DIELEKTRIČNOST

1. (LINDHARDOVA) TEORIJA SENČENJA

Določiti moramo porazdelitev gostote naboja in električni potencial, ki sta med seboj konsistentna.

Električni odziv je odvisen od frekvence in valovne dolžine motnje. Funkcija dielektričnega odziva $\varepsilon(\vec{q},\omega)$.

Predpostavimo šibko motnjo in linearen odziv materiala.

Odziv na motnjo se imenuje senčenje in je posledica odziva elektronov na zunanjo motnjo in na druge elektrone.

Obravnavamo poenostavljen problem plina prostih elektronov (soliden približek za preproste kovine).

Ločiti moramo odziv na elektromagnetno valovanje (prečna dielektrična funkcija) in odziv na motnjo v gostoti naboja (longitudinalna dielektrična funkcija). Rečemo tudi odziv tok-tok oz. odziv naboj-naboj.

Gibljiv naboj ustvarja polje, ki je vzporedno z gibalno količino naboja; predpostavimo odvisnost tipa $e^{i(\vec{q}\cdot\vec{r}-\omega t)}$.

Poseben primer bo limita $\omega\to 0$: senčenje statičnega naboja.
↳ v ožjem pomenu besede

Senčenje bo zmanjšalo doseg Coulombove interakcije.

$$\vec{E}(\vec{q},\omega) = \vec{E}_{\parallel}(\vec{q},\omega) + \vec{E}_{\perp}(\vec{q},\omega) \qquad \vec{q}\cdot\vec{E}_{\perp} = 0$$

Review: Purcell (3. izdaja), razdelek 10.11

$$\underset{\text{gostota}}{\vec{D}}(\vec{q},\omega) = \varepsilon_0 \underset{\substack{\text{dielektrična konstanta} \\ \text{"prosti naboj", "zunanji"}}}{\overset{\text{dielektričnost}}{\varepsilon}}(\vec{q},\omega) \overset{\text{jakost}}{\vec{E}}(\vec{q},\omega) = \varepsilon_0 E(\vec{q},\omega) + \overset{\text{polarizacija}}{\vec{P}}(\vec{q},\omega)$$

$\vec{P} = \chi_e \varepsilon_0 \vec{E}$ (χ_e susceptibilnost)

tukaj $e=-e_0$, obravnavamo elektrone, n je številska gostota

$$\nabla \cdot \vec{D} = e \cdot n_{ext} \quad \Rightarrow \quad i\vec{q} \cdot \vec{D}(\vec{q},\omega) = e\, n_{ext}(\vec{q},\omega)$$

$$\varepsilon_0 \nabla \cdot \vec{E} = e \cdot n_{tot} \quad \Rightarrow \quad i\vec{q} \cdot \vec{E}(\vec{q},\omega) = \frac{e}{\varepsilon_0}\left(n_{ext}(\vec{q},\omega) + n_{ind}(\vec{q},\omega)\right)$$

$\nabla \cdot \vec{P} = -e\, n_{ind}$ "inducirani", "notranji", "vezani"

$$n_{tot}(\vec{q},\omega) = n_{ext}(\vec{q},\omega) + n_{ind}(\vec{q},\omega) = \frac{n_{ext}(\vec{q},\omega)}{\varepsilon(\vec{q},\omega)} \Rightarrow \frac{1}{\varepsilon} = 1 + \frac{n_{ind}}{n_{ext}}$$

Coulombov potencial $V(r) = \frac{e_0^2}{4\pi\varepsilon_0 r} \xrightarrow{FT} V_q = \frac{e_0^2}{V\varepsilon_0 q^2}$

$\varepsilon = 1$ v vakuumu, kjer je očitno $n_{ind}=0$

Dokaz:
$$\frac{1}{V}\sum_q \frac{4\pi}{q^2} e^{i\vec{q}\cdot\vec{r}} = \frac{V}{(2\pi)^3}\frac{4\pi}{V}\underbrace{\int_0^{2\pi} d\phi}_{2\pi} \int_0^{\pi} d\theta \sin\theta \int_0^\infty dq\, e^{iqr\cos\theta}$$

$z = \cos\theta$

$$= \frac{1}{\pi}\int_0^\infty dq \int_{-1}^{1} dz\, e^{iqrz} = \frac{1}{\pi}\int_0^\infty dq \frac{1}{iqr}\left(e^{iqr} - e^{-iqr}\right)$$

