MREŽNA NIHANJA

1. SKLOPITEV MED ELEKTRONI IN IONI

valenčni elektroni in ioni (jedra + notranje lupine)
(angl. atom core, sredica?)

$$H = H_{el} + H_{ion} + H_{el-ion}$$

$$H_{el} = \sum_i \frac{p_i^2}{2m} + \frac{1}{2}\sum_{i \neq i'} \frac{e_0^2}{4\pi\varepsilon_0 |\vec{r}_i - \vec{r}_{i'}|}$$

$$H_{ion} = \underbrace{\sum_j \frac{P_j^2}{2M_j}}_{H^k_{ion}} + \underbrace{\frac{1}{2}\sum_{j \neq j'} V_{ion}(\vec{R}_j - \vec{R}_{j'})}_{H^p_{ion}}$$

$$H_{el-ion} = \sum_{ij} V_{el-ion}(\vec{r}_i - \vec{R}_j)$$

$$H\Psi = E\Psi \qquad \Psi = \Psi(\vec{r}_1, \dots, \vec{r}_N; \vec{R}_1, \dots, \vec{R}_{N'})$$

2. ADIABAT~~SKI~~NI PRIBLIŽEK

$$H = H_0 + H^k_{ion}$$

$$H_0 \psi_\alpha(\vec{r}; \vec{R}) = \varepsilon_\alpha(\vec{R}) \psi_\alpha(\vec{r}; \vec{R})$$

$$\Psi = \sum_\alpha \varphi_\alpha(\vec{R}) \psi_\alpha(\vec{r}; \vec{R})$$

$$(H - E)\Psi = \sum_\alpha (H_0 + H^k_{ion} - E)\varphi_\alpha(\vec{R}) \psi_\alpha(\vec{r}; \vec{R})$$

$$= \sum_\alpha (\varepsilon_\alpha(\vec{R}) + H^k_{ion} - E)\varphi_\alpha(\vec{R}) \psi_\alpha(\vec{r}; \vec{R}) = 0$$

Z leve množimo z $\psi_\beta^*(\vec{r}; \vec{R})$ in integriramo po elektronskih prostostnih stopnjah.

$$[H^k_{ion} + \varepsilon_\beta(\vec{R})]\varphi_\beta(\vec{R}) + \sum_\alpha \hat{A}_{\beta,\alpha}(\vec{R}) \varphi_\alpha(\vec{R}) = E \varphi_\beta(\vec{R})$$

adiabatna potencialna ploskev

$$\hat{A}_{\beta\alpha}(\vec{R}) = -\sum_j \frac{\hbar^2}{2M_j} \int d\vec{r}\, \left[\psi_\beta^*(\vec{r};\vec{R}) \frac{\partial^2}{\partial \vec{R}_j^2} \psi_\alpha(\vec{r};\vec{R}) + 2\psi_\beta^*(\vec{r};\vec{R}) \frac{\partial \psi_\alpha(\vec{r};\vec{R})}{\partial \vec{R}_j} \cdot \frac{\partial}{\partial \vec{R}_j} \right]$$

$$-\frac{\partial^2}{\partial R^2}(\psi\varphi) = -\psi\nabla^2\phi - \phi\nabla^2\psi - 2\nabla\psi\cdot\nabla\varphi$$

↳ deluje na desno

Če zanemarimo člene z $\hat{A}_{\beta\alpha}(\vec{R})$, dobimo

$$[H^{k}_{ion}(\vec{R}) + \varepsilon_\beta(\vec{R})]\varphi_\beta(\vec{R}) = E\varphi_\beta(\vec{R})$$ Rešujemo samo-usklajeno.

Razklopili smo dinamiko elektronov in ionov. Born-Oppenheimerjev približek. Povprečna porazdelitev elektronov določa gibanje ionov, trenutni položaji ionov določajo gibanje elektronov. Ioni počasnejši kot elektroni, obravnavamo ločeno. Sklopitev smatramo kot majhno perturbacijo.

Dobro deluje, če so nihajne frekvence manjše od vzbujenih energij za elektrone. $\hbar\omega \ll E_{el}^{vzb.} - E_{el}^{G.S.}$

Majhna nihanja: konstanta vzmeti $k \sim \frac{\partial^2 E}{\partial R^2} \sim \frac{E_{el}}{a_B^2}$

Bohrov radij $a_B = \frac{4\pi\varepsilon_0 \hbar^2}{m e_0^2}$ $\qquad E_H = \frac{\hbar^2}{m a_B^2}$

$$E_{ioni}^2 \sim (\hbar\omega)^2 \sim \frac{k}{M} \sim \frac{E_{el}}{M a_B^2} \sim \frac{m}{M} E_{el}^2 \Rightarrow E_{ion} \sim \sqrt{\frac{m}{M}} E_{el}$$

To je ocena, koliko energije je v vibracijskem podsistemu.

Ocena napak zaradi zanemaritve $\langle \hat{A}_{\beta\beta} \rangle$.

Tesno vezani elektroni: $\Psi(\vec{r};\vec{R}) = \prod_j \phi_j(\vec{r}_j - \vec{R}_j)$ $\qquad \nabla_{\vec{R}_j} = -\nabla_{\vec{r}_j}$

$$\Delta E_1 \propto \sum_j \frac{m}{M_j} \int d\vec{r}_j\, \phi_j(\vec{r}_j - \vec{R}_j)\left(-\frac{\hbar^2 \nabla_{\vec{r}_j}^2}{2m}\right)\phi_j(\vec{r}_j - \vec{R}_j) = \frac{m}{M_j} E^{k}_{el} \qquad \frac{m}{M_j} \sim \frac{1}{1000}$$

$$\Delta E_2 \propto \int d\vec{r}\, \psi^*(\vec{r};\vec{R}) \frac{\partial}{\partial \vec{R}} \psi(\vec{r};\vec{R}) = \frac{\partial}{\partial \vec{R}} \int \psi^*\psi\, d\vec{r} = 0$$

Če funkcija realna.

Do tu, 26. 2. 2024 (2. ura)

3) VIBRONSKA SKLOPITEV

Recimo, da smo rešili z adiabatskim približkom ali čim podobnim.

