varepsilon_{k-q}}$ pri $q=2k_F$)

D) Vplyv fonónov na elektrónové spektrum

uvažujme pre jednoduchosť $T=0$. Z rovnice 8 máme $(N_q = 0)$

$$E(T) = \sum_{k\sigma} \varepsilon_k f_{k\sigma} + \frac{1}{N} \sum_{kq\sigma} |g_q|^2 \frac{f_{k\sigma}(1-f_{k-q\sigma})}{\varepsilon_k - \varepsilon_{k-q} - \hbar\omega_q}$$

energia elektrónu

$$E_{k\sigma} = \frac{\partial E}{\partial f_{k\sigma}} = \varepsilon_k + \frac{1}{N}\sum_q |g_q|^2 \left[\frac{1-f_{k-q}}{\varepsilon_k - \varepsilon_{k-q} - \hbar\omega_q} - \frac{f_{k+q}}{\varepsilon_{k+q} - \varepsilon_k - \hbar\omega_q} \right]$$

$$E_k = \varepsilon_k + \frac{1}{N}\sum_{k'} |g_{k-k'}|^2 \left[\frac{1-f_{k'}}{\varepsilon_k - \varepsilon_{k'} - \hbar\omega_{k-k'}} - \frac{f_{k'}}{\varepsilon_{k'} - \varepsilon_k - \hbar\omega_{k-k'}} \right]$$

v tomto odseku predpokladáme $\varepsilon_k = 0$ na Fermiho ploche

očakávame: suma cez k' dominovaná bodmi blízko Fermiho plochy

potom $\omega_{k-k'} \approx \omega(\theta)$ kde θ je uhol medzi k, k'

(predpokladáme k blízko Fermiho plochy)

$$E_k \approx \varepsilon_k + N(0) \int \frac{d\Omega'}{4\pi} |g(\theta)|^2 \left[\underbrace{\int_0^\infty \frac{d\varepsilon'}{\varepsilon_k - \varepsilon' - \hbar\omega(\theta)} - \int_{-\infty}^0 \frac{d\varepsilon'}{\varepsilon' - \varepsilon_k - \hbar\omega(\theta)}}_{(*)} \right]$$

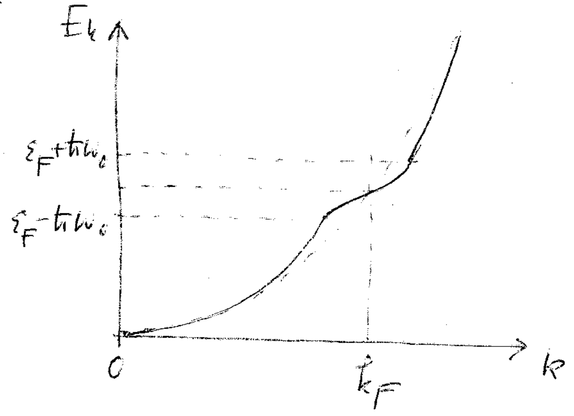
$$(*) = \int_0^\infty d\varepsilon' \left[\frac{1}{\varepsilon_k + \varepsilon' + \hbar\omega(\theta)} + \frac{1}{\varepsilon_k - \varepsilon' - \hbar\omega(\theta)} \right] = \ln \left| \frac{\varepsilon_k - \hbar\omega(\theta)}{\varepsilon_k + \hbar\omega(\theta)} \right|$$

$$\boxed{E_k \approx \varepsilon_k + N(0) \int \frac{d\Omega}{4\pi} g^2(\theta) \ln \left| \frac{\varepsilon_k - \hbar\omega(\theta)}{\varepsilon_k + \hbar\omega(\theta)} \right|}$$

$$\varepsilon_k \gg \hbar\omega \rightarrow E_k \approx \varepsilon_k - \frac{2N(0)}{\varepsilon_k} \int \frac{d\Omega}{4\pi} g^2(\theta)\, \hbar\omega(\theta)$$

$$\varepsilon_k \ll \hbar\omega \rightarrow E_k \approx (1-\lambda)\varepsilon_k$$

$$\boxed{\lambda = 2N(0) \int \frac{d\Omega}{4\pi} \frac{g^2(\theta)}{\hbar\omega(\theta)}}$$



v blízkosti Fermiho plochy sa elektróny správajú ako ťažšie častice — elektrón polarizuje mriežku

$$\boxed{\text{kvázičastica} = \text{holá častica} + \text{oblak excitácií}}$$

ukázali sme $\frac{m^*}{m} = \frac{1}{1-\lambda}$ $\xrightarrow{\text{lepšia teória}}$ $\frac{m^*}{m} = 1+\lambda$

platí pre $\lambda \ll 1$

E) Doba života elektrónov

nechajme opäť pre jednoduchosť $T=0$.

Fermiho zlaté pravidlo:

$$\frac{1}{\tau_k} = \frac{2\pi}{\hbar}\frac{1}{N}\sum_{k'} |g_{k-k'}|^2 (1-f_{k'})\, \delta(\varepsilon_{k'} - \varepsilon_k + \hbar\omega_{k-k'})$$

$$= \frac{2\pi}{\hbar} N(0) \int \frac{d\Omega}{4\pi}\, g^2(\theta) \int_0^\infty d\varepsilon'\, \delta(\varepsilon' - \varepsilon_k + \hbar\omega_{k-k'})$$

$$= \frac{2\pi}{\hbar} N(0) \int \frac{d\Omega}{4\pi}\, g^2(\theta)\, \theta(\varepsilon_k - \hbar\omega(\theta)) = \frac{2\pi}{\hbar} N(0) \frac{1}{2} \int_0^\pi d\theta \sin\theta\, g^2(\theta)\, \theta(\varepsilon_k - \hbar\omega(\theta))$$

pre $\varepsilon_k \to 0$ (t.j. elektrón blížiaci sa k Fermiho ploche)

$\theta \approx \frac{q}{k_F} \ll 1$ $\qquad \frac{1}{\tau_k} = \frac{\pi N(0)}{\hbar} \int_0^{\varepsilon_k/\hbar v k_F} d\theta\, \theta\, g^2(\theta)$

$g^2(\theta) \propto \theta \longrightarrow \boxed{\frac{1}{\tau_k} \propto \varepsilon_k^3}$ t.j. pre $\varepsilon_k \to 0$ máme $\frac{\hbar}{\tau_k} \ll \varepsilon_k$

neurčitosť energie