$x = qr \qquad \frac{dx}{x} = \frac{dq}{q}$

$$= \frac{2}{\pi}\frac{1}{r}\underbrace{\int_0^\infty dx \frac{\sin x}{x}}_{\pi/2} = 1/r$$

$$H = H_0 + V_{ext}$$

$$H_0 = \sum_{k\sigma} \frac{\hbar^2 k^2}{2m} c_{k\sigma}^\dagger c_{k\sigma} + \frac{1}{2}\sum_{k\neq 0} V_k \left(\hat{N}_k^\dagger \hat{N}_k - N\right)$$

ozadje pozitivnih ionov

$$\hat{N}_k^\dagger = \sum_{p\sigma} c_{p+k,\sigma}^\dagger c_{p\sigma} \qquad e^{i\vec{q}\cdot\vec{r}} \to \hat{N}_{-q} = \hat{N}_q^\dagger$$

$V = \frac{1}{4\pi\varepsilon_0}\frac{q}{r}$

$$V_{ext} = -V_{\vec{q}}\, N_{ext}\, e^{i(\vec{q}\cdot\vec{r}-\omega t)} \Rightarrow -V_{\vec{q}}\, \hat{N}_{-\vec{q}}\, N_{ext}\, e^{-i\omega t}$$

el. imajo neg. naboj

tu smo prešli iz prve v drugo kvantizacijo

Notacija: $\hat{n}(\vec{r}) = \psi^\dagger(\vec{r})\psi(\vec{r}) = \sum_q e^{i\vec{q}\cdot\vec{r}}\, \hat{n}_{\vec{q}}$ operatorji gostote

$\underset{\text{število}}{\hat{N}_q} = V \underset{\text{gostota}}{\hat{n}_{\vec{q}}}$ operatorji (fluktuacij) števila

$$u_{ind}(\vec{r},t) = \frac{1}{V}\langle \hat{N}_{q} \rangle e^{i\vec{q}\cdot\vec{r} - i\omega t}$$

$$\frac{1}{\varepsilon(q,t)} = 1 + \frac{\langle N_{\vec{q}} \rangle}{N_{ext}}$$

TEORIJA LINEARNEGA ODZIVA:

$$H = H_0 + V_{ext}$$

$$V_{ext} = -\hat{B}F(t)$$

$$\langle \hat{A} \rangle_t = Tr(\rho \hat{A}) = \int dt' \, R(t,t') F(t')$$

↑ funkcija odziva

$$\langle \hat{A} \rangle_t = A_0 + \frac{i}{\hbar}\int_{-\infty}^{\infty} \theta(t-t') \langle [\hat{A}(t-t'), \hat{B}(0)] \rangle_0 F(t') dt'$$

↑ vrednost v ravnovesju (v nemotenem sistemu)

↑ v Heisenbergovi sliki, $A(t) = e^{i/\hbar H_0 t} A e^{-i/\hbar H_0 t}$

$$V_{ext} = -\hat{B}F(\omega)e^{-i\omega t}$$

$$\Delta A(\omega) = \chi_{AB}(\omega) F(\omega)$$

$$\chi_{AB}(\omega) = \frac{i}{\hbar}\int_{-\infty}^{\infty} d\tau \, e^{i\omega\tau} \theta(\tau) \langle [\hat{A}(\tau), \hat{B}(0)] \rangle_0$$

Prepoznamo $\hat{B} = v_{\vec{q}} \hat{N}_{-\vec{q}} N_{ext}$ $\quad \hat{A} = \hat{N}_{q}$

$$\frac{1}{\varepsilon(q,\omega)} = 1 + \lim_{\Gamma \to 0} v_{\vec{q}} \frac{i}{\hbar}\int_0^{\infty} d\tau \, e^{i\omega\tau - \Gamma\tau} \langle [N_{\vec{q}}(\tau), N_{-\vec{q}}(0)] \rangle_0$$

↑ regularizacija integrala

$T=0$:

$$\langle \psi_0 | [N_q(\tau), N_{-q}(0)] | \psi_0 \rangle = \sum_m \Big[\langle \psi_0 | N_q(\tau) | \psi_m \rangle \langle \psi_m | N_{q}(0) | \psi_0 \rangle$$

$$- \langle \psi_0 | N_{-q}(0) | \psi_m \rangle \langle \psi_m | N_{\vec{q}}(\tau) | \psi_0 \rangle \Big]$$

$$N_{\vec{q}}(\tau) = e^{\frac{i}{\hbar} H_0 \tau} N_{\vec{q}} e^{-i/\hbar H_0 \tau}$$

$$= \sum_m |\langle \psi_0 | N_q | \psi_m \rangle|^2 \left(e^{-i(\omega_m - \omega_0)\tau} - e^{i(\omega_m - \omega_0)\tau} \right)$$

TOČEN IZRAZ

predznak!