Referenčne lege $\vec{R}^0$. V statični približek s fiksnimi jedri pri reševanju el. podproblema. Običajno velja simetrična postavitev.

$$V_{el\text{-}ion}(\vec{r},\vec{R}) = V_{el\text{-}ion}(\vec{r},\vec{R}^0) + \underbrace{\sum_\alpha \left(\frac{\partial V}{\partial R_\alpha}\right)_0 Q_\alpha + \sum_{\alpha\beta}\left(\frac{\partial^2 V}{\partial R_\alpha \partial R_\beta}\right)_0 Q_\alpha Q_\beta + \ldots}_{W}$$

$$\Psi = \sum_a \psi_a(\vec{r})\,\phi_a(\vec{R})$$ PAZI: ψ_a nima eksplicitne odvisnosti od $\vec{R}$

$$\left[H^k_{ion}(\vec{R}) + H^P_{ion}(\vec{R}) + W_{aa}(\vec{R}) + E_{el,a} - E\right]\phi_a(\vec{R}) + \sum_{b\neq a} W_{ab}(\vec{R})\,\phi_b(\vec{R}) = 0$$

$$W_{ab} = \sum_\alpha \left\langle \psi_a(\vec{r}) \right| \left(\frac{\partial V}{\partial R_\alpha}\right)_0 \left| \psi_b(\vec{r}) \right\rangle Q_\alpha$$

$$\left[H_{el}(\vec{r}) + H_{el\text{-}ion}(\vec{r},\vec{R}^0)\right]\psi_a(\vec{r}) = E_{el,a}\psi_a(\vec{r})$$

Ocena:

$$\langle A_{ab}\rangle \sim \frac{\hbar^2}{2M}\underbrace{\int d\vec{r}\,\psi_a^* \frac{\partial}{\partial R}\psi_b}_{\Downarrow\ \partial/\partial r} \int d\vec{R}\,\phi_a^* \frac{\partial}{\partial R}\phi_b$$

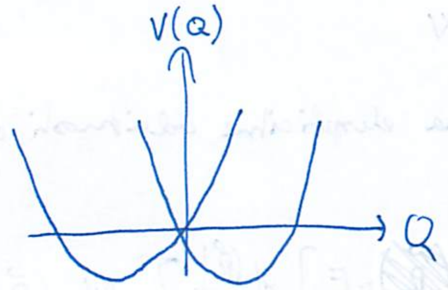
To bolj spada v prejšnji razdelek!

$$\sim \frac{1}{M}\langle p_{el}\rangle\langle p_{ion}\rangle \sim \frac{1}{M}\sqrt{mE^k_{el}}\sqrt{mE^k_{ion}} \sim \left(\frac{m}{M}\right)^{3/4} E^k_{el}$$

4. JAHN-TELLERJEV POJAV

Ena prvih aplikacij teorije grup v trdni snovi (1937).

Izrek: Če ima nelinearen sistem atomov več potencialnih ploskev, ki sovpadajo v eni točki, potem vsaj ena izmed teh ploskev nima minimuma v tej točki.



Deformacija
- statična: el. degeneracija odpravljena.
- dinamična: skakanje med različnimi minimumi.

Grupa G opisuje nedeformiran sistem. Simetrija se reducira na podgrupo S. Q_α pripada eni izmed degeneriranih ireducibilnih reprezentacij grupe G. V grupi S je Q_α invarianten (trivialna popolnoma simetrična upodobitev).

Renner-Tellerjev pojav: deformacija zaradi kvadratičnih členov.

$$M=\begin{pmatrix} M_{11} & M_{12}e^{i\alpha} \\ M_{12}e^{-i\alpha} & M_{22} \end{pmatrix} \qquad D = S^\dagger M S \qquad S=\begin{pmatrix} \cos\varphi\, e^{i\alpha} & \sin\varphi\, e^{i\alpha} \\ -\sin\varphi & \cos\varphi \end{pmatrix}$$

$$D_{1,2} = \Sigma \mp \sqrt{\Delta^2 + M_{12}^2} \qquad \Sigma = \frac{M_{11}+M_{22}}{2} \qquad \Delta = \frac{M_{11}-M_{22}}{2} \qquad \varphi = \frac{1}{2}\arctan\frac{2M_{12}}{M_{22}-M_{11}}$$

Primer: - dve elektronski stanji, $|1\rangle$ in $|2\rangle$

- dve nihajni prostostni stopnji, x, y $\qquad \hbar = 1 \quad M = 1$

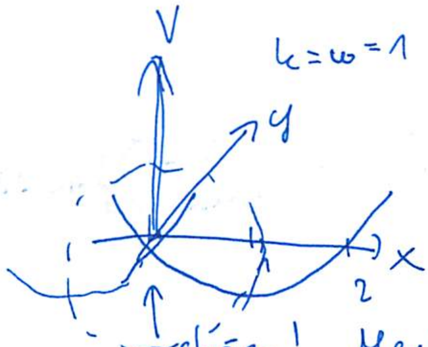
$$\hat{H} = -\frac{1}{2}\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}\right) + \sum_{ij} |i\rangle V_{ij} \langle j|$$

kinetična energija ionov $\qquad$ adiabatni el. potencial, odvisen od položaja ionov

$$\underline{V} = \frac{\omega}{2}(x^2+y^2)\,\underline{1} + k(x\sigma^x + y\sigma^y) = \begin{bmatrix} \frac{\omega}{2}\rho^2 & k(x-iy) \\ k(x+iy) & \frac{\omega}{2}\rho^2 \end{bmatrix} = \begin{bmatrix} \frac{\omega}{2}\rho^2 & k\rho e^{-i\theta} \\ k\rho e^{i\theta} & \frac{\omega}{2}\rho^2 \end{bmatrix}$$

$x = \rho\cos\theta \quad y = \rho\sin\theta$

Lastni vrednosti $V_{1,2} = \frac{\omega}{2}\rho^2 \pm k\rho$ $\qquad |\psi_1\rangle = \begin{bmatrix} e^{-i\theta}/\sqrt{2} \\ -1/\sqrt{2} \end{bmatrix} \quad |\psi_2\rangle = \begin{bmatrix} e^{-i\theta}/\sqrt{2} \\ 1/\sqrt{2} \end{bmatrix}$



stožec! Mexican hat potential

Minimum pri $\rho_0 = \frac{k}{\omega}$, degenerirano po θ

$$\frac{\partial}{\partial x} = \cos\theta\frac{\partial}{\partial\rho} - \frac{\sin\theta}{\rho}\frac{\partial}{\partial\theta}$$
$$\frac{\partial}{\partial y} = \sin\theta\frac{\partial}{\partial\rho} + \frac{\cos\theta}{\rho}\frac{\partial}{\partial\theta}$$

Tenzor sklopitev $H_{n,ij} = \langle\psi_i|\nabla|\psi_j\rangle$.

Poskrbeti moramo, da so diagonalni deli enaki 0. Avtomatično velja za realne valovne funkcije. Tukaj moramo sami poskrbeti za primerno izbiro faze.

$$|\tilde{\psi}_1\rangle = \begin{bmatrix} e^{-i\theta/2}/\sqrt{2} \\ -e^{i\theta/2}/\sqrt{2} \end{bmatrix} \qquad |\tilde{\psi}_2\rangle = \begin{bmatrix} e^{-i\theta/2}/\sqrt{2} \\ e^{i\theta/2}/\sqrt{2} \end{bmatrix}$$

$H_{n,12} = \langle\tilde{\psi}_1|\nabla|\tilde{\psi}_2\rangle = \frac{1}{\rho}(-\sin\theta, \cos\theta)\, i/2$ $\qquad$ Divergira pri $\rho \to 0$.