$$\frac{1}{\varepsilon(\vec{q},\omega)} = 1 + \frac{V_q}{\hbar}\sum_m |\langle\psi_0|\hat{N}_{\vec{q}}|\psi_m\rangle|^2 \left(\frac{1}{\omega_m-\omega_0+\omega+i0^+} + \frac{1}{\omega_m-\omega_0-\omega-i0^+}\right)\cdot(-1)$$

$$= 1 + \frac{V_q}{\hbar}\sum_m |\langle\psi_0|\hat{N}_{\vec{q}}|\psi_m\rangle|^2 \frac{2(\omega_m-\omega_0)}{(\omega_m-\omega_0)^2-(\omega+i0^+)^2}\cdot(-1) = 1 + V_q\,\chi(\vec{q},\omega)$$

dinamična nabojska susceptibilnost

Do tu, 27.5.2024

Prosti elektroni: osnovno stanje je zapolnjena Fermijeva krogla, vzbuditve pa ustrezajo premiku elektrona iz notranjosti nad površino, torej nastanek para elektron-vrzel.

$$\langle\psi_{\vec{k}\vec{q}\sigma}|\hat{N}_{\vec{q}'}|\psi_0\rangle = \begin{cases} \delta_{\vec{q}\vec{q}'} & |\vec{k}|<k_F,\ |\vec{k}+\vec{q}|>k_F \\ 0 & \text{sicer}\end{cases}$$

Restrikcijo upoštevamo s faktorjem $f_{\vec{k}}(1-f_{\vec{k}+\vec{q}})$. (Rezultat pravzaprav velja tudi za $T>0$.)
V prvem členu še substituiramo $\vec{k}+\vec{q}\to-\vec{k}$.

$$\frac{1}{\varepsilon(\vec{q},\omega)} = 1 + V_q\sum_{k\sigma}\left(\frac{f_{-\vec{k}-\vec{q}}(1-f_{-\vec{k}})}{\hbar\omega+\varepsilon_{-\vec{k}}-\varepsilon_{-\vec{k}-\vec{q}}+i0^+} - \frac{f_{\vec{k}}(1-f_{\vec{k}+\vec{q}})}{\hbar\omega-\varepsilon_{\vec{k}+\vec{q}}+\varepsilon_{\vec{k}}+i0^+}\right)\cdot(-1)$$

$\varepsilon_{-\vec{k}}=\varepsilon_{\vec{k}}$, $f_{-\vec{k}}=f_{\vec{k}}$

$$\frac{1}{\varepsilon(\vec{q},\omega)} = 1 + V_q\,\Pi_0(\vec{q},\omega) \qquad \Pi_0(\vec{q},\omega) = \sum_{k\sigma}\frac{f_{\vec{k}}-f_{\vec{k}+\vec{q}}}{\hbar\omega-\varepsilon_{\vec{k}+\vec{q}}+\varepsilon_{\vec{k}}+i0^+}\ \checkmark$$

PRIBLIŽEK

Polarizacijska funkcija
(pogost zapis je tudi $\chi_0(\vec{q},\omega)$.)

Enak rezultat dobimo tudi v okviru Hartree-Focka, le ε_k, ε_{k+q} nadomestimo s HF izrazi.
Korak dlje je približek naključne faze (RPA), ki ga dobimo z nadomestitvijo $V_q\to V_q/\varepsilon(\vec{q},\omega)$. Tako vgradimo v teorijo samousklajenost.

(3.)

$$\frac{1}{\varepsilon} = 1 + \frac{V_q}{\varepsilon}\Pi_0 = 1 + V_q\Pi_0\left(1 + V_q\Pi_0\left(1 + V_q\Pi_0\right)\dots\right)$$

$$= 1 + V_q\Pi_0 + (V_q\Pi_0)^2 + \dots$$

$$= \frac{1}{1 - V_q\Pi_0}$$

$$\underset{\text{PRIBLIŽEK}}{\varepsilon^{RPA}} = 1 - V_q\Pi_0 = 1 - \frac{e_0^2}{V\varepsilon_0 q^2}\sum_{k,\sigma}\frac{f_{\vec{k}} - f_{\vec{k}+\vec{q}}}{\hbar\omega + \varepsilon_{\vec{k}} - \varepsilon_{\vec{k}+\vec{q}} + i0^+}$$ (Lindhardova enačba)

2. LASTNOSTI DIELEKTRIČNE FUNKCIJE

Dinamični strukturni faktor $S(\vec{q},\omega) = \frac{1}{2\pi}\int e^{+i\omega t}\langle N_{\vec{q}}(t)N_{-\vec{q}}(0)\rangle dt$

$$\overset{T=0}{=} \sum_m |\langle \psi_0|N_{\vec{q}}|\psi_m\rangle|^2\,\delta(\omega - \omega_{om})$$

$$\mathrm{Im}\frac{1}{\varepsilon(\vec{q},\omega)} = -\frac{\pi}{\hbar}V_q\left[S(\vec{q},\omega) - S(\vec{q},-\omega)\right]$$ energy-loss function

f-sum rule: $\int_{-\infty}^{\infty} d\omega\,\omega\,S(q,\omega) = \frac{(N/V)\hbar q^2}{2m}$

$$\varepsilon^{RPA} = \varepsilon_1 + i\varepsilon_2$$

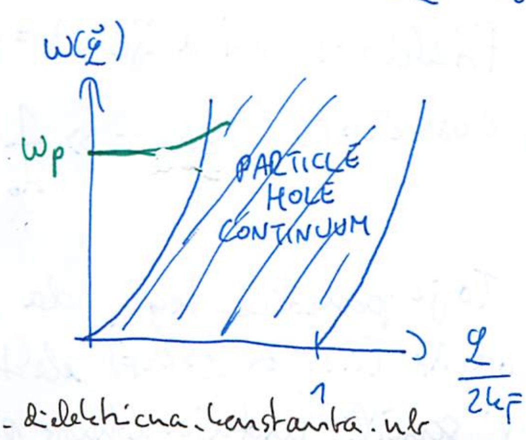
$$\varepsilon_1 = 1 + V_q\sum_{k\sigma}\frac{f_{\vec{k}+\vec{q}} - f_{\vec{k}}}{\hbar\omega - \varepsilon_{\vec{k}+\vec{q}} + \varepsilon_{\vec{k}}}$$

$$\varepsilon_2 = \pi V_q\sum_{k\sigma}\left(f_{\vec{k}} - f_{\vec{k}+\vec{q}}\right)\delta\left(\hbar\omega - \varepsilon_{\vec{k}+\vec{q}} + \varepsilon_{\vec{k}}\right)$$

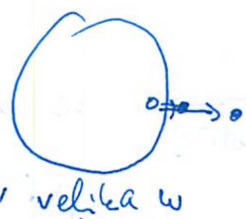
$$\mathrm{Im}\frac{1}{\varepsilon} = -\frac{\varepsilon_2}{\varepsilon_1^2 + \varepsilon_2^2}$$

$\varepsilon_2 \neq 0$ če $\hbar\omega = \varepsilon_{\vec{k}+\vec{q}} - \varepsilon_{\vec{k}} = \frac{\hbar^2}{2m}(2\vec{k}+\vec{q})\cdot\vec{q}$

Enačba za vsako ω podaja razpon $\vec{q}$, kjer je možna absorbcija energije.



majhna ω
velik q



~ velika ω
majhen q

glej RPA-dielektricna_konstanta.nb

7. STATIČNO SENČENJE

$\omega \to 0$:

$$\varepsilon(q,0) = 1 - V_q \sum_{k\sigma} \frac{f_k - f_{k+q}}{\varepsilon_k - \varepsilon_{k+q}} \simeq 1 + V_q \sum_{k\sigma} \left(-\frac{\partial f}{\partial \varepsilon}\right) \quad \text{za } q \to 0$$

Dvojna limita: najprej $\omega \to 0$, potem $q \to 0$.

$$= 1 + \frac{e_0^2}{\varepsilon_0 q^2} \int \left(-\frac{\partial f}{\partial \varepsilon}\right) N(\varepsilon)\, d\varepsilon = 1 + \frac{e_0^2}{\varepsilon_0 q^2} N_0$$

Thomas-Fermijeva senčitvena funkcija

$$\varepsilon(q) = 1 + \frac{\lambda_0^2}{q^2} \qquad \lambda_0 = \frac{e_0^2}{\varepsilon_0} N_0 \qquad \text{za } k_B T \ll \varepsilon_F$$

Boljši zapis $\lambda_0 \to q_{TF}$

$$V_{eff}(r) = \frac{V(r)}{\varepsilon} \Rightarrow V_{eff}(q) = \frac{V(q)}{\varepsilon_q} = \frac{e_0^2}{V\varepsilon_0(q^2+\lambda_0^2)}$$

$e_0^2/\varepsilon_0 q^2 V$

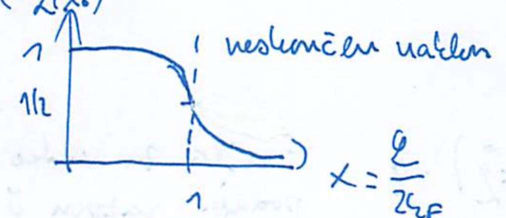
$$\Rightarrow V_{eff}(r) = \frac{e_0^2}{4\pi\varepsilon_0 r} e^{-\lambda_0 r} \qquad \text{Velja za } q \to 0.$$

Zasenčitvena razdalja $r_{scr} = \frac{1}{\lambda_0}$.