Mimogrede: $\tilde{\psi}_1(\theta)$ in $\tilde{\psi}_2(\theta)$ sta isto fizično stanje. Velja pa $\tilde{\psi}_1(\theta+2\pi) = -\tilde{\psi}_1(\theta)$. To ima merljive posledice.
Splošna lastnost disperzij v obliki stožca.

5. MATRIKA KONSTANT VZMETI

(angl. atomic force constants)

$\vec{R}_{nk} = \vec{R}_n + \vec{r}_k + \vec{u}_{nk}(t)$ momenti $\vec{p}_{nk}$

Gledamo odmike: $H = H_{ion}(\vec{R}) + E_{el}(\vec{R}) \longrightarrow H = H_{kin}(\vec{p}) + U(\vec{u})$

Harmonični približek:

$$U(\vec{u}) = U_0 + \frac{1}{2} \sum_{\substack{nk\alpha \\ n'k'\alpha'}} u_{nk\alpha} \underbrace{\frac{\partial^2 U}{\partial u_{nk\alpha}\partial u_{n'k'\alpha'}}}_{D} u_{n'k'\alpha'}$$

a) simetrična $3NK \times 3NK$ matrika

b) $\sum_{n'k'} D_{nk\alpha, n'k'\alpha'} = 0$ Homogen premik $F_{nk\alpha} = -\frac{\partial U}{\partial u_{nk\alpha}} = \sum D_{nk\alpha, n'k'\alpha'} u_{n'k'\alpha'}$

konst.

Manj pomembno:

c) $\sum_{n'k'} D_{nk\alpha, n'k'\alpha} R^0_{n'k'\gamma} = \sum D_{nk\alpha, n'k'\gamma} R^0_{n'k'\alpha}$ za vse $\alpha' \neq \gamma$

Čisti zasuk $\vec{u}_{n'k'} = \vec{w} \times \vec{R}^0_{nk}$

d) Vse simetrijske lastnosti kristala.

Medatomski potencial

$$U = \frac{1}{2} \sum_{nn'} \phi(\vec{R}_n + \vec{u}_n - (\vec{R}_{n'} + \vec{u}_{n'}))$$

$$= U_0 + \frac{1}{4} \sum_{nn'} (\vec{u}_n - \vec{u}_{n'}) \underbrace{\left.\frac{\partial^2 \phi}{\partial \vec{r} \partial \vec{r}}\right|_{\vec{R}_n - \vec{R}_{n'}}}_{\underline{\underline{\Phi}}(\vec{R}_n - \vec{R}_{n'})} (\vec{u}_n - \vec{u}_{n'}) = U_0 + \frac{1}{2} \sum \vec{u}_n \underline{\underline{D}}_{nn'} \vec{u}_{n'}$$

$$\underline{\underline{D}}_{nn'} = \delta_{nn'} \sum_m \underline{\underline{\Phi}}(\vec{R}_n - \vec{R}_m) - \underline{\underline{\Phi}}(\vec{R}_n - \vec{R}_{n'})$$

Prvi člen je vpliv vseh ostalih atomov, če jih premaknemo za negativen odmik obravnavanega.

Dva atoma, prim. pri $n=0$, premaknemo atom n'.

$$\vec{F}_{n' \to 0} = k_{n'} \hat{e}_{n'} (\hat{e}_{n'} \cdot \vec{u}_{n'}) \quad \Rightarrow \quad \underline{\underline{D}}_{0n'} = -k_{n'} \hat{e}_{n'} \otimes \hat{e}_{n'}$$

oz. $D_{0n'\,\alpha\beta} = -k_{n'} e_{n'\alpha} e_{n'\beta}$

$$D_{00\,\alpha\beta} = \sum_{n'} k_{n'} e_{n'\alpha} e_{n'\beta}$$

6. KLASIČNA NIHANJA

$$E_{kin} = \frac{1}{2} \sum_{nk} M_k \dot{\vec{u}}_{nk}^2$$

$$M_k \ddot{\vec{u}}_{nk} = -\frac{\partial U}{\partial \vec{u}_{nk}} = -\sum \underline{\underline{D}}_{nk,n'k'} \vec{u}_{n'k'}$$

Rešujemo v recipročnem prostoru.

Nastavek: $\vec{u}_{nk}^{(j)}(q,t) = \frac{u_0}{\sqrt{M_k N}} \vec{\varepsilon}_{k\vec{q}j}\, e^{i(\vec{q}\cdot\vec{R}_n - \omega_{\vec{q}j} t)}$

polarizacija — lastna frekvenca

$j = 1, \dots, 3K$: nihajni načini oz. veje (angl. normal mode). Kolektivni nihajni načini.

$$\underline{\underline{\mathcal{D}}}_{kk'}(\vec{q}) = \sum_{\vec{R}_n - \vec{R}_{n'}} \frac{1}{\sqrt{M_k M_{k'}}} \underline{\underline{D}}_{nk,n'k'}\, e^{-i\vec{q}\cdot(\vec{R}_n - \vec{R}_{n'})}$$

$$\omega_{\vec{q}j}^2 \vec{\varepsilon}_{k\vec{q}j} = \sum_{k'} \underline{\underline{\mathcal{D}}}_{kk'}(\vec{q})\, \vec{\varepsilon}_{k'\vec{q}j}$$

Do tu, 27.2.2024

a) $\underline{\underline{\mathcal{D}}}_{k'k}^*(\vec{q}) = \underline{\underline{\mathcal{D}}}_{kk'}(\vec{q})$ Hermitska, pozitivno definitna.

$\underline{\underline{D}}_{k'k}^{n'n} = \underline{\underline{D}}_{kk'}^{nn'}$ realna simetrična

$\underline{\underline{\mathcal{D}}}_{kk'}(\vec{q}) = \underline{\underline{\mathcal{D}}}_{k'k}(-\vec{q}) \quad \Rightarrow \quad \omega_{-\vec{q}j} = \omega_{\vec{q}j}$ in $\vec{\varepsilon}_{k-\vec{q}j} = \vec{\varepsilon}_{k\vec{q}j}^*$

b) $\sum_{k=1}^{K} \vec{\varepsilon}_{k\vec{q}j}^{\,*} \cdot \vec{\varepsilon}_{k\vec{q}j'} = \delta_{jj'}$

c) $\omega_{\vec{q}j}$ je definirana v 1. B.C. Ima vse sim. lastnosti točkovne grupe.

d) Akustične veje: $\omega_{\vec{q}j} \to 0$ $\qquad \vec{\varepsilon}_{k\vec{q}j} = \frac{\vec{u}}{\sqrt{M_k}}$