Pri večjih q velja $\varepsilon(q) = 1 + \frac{\lambda_q^2}{q^2}$

$$F(q) = \left(\frac{\lambda_q}{\lambda_0}\right)^2 = \frac{1}{2} + \frac{1-x^2}{4x} \ln\left|\frac{1+x}{1-x}\right| \qquad x = \frac{q}{2k_F} \qquad \text{Lindhardova funkcija}$$

$F(q) = (\lambda_q/\lambda_0)^2$



$$V_{eff}(q) = \frac{e_0^2}{\varepsilon_0(q^2+\lambda_q^2)} \Rightarrow V_{eff}(r) \cong \frac{e^2}{\varepsilon_0 k_F^2 r^3} \cos(2k_F r) \qquad \text{za } r \gg \frac{1}{\lambda_0}$$

Friedelove oscilacije, $\lambda = \frac{\pi}{k_F}$

$$r_{scr}(q) = \frac{1}{\lambda_0 \sqrt{F(q)}}$$

se povečuje, ko q veliča. To je posledica tega, da se pri razdaljah manjših od λ_F (i.e. za $q > 2k_F$) elektroni ne morejo razporediti, da bi senčili motnjo. Kvantni pojav.

8. PLAZMONI

Če $\varepsilon=0$, lahko elektroni zanihajo v odsotnosti zunanjega polja; kolektivna vzbuditev vseh elektronov.

$\hbar\omega \gg \varepsilon_{k+q}-\varepsilon_k \Rightarrow \varepsilon_2=0$ $\quad k+q \to k$

$$\varepsilon_1(q,\omega) = 1+V_q\sum_{k\sigma}\left(\frac{f_k}{\hbar\omega-\varepsilon_k+\varepsilon_{k-q}}-\frac{f_k}{\hbar\omega-\varepsilon_{k+q}+\varepsilon_k}\right)$$

$$= 1+V_q\sum_{k\sigma} f_k\frac{2\varepsilon_k-\varepsilon_{k+q}-\varepsilon_{k-q}}{(\hbar\omega-\varepsilon_k+\varepsilon_{k-q})(\hbar\omega-\varepsilon_{k+q}+\varepsilon_k)} \quad \leftarrow -\hbar^2 q^2/m \quad \leftarrow \hbar^2\omega^2$$

$$= 1-\underset{\uparrow \atop \frac{e_0^2}{V\varepsilon_0 q^2}}{V_q}\frac{q^2}{m\omega^2}\underbrace{\sum_{k\sigma} f_k}_{N} = 1-\frac{e_0^2(N/V)}{\varepsilon_0 m\omega^2}$$

$$\varepsilon_1(q,\omega)\simeq 1-\frac{\omega_p^2}{\omega^2} \qquad \omega_p^2=\frac{e_0^2}{\varepsilon_0 m}\rho \quad \text{plazemska frekvenca}$$

klasično: $\vec{E} = -\vec{P}/\varepsilon_0 = \rho\, e_0\vec{r}/\varepsilon_0$

$$m\ddot{\vec{r}} = -\frac{e_0^2}{\varepsilon_0}\rho\,\vec{r} \Rightarrow \ddot{\vec{r}} = -\omega_p^2\vec{r}$$

kvantni popravki:

$$\omega_p(q)^2 = \omega_p^2\left(1+\frac{3}{10}\frac{q^2\hbar^2k_F^2}{m^2\omega_p^2}+\dots\right)$$

V limiti $q\to 0$ so plazmoni edina vzbuditev elektronskega plina.

5. DIELEKTRIČNA KONSTANTA IZOLATORJA

V kovinah $\varepsilon(q\to 0)$ divergira kot $1/q^2$.

V izolatorjih $\varepsilon(q\to 0) = \varepsilon$ zaradi energijske reže.

Nečistoča v kovini ima potencial $V(r) \sim \frac{1}{4\pi\varepsilon_0 \varepsilon r}$ za velike r, kar omogoča nastanek donorskih in akceptorskih stanj ter ekscitonov.

$$\varepsilon = 1 + \frac{(\hbar\omega_p)^2}{E_{gap}^2}$$ ← plazemska frekvenca valenčnih elektronov

6. KRAMERS-KRONIGOVE ZVEZE

$\varepsilon_1(\omega)$ soda funkcija, $\varepsilon_2(\omega)$ liha funkcija

$$\varepsilon_1(\omega) = 1 + \frac{2}{\pi} P \int_0^\infty d\omega' \, \varepsilon_2(\omega') \frac{\omega'}{\omega'^2 - \omega^2}$$

$$\varepsilon_2(\omega) = \frac{2\omega}{\pi} P \int_0^\infty d\omega' \, \frac{\varepsilon_1(\omega) - 1}{\omega'^2 - \omega^2}$$

Posledica kavzalnosti.

Bolje: Točna verzija za $\mathrm{Re}\frac{1}{\varepsilon}$ in $\mathrm{Im}\frac{1}{\varepsilon}$!

8 7. POVEZAVA S PREVODNOSTJO

$\chi = \varepsilon - 1$ opisuje odziv gostote naboja na zunanji potencial

σ opisuje odziv gostote toka na zunanje polje

Kontinuitetna enačba: $\nabla \cdot \vec{j} + e\, n_{ind} = 0$ Review: Purcell, razdelek 10.14

$$i\vec{q} \cdot \vec{j}(\vec{q},\omega) + e(-i\omega)\, n_{ind}(\vec{q},\omega) = 0$$

$$\vec{j}(\vec{q},\omega) = \sigma(\vec{q},\omega)\, \vec{E}(\vec{q},\omega)$$

$$\vec{q}\cdot\vec{j} = e\omega\, n_{ind} = \sigma\, \vec{q}\cdot\vec{E} = \sigma \frac{e}{i\varepsilon_0}(n_{ext} + n_{ind})$$

$$\frac{n_{ind}}{n_{ind} + n_{ext}} = \frac{\sigma}{i\omega\varepsilon_0}$$

$$\frac{n_{ind}/n_{ext}}{1 + n_{ind}/n_{ext}} = \frac{\varepsilon^{-1} - 1}{\varepsilon^{-1}} = \frac{\sigma}{i\omega\varepsilon_0}$$

$$1 - \varepsilon = \frac{\sigma}{i\omega\varepsilon_0}$$

$$\varepsilon(\vec{q},\omega) = 1 - \frac{\sigma(\vec{q},\omega)}{i\omega\varepsilon_0}$$

Ekvivalentna izpeljava: $\vec{j} = \frac{d\vec{P}}{dt}$

f-sum rule: $\int_0^\infty d\omega \; \mathrm{Re}\,\sigma(\omega) = \frac{\omega_p^2}{8}$

78. VSOTNA PRAVILA

(Dokaz: Mahan, razdelek 5.7)

1. $$\int_0^\infty d\omega\, \omega\, \varepsilon_2(\vec{q},\omega) = \frac{\pi}{2}\omega_p^2$$

stisljivost $\varkappa = \frac{3}{2(N/V)\varepsilon_F} = \frac{N_0}{(N/V)^2}$

2. $$\lim_{q\to 0}\int_0^\infty \frac{d\omega}{\omega}\varepsilon_2(\vec{q},\omega) = \frac{\pi}{2}V_q^2 N \varkappa V$$

3. $$\int_0^\infty d\omega\, \omega\, \mathrm{Im}\left[\frac{1}{\varepsilon(\vec{q},\omega)}\right] = -\frac{\pi}{2}\omega_p^2$$ longitudinal f-sum rule

4. $$\lim_{q\to 0}\int_0^\infty \frac{d\omega}{\omega}\mathrm{Im}\left[\frac{1}{\varepsilon(\vec{q},\omega)}\right] = -\frac{\pi}{2}$$

3. in 4. sta eksaktni, 1. in 2. pogosto veljata (recimo za RPA).

1., 2. in 4. so posledica kavzalnosti (Kramers-Kronig).

Z 4. pravilom lahko pokažemo, da plazmoni zapolnijo vsotno pravilo pri $q\to 0$, zato pri $q=0$ ni drugih vzbuditev.

9. RPA = RANDOM PHASE APPROXIMATION (ua liho v 2024)

To je teoretična utemeljitev vsega, kar smo delali do zdaj.

$$H = \sum \frac{p_i^2}{2m} + \frac{e_0^2}{8\pi\varepsilon_0} \sum_{i\neq j} \frac{1}{|\vec{r}_i - \vec{r}_j|}$$

$$\frac{e_0^2}{8\pi\varepsilon_0} \sum_{i\neq j} \frac{1}{|\vec{r}_i - \vec{r}_j|} = \frac{e_0^2}{2V\varepsilon_0} \sum_{i\neq j} \sum_{k} \frac{e^{i\vec{k}\cdot(\vec{r}_i - \vec{r}_j)}}{k^2}$$

Ločimo $k<k_c$ in $k>k_c$

Za $k<k_c$ uvedemo opis s poljem

$$\vec{A}(\vec{r}_i) = \frac{1}{\sqrt{V\varepsilon_0}} \sum_{k}{}' \hat{k} Q_k e^{i\vec{k}\cdot\vec{r}_i}$$

$$\vec{E} = -\dot{\vec{A}} = -\frac{1}{\sqrt{V\varepsilon_0}} \sum_{k} \hat{k} \dot{Q}_k e^{i\vec{k}\cdot\vec{r}_i} = -\frac{1}{\sqrt{V\varepsilon_0}} \sum_{k} \hat{k} P_k^* e^{i\vec{k}\cdot\vec{r}_i}$$

$\vec{Q}_k$ in $\vec{P}_k$ sta kolektivni koordinati polja, ki opisuje Coulombovo interakcijo elektronov.

V H to vpeljemo z $\vec{p}_i \to \vec{p}_i + e\vec{A}(\vec{r}_i)$ in dodamo energijo $\frac{\varepsilon_0}{2}\int E^2 d^3\vec{r}$.