Analogija z Goldstonovim izrekom. Goldstone: če je zlomljena zvezna simetrija, obstajajo "brezmasne" vzbuditve.
V sistemih z Lorentzevo invarianco je število Goldstonovih bozonov enako številu generatorjev simetrije, ki je zlomljena.
↳ cf. Watanabe, Murayama 2012

e) Dolgovalovna limita

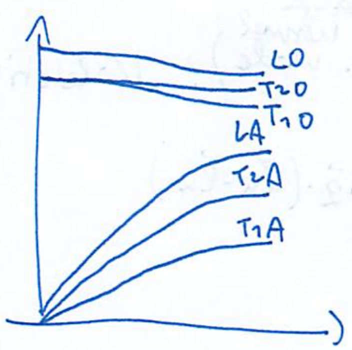
$$\vec{u}_n^{(j)} = \frac{1}{\sqrt{N}} \vec{\varepsilon}_j \, e^{i(\vec{q}\cdot\vec{R}_n - \omega_{\vec{q}j} t)}$$

$$M \omega_{\vec{q}j}^2 \vec{\varepsilon}_j = \sum_{n'} D_{nn'} e^{i\vec{q}\cdot(\vec{R}_n - \vec{R}_{n'})} \vec{\varepsilon}_j \doteq q^2 \,\underline{\underline{\tilde{D}}}(\hat{e}_q) \vec{\varepsilon}_j$$

$$\underline{\underline{\tilde{D}}}(\hat{e}_q) = -\frac{1}{2}\sum_{n'} \underline{\underline{D}}_{nn'} \left[\hat{e}_q \cdot (\vec{R}_n - \vec{R}_{n'})^2 \right]$$

$j = L, T_1, T_2 \qquad \vec{\varepsilon}_L \sim \hat{e}_{\vec{q}} \qquad \vec{\varepsilon}_{T_1}, \vec{\varepsilon}_{T_2} \sim \perp \hat{e}_{\vec{q}}$

$$c_j^2(\hat{e}_{\vec{q}}) = \left(\frac{\omega_{\vec{q}j}}{q}\right)^2 = \frac{1}{M} \vec{\varepsilon}_j \,\underline{\underline{\tilde{D}}}(\hat{e}_{\vec{q}}) \vec{\varepsilon}_j$$



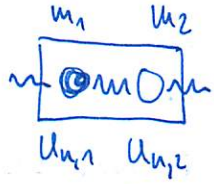
optični — oscilirajo iz faze, če različno nabiti, se sklapljajo z em poljem

akustične — oscilirajo v fazi

SEMINAR:

Veriga z bazo

$m_1 > m_2$



$$U = \frac{k}{2} \sum_n (u_{n,2} - u_{n,1})^2 + (u_{n+1,1} - u_{n,2})^2 \qquad E_{kin} = \frac{1}{2} \sum_n m_1 \dot{u}_{n1}^2 + m_2 \dot{u}_{n2}^2$$

$$D_{nk,n'k'} = \frac{\partial U}{\partial u_{nk} \partial u_{n'k'}} \qquad \mathcal{D}_{kk'}(\vec{q}) = \sum_{n'} \frac{1}{\sqrt{m_k m_{k'}}} D_{nk,n'k'} e^{i\vec{q}(R_{n'}-R_n)}$$

$n = n'$ $\quad D^0_{n,n} = \begin{bmatrix} 2k & -k \\ -k & 2k \end{bmatrix}$ $\qquad \mathcal{D}_{11} = \frac{2k}{m_1} \qquad \mathcal{D}_{22} = \frac{2k}{m_2}$

$n' = n+1$ $\quad D^+_{n,n+1} = \begin{bmatrix} 0 & -k \\ 0 & 0 \end{bmatrix}$ $\qquad \mathcal{D}_{12} = \frac{-k}{\sqrt{m_1 m_2}} (1 + e^{-iqa}) = \mathcal{D}_{21}^*$

$n' = n-1$ $\quad D^-_{n,n-1} = \begin{bmatrix} 0 & 0 \\ -k & 0 \end{bmatrix}$

$$\omega_q^2 = \frac{k}{m_1 m_2} \left[(m_1 + m_2) \pm \sqrt{(m_1 - m_2)^2 + 2 m_1 m_2 (1 + \cos qa)} \right]$$

$$\omega^2_{q=0} = \begin{cases} 0 & \text{akustična} \\ \frac{2k}{m^*} & \text{optična} \end{cases} \qquad \omega^2_{q=\pi/a} = \begin{cases} 2k/m_1 \\ 2k/m_2 \end{cases}$$

atomi enega tipa ležijo na vozlih valovanja s periodo 2a.

$\frac{1}{m^*} = \frac{1}{m_1} + \frac{1}{m_2}$ ker gre za relativno gibanje enih proti drugim

$$\omega_{q,A} = cq \qquad c = \sqrt{\frac{k}{2M}} \cdot a \qquad M = m_1 + m_2$$

7. TEORIJA ELASTIČNOSTI

Mikroskopsko strukturo bi radi zanemarili. Simetrijske lastnosti vseeno ostanejo pomembne. Posledica reda dolgega dosega.

Enoatomni kristal, zvezna limita: $\vec{u}_{n\kappa}(t) \to \vec{u}(\mathring{R}_{n\kappa}, t) \to \vec{u}(\vec{r}, t)$

$$U = \frac{1}{2} \sum_{\substack{\alpha\beta \\ nn'}} u_\alpha(\vec{R}_n) D_{\alpha\beta}(\vec{R}_n - \vec{R}_{n'}) u_\beta(\vec{R}_{n'})$$

$n \leftrightarrow n'$

$$= \frac{1}{4} \sum_{\substack{\alpha\beta \\ nn'}} u_\alpha(\vec{R}_n) D_{\alpha\beta}(\vec{R}_n - \vec{R}_{n'}) u_\beta(\vec{R}_{n'}) + u_\alpha(\vec{R}_{n'}) D_{\alpha\beta}(\vec{R}_{n'} - \vec{R}_n) u_\beta(\vec{R}_n)$$

$D_{\alpha\beta}(\vec{R}_{n'} - \vec{R}_n) = D_{\alpha\beta}(\vec{R}_n - \vec{R}_{n'})$

to velja za enoatomni kristal, ki ima center inverzije!

$$= -\frac{1}{4} \sum_{\substack{\alpha\beta \\ nn'}} \left(u_\alpha(\vec{R}_n) - u_\alpha(\vec{R}_{n'})\right) D_{\alpha\beta}(\vec{R}_n - \vec{R}_{n'}) \left(u_\beta(\vec{R}_n) - u_\beta(\vec{R}_{n'})\right)$$

$$u_\alpha(\vec{R}_{n'}) - u_\alpha(\vec{R}_n) = \sum_\gamma (R_{n'\gamma} - R_{n\gamma}) \left.\frac{\partial u_\alpha}{\partial x_\gamma}\right|_{\vec{r} = \vec{R}_n}$$

$$U = -\frac{1}{4} \sum_n \sum_{\vec{R}} \sum_{\substack{\alpha\beta \\ \gamma\delta}} R_\gamma D_{\alpha\beta}(\vec{R}) R_\delta \frac{\partial u_\alpha}{\partial x_\gamma} \frac{\partial u_\beta}{\partial x_\delta}$$

po vseh celicah

razmiki

$$\boxed{\begin{gathered} \mathcal{L} = T - U = \mathcal{L}(u, \dot{u}, \tfrac{\partial}{\partial x_\gamma} u) \\ \frac{\partial}{\partial t}\left(\frac{\partial \mathcal{L}}{\partial \dot{u}_\alpha}\right) = \frac{\partial \mathcal{L}}{\partial u_\alpha} - \frac{\partial}{\partial x_\gamma}\left(\frac{\partial \mathcal{L}}{\partial\left(\frac{\partial u_\alpha}{\partial x_\gamma}\right)}\right) \end{gathered}}$$

Tenzor elastičnosti (elastic stiffness):

$$C_{\alpha\beta\gamma\delta} = -\frac{1}{2} \frac{1}{V_0} \sum_{\vec{R}} R_\gamma D_{\alpha\beta}(\vec{R}) R_\delta$$

volumen osnovne celice

$$\rho \ddot{u}_\alpha = \sum_{\beta\gamma\delta} C_{\alpha\beta\gamma\delta} \frac{\partial^2 u_\beta}{\partial x_\gamma \partial x_\delta}$$

Simetrije:

a) $C_{\alpha\beta\gamma\delta} = C_{\beta\alpha\gamma\delta}$ $\qquad C_{\alpha\beta\gamma\delta} = C_{\alpha\beta\delta\gamma}$

b) $C_{(\alpha\beta)(\gamma\delta)} = C_{(\gamma\delta)(\alpha\beta)}$

c) Invariantnost na rotacijo: $C_{\alpha\beta\gamma\delta} = C_{\alpha\delta\gamma\beta}$ $\qquad \frac{\partial u_\beta}{\partial x_\delta} = -\frac{\partial u_\delta}{\partial x_\beta}$

Deformacijski tenzor: $\varepsilon_{\alpha\beta} = \frac{1}{2}\left(\frac{\partial u_\alpha}{\partial x_\beta} + \frac{\partial u_\beta}{\partial x_\alpha}\right)$
[strain tensor]

$$\rho \ddot{u}_\alpha = C_{\alpha\beta\gamma\delta} \frac{\partial}{\partial x_\beta} \varepsilon_{\gamma\delta}$$

Tenzor napetosti: $\sigma_{\alpha\beta} = C_{\alpha\beta\gamma\delta}\, \varepsilon_{\gamma\delta}$
[stress tensor]

$$\rho \ddot{u}_\alpha = \frac{\partial}{\partial x_\beta} \sigma_{\alpha\beta}$$

$$dF_\alpha = -\sigma_{\alpha\beta}\, \hat{n}_\beta\, d\Sigma$$

$$f = f_0 + \frac{1}{2} C_{\alpha\beta\gamma\delta}\, \varepsilon_{\alpha\beta}\, \varepsilon_{\gamma\delta} + \mathcal{O}(\varepsilon^3)$$

To je simetrizirana oblika potencialne energije iz začetka tega razdelka!

$$\sigma_{\alpha\beta} = \frac{\partial f}{\partial \varepsilon_{\alpha\beta}} \qquad C_{\alpha\beta\gamma\delta} = \frac{\delta \sigma_{\alpha\beta}}{\delta \varepsilon_{\gamma\delta}}$$

Voigtov zapis:

$\vec{\sigma} = (C)\, \vec{\varepsilon}$ $\qquad \frac{6(6+1)}{2} = 21$ neodvisnih elementov

$$\underline{\underline{\sigma}} = \begin{pmatrix} \sigma_{xx}^{1} & \sigma_{xy}^{6} & \sigma_{xz}^{5} \\ & \sigma_{yy}^{2} & \sigma_{yz}^{4} \\ & & \sigma_{zz}^{3} \end{pmatrix}$$

$\vec{\sigma} = (\sigma_{xx}, \sigma_{yy}, \sigma_{zz}, \sigma_{yz}, \sigma_{xz}, \sigma_{xy})$

$\vec{\varepsilon} = (\varepsilon_{xx}, \varepsilon_{yy}, \varepsilon_{zz}, 2\varepsilon_{yz}, 2\varepsilon_{xz}, \underbrace{2\varepsilon_{xy}}_{=\gamma_{xy}})$

$= \gamma_{xy}$ engineering shear strain

Kubičen: $C_{11} = C_{22} = C_{33}$ vsi ostali so enaki nič
$C_{12} = C_{23} = C_{31}$
$C_{44} = C_{55} = C_{66}$

SEMINAR!

Izotropen: kot kubičen + $C_{11} = C_{12} + 2C_{44}$

NEUMANNOVO NAČELO: Simetrijski elementi fizikalne lastnosti kristala morajo vključevati vse simetrijske lastnosti točkovne grupe kristala.

8. FONONI

$$\vec{u}_{nk}(t) = \sum_{\vec{q}j} Q_{\vec{q}j}(t)\, \vec{u}^{\,0}_{nk\vec{q}j} \qquad \vec{u}^{\,0}_{nk\vec{q}j} = \frac{1}{\sqrt{M_k N}}\, \vec{\varepsilon}_{k\vec{q}j}\, e^{i\vec{q}\cdot\vec{R}_n}$$

Delamo s kompleksnimi odmiki in zahtevamo $Q_{\vec{q}j} = Q^{*}_{-\vec{q}j}$, kar skupaj z $\vec{\varepsilon}_{k\vec{q}j} = \vec{\varepsilon}^{\,*}_{k-\vec{q}j}$ jamči, da so odmiki realni.

$$E_{kin} = \frac{1}{2}\sum_{nk} M_k \dot{u}_{nk}^2 = \frac{1}{2}\sum_{\substack{nk\\ \vec{q}j\\ \vec{q}'j'}} M_k \frac{1}{M_k N}\, \vec{\varepsilon}^{\,*}_{k\vec{q}j}\cdot\vec{\varepsilon}_{k\vec{q}'j'}\, e^{i(\vec{q}-\vec{q}')\cdot\vec{R}_n}\, \dot{Q}_{\vec{q}j}(t)\dot{Q}_{\vec{q}'j'}(t)$$