Kvantiziramo $\vec{p}_i, \vec{r}_i$ in $\vec{P}_k, \vec{Q}_k$

Obstaja vez $\varepsilon_0 \nabla\cdot\vec{E} = \rho \Rightarrow \vec{P}_k = i\sqrt{\frac{e_0^2}{V\varepsilon_0 k^2}} \sum_j e^{i\vec{k}\cdot\vec{r}_j}$

$$H = \sum_i \frac{p_i^2}{2m} + \frac{e_0^2}{2V\varepsilon_0} \sum_{i,j} \sum_{k>k_c} \frac{e^{i\vec{k}\cdot(\vec{r}_i - \vec{r}_j)}}{k^2} - \frac{ne^2}{2\varepsilon_0} \sum_{k>k_c} \frac{1}{k^2}$$

Plin elektronov z zasenčeno interakcijo

$$+ \frac{1}{2} \sum_{k<k_c} \left(P_k^* P_k + \omega_p^2 Q_k^* Q_k - \frac{ne^2}{\varepsilon_0 k^2} \right)$$

Plazemske oscilacije

$$+ \frac{e_0}{\sqrt{V\varepsilon_0} m} \sum_{k<k_c} Q_k \hat{k} \cdot \sum_i \left(\vec{p}_i - \frac{\hbar \vec{k}}{2} \right) e^{i\vec{k}\cdot\vec{r}_i}$$

interakcija med elektroni in plazmoni

$$+ \frac{e_0^2}{2V\varepsilon_0 m} \sum_{k,k'} \hat{k}\cdot\hat{k}' Q_k Q_{k'} \sum_i e^{i(\vec{k}+\vec{k}')\cdot\vec{r}_i}$$

odpade, ker položaji $\vec{r}_i$ naključno porazdeljeni

$$H = \sum_{k\sigma} \frac{\hbar^2 k^2}{2m} c_{k\sigma}^\dagger c_{k\sigma} + \sum_{k>k_c} \frac{e_0^2}{2V\varepsilon_0 k^2} \sum_{\substack{\sigma\sigma' \\ pp'}} c_{p+k\sigma}^\dagger c_{p'-k\sigma'}^\dagger c_{p'\sigma'} c_{p\sigma} + \sum_k \hbar\omega_p (a_k^\dagger a_k + 1/2)$$

$$+ \sum_{k<k_c} \sqrt{\frac{e_0^2 \hbar^3}{V\varepsilon_0 \omega_p m^2 k^3}} \sum_{p\sigma} (2\vec{k}\cdot\vec{p} + k^2)(a_k c_{p+k\sigma}^\dagger c_{p\sigma} + a_{-k}^\dagger c_{p+k\sigma}^\dagger c_{p\sigma})$$

$$+ \ldots (aa + a^\dagger a^\dagger + a^\dagger a + aa^\dagger) c^\dagger c$$

dvoplazmonski procesi, sklapljajo različne k in k'

Do TU, 28/5/2024

STISLJIVOST EL. PLINA

$$\varkappa = -\frac{1}{V}\left(\frac{\partial V}{\partial P}\right)_T$$

$$P = \frac{2}{5}\,\frac{E_F N}{V} \qquad E_F = \frac{\hbar^2}{2m}\left(3\pi^2 \frac{N}{V}\right)^{2/3} \qquad P \propto V^{-5/3}$$

$$\ln P = -\frac{5}{3}\ln V$$

$$\frac{V}{P}\frac{\partial P}{\partial V} = \qquad \frac{\partial \ln P}{\partial \ln V} = -\frac{5}{3}$$

$$\left.\begin{array}{l} \varkappa = \dfrac{3}{5}\,\dfrac{1}{P} = \dfrac{3}{2(N/V)E_F} \\[2em] \text{DOS} \quad g(\varepsilon_F) = N_0 = \dfrac{3(N/V)}{2\varepsilon_F} \end{array}\right\} \quad \varkappa = \frac{N_0}{(N/V)^2}$$

Compressibility sum rule: (Arovas p. 450)

$$\langle \delta n \rangle = \hat{\chi}(q=0, \omega=0)\,\delta\mu \quad \Rightarrow \quad \varkappa = \frac{2}{\hbar n^2}\lim_{q\to 0}\int_{-\infty}^{\infty} d\omega\,\frac{S(\vec{q},\omega)}{\omega}$$

$$\delta n(\vec{q},\omega) = \hat{\chi}(q,\omega)\,\underbrace{\phi(\vec{q},\omega)}_{\text{potencial v energijskih enotah}} \qquad \hat{\chi}(q,\omega) = \frac{1}{\hbar}\int_{-\infty}^{\infty} d\nu\, S(q,\nu)\left\{\frac{1}{\omega+i\delta+\nu} - \frac{1}{\omega+i\delta-\nu}\right\}$$