(2) $\sum_k \to \delta_{jj'}$ (1.) $\sum_n \to N\delta_{\vec{q}\vec{q}'}$

$$E_{kin} = \frac{1}{2}\sum_{\vec{q}j} |\dot{Q}_{\vec{q}j}|^2$$

$$U = \frac{1}{2}\sum_{\substack{nk\\ n'k'}} \vec{u}_{nk}\, \underline{\underline{D}}_{nk,n'k'}\, \vec{u}_{n'k'} = \frac{1}{2}\sum_{\substack{nk\\ n'k'\\ \vec{q}j\\ \vec{q}'j'}} \frac{1}{\sqrt{M_k M_{k'}}\, N}\, \vec{\varepsilon}^{\,*}_{k\vec{q}j}\, D_{nk,n'k'}\, \vec{\varepsilon}_{k'\vec{q}'j'}\, e^{i(\vec{q}'\vec{R}_{n'} - \vec{q}\cdot\vec{R}_n)}\, Q_{\vec{q}j} Q_{\vec{q}'j'}$$

$$\underline{\underline{\mathcal{D}}}_{kk'} = \sum_{n'} \frac{1}{\sqrt{M_k M_{k'}}}\, D_{nk,n'k'}\, e^{-i\vec{q}\cdot(\vec{R}_n - \vec{R}_{n'})}$$

$$= \frac{1}{2}\sum_{\substack{kk'\\ \vec{q}jj'}} \vec{\varepsilon}^{\,*}_{k\vec{q}j}\, \underbrace{\underline{\underline{\mathcal{D}}}_{kk'}\, \vec{\varepsilon}_{k'\vec{q}j'}}\, Q_{\vec{q}j}(t) Q_{\vec{q}j'}(t)$$

(1) $\sum_{k'} \to \omega^2_{\vec{q}j}\, \varepsilon_{k\vec{q}j'}$ (2) $\sum_k \to \delta_{jj'}$

$$U = \frac{1}{2}\sum_{\vec{q}j} |Q_{\vec{q}j}|^2\, \omega^2_{\vec{q}j}$$

Posplošen moment: $P_{\vec{q}j} = \dfrac{\partial E_{kin}}{\partial \dot{Q}^{*}_{\vec{q}j}} = \dot{Q}_{\vec{q}j}$

Harmonski oscilatorji: $\ddot{Q}_{\vec{q}j} + \omega^2_{\vec{q}j} Q_{\vec{q}j} = 0$

$$H = \frac{1}{2}\sum_{\vec{q}j} |P_{\vec{q}j}|^2 + \omega^2_{\vec{q}j}|Q_{\vec{q}j}|^2$$

Kanonična kvantizacija: $[Q_{\vec{q}j}, P_{\vec{q}'j'}] = i\hbar\, \delta_{\vec{q}\vec{q}'}\delta_{jj'}$

$$Q_{\vec{q}j} = \sqrt{\frac{\hbar}{2\omega_{\vec{q}j}}}\left(a_{\vec{q}j} + a^{+}_{-\vec{q}j}\right) \qquad P_{\vec{q}j} = i\sqrt{\frac{\hbar\omega_{\vec{q}j}}{2}}\left(a^{+}_{\vec{q}j} - a_{-\vec{q}j}\right)$$

$$H = \sum_{\vec{q}j} \hbar\omega_{\vec{q}j}\left(a^{+}_{\vec{q}j} a_{\vec{q}j} + 1/2\right)$$

$$\langle a^{+}_{\vec{q}j} a_{\vec{q}j}\rangle_T = \frac{1}{e^{\hbar\omega_{\vec{q}j}/k_B T} - 1}$$

9. GOSTOTA STANJ

$$D(\omega) = \frac{1}{V} \sum_{\vec{q}\,j} \delta(\omega - \omega_{\vec{q}j}) = \sum_j D_j(\omega)$$

$$D_j(\omega) = \int \frac{d^3\vec{q}}{(2\pi)^3}\, \delta(\omega - \omega_{\vec{q}j}) = \oint\!\int \frac{dS_{\vec{q}}\, dq_\perp}{(2\pi)^3}\, \delta\big(\omega - (\omega + \nabla_q \omega_{\vec{q}j} \cdot q_\perp)\big)$$

$$= \oint \frac{dS_{\vec{q}}}{(2\pi)^3} \frac{1}{|\nabla_q \omega_{\vec{q}j}|}$$

Kritične točke: $\nabla \omega_{\vec{q}j} = 0$

a) $\omega = cq \quad D \propto \oint \frac{dS_q}{(2\pi)^3} \frac{1}{c} \propto q^2 \propto \omega^2$

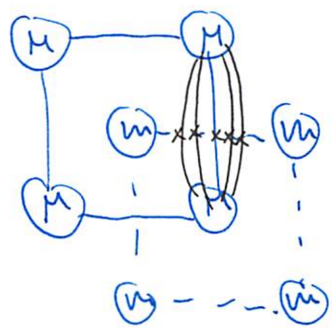
b) Min: $\omega = \omega_c + \alpha q^2 \quad D \propto \frac{q^2}{q} = q \propto \sqrt{\omega - \omega_c}$

c) Max: $\omega = \omega_c - \alpha q^2 \implies D \propto \sqrt{\omega_c - \omega}$

d) Sedelne točke: na eni strani končen odvod, na drugi neskončen.

Nujno vsaj ena točka tipa S_1 in ena tipa S_2, ter odvod $-\infty$ pri max.
Razlog so topološke lastnosti periodičnih zveznih funkcij.

V 2D:

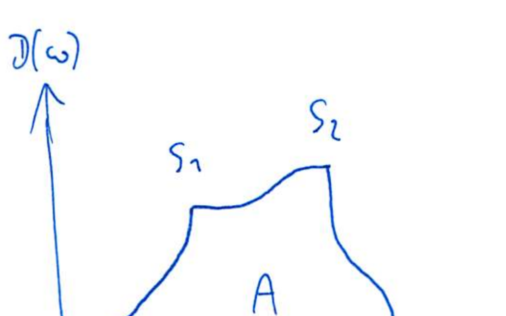


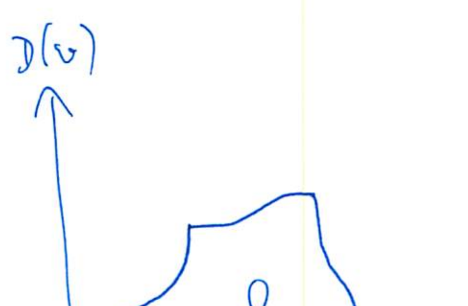
x: min na poti od enega M do drugega

Dobimo pot od m do m.

Na tej poti $\exists$ en maksimum.

To je sedelna točka!



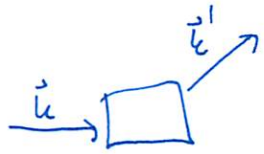


DO TU 4.3.2024

10. SIPANJE NEVTRONOV

Nevtroni čutijo jedra (močna interakcija), točkama.

En atom na celico. Potencial: $V(\vec r) = \sum_j v(\vec r - \vec R_j) = \tilde a \sum_j \delta(\vec r - \vec R_j)$



Začetno: $\phi_a = \frac{1}{\sqrt V} e^{i\vec k\cdot\vec r}$ $\quad \psi_a, \varepsilon_a \quad E = \varepsilon_a + \frac{\hbar^2 k^2}{2M_n}$

Končno: $\phi_b = \frac{1}{\sqrt V} e^{i\vec k'\cdot\vec r}$ $\quad \psi_b, \varepsilon_b \quad E' = \varepsilon_b + \frac{\hbar^2 k'^2}{2M_n}$

Celotna valovna: $\Phi = \phi\psi$

Fermijevo zlato pravilo:

$$P = \frac{2\pi}{\hbar}\sum_b \left|\langle\Phi_b|V(\vec r)|\Phi_a\rangle\right|^2 \delta(E'-E)$$

$$\langle\Phi_b|V(\vec r)|\Phi_a\rangle = \frac{\tilde a}{V}\sum_j\int d\vec r\, \langle\psi_b|e^{-i\vec k'\cdot\vec r}\,\delta(\vec r-\vec R_j)\,e^{i\vec k\cdot\vec r}|\psi_a\rangle$$

$$= \frac{\tilde a}{V}\sum_j \langle\psi_b|e^{i(\vec k-\vec k')\cdot\vec R_j}|\psi_a\rangle$$

$\vec q = \vec k - \vec k'$

$$P = \frac{2\pi\tilde a^2}{\hbar V^2}\sum_b \delta(\varepsilon_b-\varepsilon_a-\hbar\omega)\left|\langle\psi_b|\sum_j e^{i\vec q\cdot\vec R_j}|\psi_a\rangle\right|^2$$

$\hbar\omega$ je energija, ki jo pridobi kristal. $\hbar\vec q$ je gibalna količina, ki jo preda n.
Povprečimo po začetnih stanjih kristala z utežjo $p_a = e^{-\beta\varepsilon_a}/Z$.

DINAMIČNI STRUKTURNI FAKTOR:

$$S(\vec q,\omega) = \sum_a \frac{e^{-\beta\varepsilon_a}}{Z}\,\frac{1}{N}\sum_b \delta\left(\omega-\frac{\varepsilon_b-\varepsilon_a}{\hbar}\right)\left|\langle\psi_b|\sum_j e^{i\vec q\cdot\vec R_j}|\psi_a\rangle\right|^2$$

$$\delta(\omega) = \frac{1}{2\pi}\int dt\, e^{i\omega t}$$

$$S(\vec q,\omega) = \sum_{a,b}\frac{e^{-\beta\varepsilon_a}}{Z}\,\frac{1}{2\pi N}\int dt\, e^{i\omega t}\sum_{ij}\langle\psi_a|\overbrace{e^{i\frac{\varepsilon_a}{\hbar}t}e^{-i\vec q\cdot\vec R_i}e^{-i\frac{\varepsilon_b}{\hbar}t}}^{e^{-i\vec q\cdot\vec R_i(t)}}\overbrace{|\psi_b\rangle\langle\psi_b|}^{\sum_b \Rightarrow 1}e^{i\vec q\cdot\vec R_j}|\psi_a\rangle$$

$$= \frac{1}{2\pi N}\int dt\, e^{i\omega t}\left\langle\hat\rho(\vec q,t)\,\hat\rho(-\vec q,0)\right\rangle_T \qquad \langle\hat O\rangle_T = \frac{1}{Z}\mathrm{Tr}\left[e^{-\beta H}\hat O\right]$$

$$\hat\rho(\vec q,t) = \sum_i e^{-i\vec q\cdot\hat{\vec R}_i(t)}$$

$$\vec{R}_j = \vec{R}_j^{\,0} + \vec{u}_j$$

$$S(\vec{q},\omega) = \frac{1}{2\pi N}\int dt\, e^{i\omega t}\sum_{ij} e^{-i\vec{q}\cdot(\vec{R}_i^{\,0}-\vec{R}_j^{\,0})} f_{ij}(t) \qquad f_{ij}(t) = \left\langle e^{-i\vec{q}\cdot\vec{u}_i(t)}\, e^{i\vec{q}\cdot\vec{u}_j(0)}\right\rangle_T$$

$$P = \frac{N}{\hbar^2 V^2}\,\tilde{a}^2\, S(\vec{q},\omega)$$

upadni fluks $\quad j = \frac{\hbar k}{M_n V}$

SIPALNI PRESEK: $\quad \frac{dn}{dt} = j\,\frac{d\sigma}{d\Omega\, dE}\, d\Omega\, dE$

$$\frac{d\sigma}{d\Omega\, dE} = \frac{k'}{k}\,\frac{a^2}{\hbar}\, N S(\vec{q},\omega) \qquad \tilde{a} = \frac{2\pi\hbar^2 a}{M_n} \qquad a\text{: sipalna razdalja.}$$

Predfaktor je povezan z gostoto končnih stanj in s spremembo hitrosti delcev ob neelastičnih trkih.

ELASTIČNO SIPANJE

Limita $\omega \to 0 \qquad f_{ij}(t\to\infty) \to \left\langle e^{-i\vec{q}\cdot\vec{u}_i}\right\rangle_T \left\langle e^{i\vec{q}\cdot\vec{u}_j}\right\rangle_T = e^{-2W}$

Neodvisnost odmikov oz. ergodičnost.

$$S_{el}(\vec{q},\omega) = \tilde{S}(\vec{q})\,\delta(\omega)$$

$$\tilde{S}(\vec{q}) = \frac{1}{N}\sum_{ij} e^{-i\vec{q}\cdot(\vec{R}_i^{\,0}-\vec{R}_j^{\,0})}\, e^{-2W} = e^{-2W} N \sum_{\vec{G}} \delta_{\vec{q},\vec{G}}$$

$$\vec{u}_j = \frac{1}{\sqrt{NM}}\sum_{\vec{k}\lambda} Q_{k\lambda}\,\vec{\varepsilon}_{k\lambda}\, e^{i\vec{k}\cdot\vec{R}_j^{\,0}} \qquad Q_k = \sqrt{\frac{\hbar}{2\omega_k}}\,(a_k + a_{-k}^\dagger) \qquad k = (\vec{k},\lambda),\ -k = (-\vec{k},\lambda)$$

$$e^{-W} = \left\langle e^{i\vec{q}\cdot\vec{u}_j}\right\rangle = \left\langle \prod_{k>0,\lambda} \exp\left[i\frac{\vec{q}\cdot\vec{\varepsilon}_{k\lambda}}{\sqrt{NM}}\left(e^{i\vec{k}\cdot\vec{R}_j^{\,0}} Q_{k\lambda} + e^{-i\vec{k}\cdot\vec{R}_j^{\,0}} Q_{-k\lambda}\right)\right]\right\rangle_T$$

$$= \left\langle \prod_{\substack{k>0\\ \lambda}} \exp\left[\alpha_k(a_k + a_{-k}^\dagger) - \alpha_k^*(a_{-k} + a_k^\dagger)\right]\right\rangle_T = \underbrace{\left\langle \prod_{\substack{k\\ \lambda}} \exp\left(\alpha_k a_k - \alpha_k^* a_k^\dagger\right)\right\rangle_T}_{e^{-W_k}}$$

$$\alpha_k = \frac{i\vec{q}\cdot\vec{\varepsilon}_k\sqrt{\hbar}}{\sqrt{NM2\omega_k}}\, e^{i\vec{k}\cdot\vec{R}_j^{\,0}}$$

$$e^{-W} = \prod_k e^{-W_k}$$
$$W = \sum_k W_k$$

11. OPERATORJI PREMIKA

$$D(z) = e^{z a^\dagger - \bar{z} a} \qquad [a, a^\dagger] = 1 \qquad a|n\rangle = \sqrt{n}\,|n-1\rangle$$
$$a^\dagger |n\rangle = \sqrt{n+1}\,|n+1\rangle$$

unitaren. Velja $D(-z) = D(z)^\dagger$.