DETAJLI

$$\psi^\dagger(\vec r)\psi(\vec r) = \sum \delta(\vec r - \hat{\vec r}_i) = n(\vec r)$$ operator številske gostote

prva kvantizacija, en delec $\qquad$ druga več delcev $\qquad$ druga kvantizacija

$$e^{i\vec q\cdot\vec r} \Rightarrow \sum_i e^{i\vec q\cdot\vec r_i} = \int e^{i\vec q\cdot\vec r} \underbrace{\psi^\dagger(r)\psi(r)}_{\sum_{\vec k} e^{i\vec k\cdot\vec r}\hat n_{\vec k}} dr$$

$$= V\sum_k \delta_{\vec q,-k} n_k = N_{-\vec q} = N^\dagger_{\vec q}$$

$$\psi(\vec r) = \sum_m \varphi_m(\vec r) c_m$$

$$\varphi_m(\vec r) = \frac{1}{\sqrt V} e^{i\vec k\cdot\vec r} \quad \text{za } m = \vec k$$

$$n(\vec r) = \psi^\dagger(\vec r)\psi(\vec r) = \sum_{k',k} e^{-i(k'-k)\cdot r}\frac{1}{V} c^\dagger_{k'} c_k \qquad q = k'-k$$

ker $n = n^*$

$$= \sum_q e^{-iq\cdot r} \underbrace{\frac{1}{V}\sum_k c^\dagger_{k+q} c_k}_{n^\dagger_{\vec q}} = \sum_q e^{iqr} n_{\vec q}$$

$$n_0 = \frac{1}{V}\sum_k c^\dagger_k c_k = \hat n$$ operator gostote

Coulombova interakcija:

$$c^\dagger_{p+k\sigma} c^\dagger_{q-k\sigma'} c_{q\sigma'} c_{p\sigma} = -c^\dagger_{p+k\sigma}\left(\delta_{\sigma\sigma'}\delta_{q-k,p} - c_{p\sigma} c^\dagger_{q-k\sigma'}\right) c_{q\sigma'}$$

$$\downarrow \sum_{p,q\sigma\sigma'}$$

$$= N_{\hat k} N_{-\hat k} - \underbrace{\sum_{q\sigma} c^\dagger_{q\sigma} c_{q\sigma}}_{N}$$

Sum-rule in plazmoni:

$\vec{q} \to 0$ $\lim_{q\to 0} \varepsilon(\vec{q},\omega) = 1 - \frac{\omega_p^2}{\omega^2} + \mathcal{O}(\omega^{-4})$

$$\lim_{q\to 0} \left[\frac{1}{\varepsilon} - 1\right] = \frac{\omega^2}{\omega^2 - \omega_p^2} - 1 = \frac{\omega_p^2}{\omega^2 - \omega_p^2} = \frac{\omega_p^2}{(\omega-\omega_p)(\omega+\omega_p)}$$

$$= \frac{\omega_p}{2}\left(\frac{1}{\omega-\omega_p} - \frac{1}{\omega+\omega_p}\right)$$

Spomnimo se, da moramo v resnici vzeti $\omega \to \omega + i\delta$. Zato je

$$\lim_{q\to 0} \operatorname{Im}\left[\frac{1}{\varepsilon} - 1\right] = -\pi \frac{\omega_p}{2}\left[\delta(\omega-\omega_p) - \delta(\omega+\omega_p)\right]$$

$\frac{1}{x+i\delta} = P\frac{1}{x} - i\pi\,\delta(x)$

$$\lim_{q\to 0} \int_0^\infty \omega\, d\omega \operatorname{Im}\left[\frac{1}{\varepsilon} - 1\right] = -\frac{\pi}{2}\omega_p^2$$

$$\lim_{q\to 0} \int_0^\infty \frac{1}{\omega}\, d\omega \operatorname{Im}\left[\frac{1}{\varepsilon} - 1\right] = -\frac{\pi}{2}$$

Plazmoni torej zapolnijo vsotno pravilo pri $q \to 0$, ni drugih prispevkov.

$$\hbar\omega_{\vec{q}} = \frac{\hbar^2}{2m}(2\vec{k} + \vec{q})\cdot\vec{q}$$

$\vec{k}$ v smeri $\vec{q}$ ali v nasprotni smeri. $k = k_F$

$\omega_q = \frac{\hbar}{2m}(2kq + q^2) \quad \to \quad q = -k_F + \sqrt{k_F^2 + \frac{2m\omega}{\hbar}} \quad \Rightarrow \quad q = 0$ za $\omega = 0$

$\omega_q = \frac{\hbar}{2m}(-2kq + q^2) \quad \to \quad q = k_F + \sqrt{k_F^2 + \frac{2m\omega}{\hbar}} \quad \Rightarrow \quad q = 2k_F$ za $\omega = 0$