Weylova formula: $e^A e^B = e^{1/2 [A,B]} e^{A+B}$ (the "disentangling theorem")
(Baker-Campbell-Hausdorff)
Glauberjeva formula
$[A,[A,B]]=0$ in $[B,[A,B]]=0$

normalno urejeno — antinormalno urejeno

$$D(z) = e^{-\frac{1}{2}|z|^2} e^{z a^\dagger} e^{-\bar{z} a} = e^{\frac{1}{2}|z|^2} e^{-\bar{z} a} e^{z a^\dagger}$$

$$D(z)|0\rangle = e^{-\frac{1}{2}|z|^2} \sum_{n=0}^{\infty} \frac{z^n}{\sqrt{n!}} |n\rangle = |z\rangle \quad \text{koherentno stanje}$$

Adicijska formula:

$$D(z) D(z') = e^{\frac{1}{2}[z a^\dagger - \bar{z} a,\, z' a^\dagger - \bar{z}' a]} D(z+z')$$

$$= \underbrace{e^{\frac{1}{2} z \circ z'}}_{\text{čista faza}} D(z+z') \qquad z \circ z' = z\bar{z}' - \overline{z\bar{z}'} = 2\,\mathrm{Im}(z\bar{z}');$$
$$z \circ z = 0 \qquad z_1 \circ z_2 = -z_2 \circ z_1$$

$$\frac{\partial}{\partial z} \Rightarrow -\frac{1}{2} z D(z) - D(z) a = \frac{1}{2} z D(z) - a D(z) \Rightarrow [a, D(z)] = z D(z)$$

Premik operatorja:

$$D(z) a D(z)^\dagger = a - z$$

$$a D(z) - D(z) a = z D(z)$$
$$[a, D(z)] = z D(z)$$

Kvaziamična formula:

$$D(z) D(z') D(z)^\dagger = e^{z \circ z'} D(z')$$

Premik koh. stanja:

$$D(z)|\alpha\rangle = e^{\frac{1}{2} z \circ \alpha} |z+\alpha\rangle$$

Cahill-Glauber formula (1969): DOKAZ: SEMINAR!

$$\langle m | D(z) | n \rangle = \sqrt{\frac{n!}{m!}}\, z^{m-n} e^{-|z|^2/2} L_n^{(m-n)}(|z|^2)$$

↑ pridruženi laguerr

$$\langle n | D(z) | n \rangle = e^{-|z|^2/2} L_n(|z|^2)$$

↑ laguerr polinom $L_n(x) = \sum_{k=0}^{n} \binom{n}{k} \frac{(-1)^k}{k!} x^k$

$$\sum_{n=0}^{\infty} t^n L_n(x) = \frac{1}{1-t} e^{-\frac{tx}{1-t}}$$

generacijska funkcija

Do tu, 5.3.2024

Primer:

$$W = \sum_k W_k \qquad e^{-W_k} = \left\langle \exp\left(\alpha_k a_k - \alpha_k^* a_k^\dagger\right)\right\rangle_T \qquad \prod_k$$

$$z = -\alpha_k^* \qquad a_k \to a \qquad \gamma = \hbar\omega_k$$

$$e^{-W_k} = \frac{1}{Z}\mathrm{Tr}\Big(e^{-\gamma a^\dagger a} \underbrace{e^{z a^\dagger - \bar z a}}_{D(z)} \Big)$$

$$= \frac{1}{Z}\sum_{n=0}^{\infty} e^{-\gamma n}\langle n | D(z) | n\rangle$$

$$= \frac{1}{Z}\sum_{n=0}^{\infty} e^{-\gamma n} e^{-|\alpha|^2/2} L_n(|\alpha|^2)$$

$$= \cancel{\frac{1}{Z}}\, e^{-|\alpha|^2/2} \underbrace{\sum_{n=0}^{\infty} t^n L_n(x)}_{\cancel{\frac{1}{1-t}}\, e^{-\frac{tx}{1-t}}} \qquad t = e^{-\gamma} \quad x = |\alpha|^2$$

$$\frac{\partial t}{\partial \gamma} = -t$$

$$Z = \mathrm{Tr}\left[e^{-\gamma a^\dagger a}\right] = \sum_{n=0}^{\infty} (e^{-\gamma})^n = \sum_{n=0}^{\infty} t^n = \frac{1}{1-t}$$

$$\langle n\rangle = \frac{1}{Z}\underbrace{\frac{\partial}{\partial(-\gamma)}}_{-\frac{\partial Z}{\partial t}\frac{\partial t}{\partial \gamma}} Z = \frac{1}{Z}\sum_{n=0}^{\infty} n t^n = \frac{t}{1-t}$$

$$W_k = e^{-|\alpha|^2/2}\, e^{-\langle n\rangle|\alpha|^2}$$

$$e^{-W_k} = e^{-|\alpha_k|^2\left(\langle n_k\rangle + \frac{1}{2}\right)} \qquad \text{Debye-Wallerjev faktor}$$

$$|\alpha_k|^2 = \frac{(\vec{q}\cdot\vec{\varepsilon}_k)^2\hbar}{2NM\omega_k}$$

12. NEELASTIČNO SIPANJE

$$S(\vec q,\omega) = \frac{1}{2\pi N}\int dt\, e^{i\omega t}\sum_{ji} e^{-i\vec q\cdot(\vec R_i^0-\vec R_j^0)} f_{ij}(t)$$

$$f_{ij}(t) = \left\langle e^{-i\vec q\cdot\vec u_i(t)}\, e^{i\vec q\cdot\vec u_j(0)}\right\rangle_T \overset{\text{domača naloga!}}{=} \prod_k \left\langle e^{-(\tilde\alpha_k a_k - \tilde\alpha_k^* a_k^\dagger)}\, e^{\alpha_k a_k - \alpha_k^* a_k^\dagger}\right\rangle_T$$

$$\tilde\alpha_k = \frac{i\vec q\cdot\vec\varepsilon_k\sqrt{\hbar}}{\sqrt{2NM\omega_k}}\, e^{i\vec k\cdot\vec R_i^0}\, e^{-i\omega_k t}$$ (časovna odvisnost anihilacijskega)

$$z' = \tilde\alpha_k^*$$

$$f_{ij}^{(k)}(t) = \frac{1}{Z}\,\mathrm{Tr}\left[e^{-\gamma a^\dagger a} D(z')D(z)\right]$$

$$= \frac{1}{Z}\,\mathrm{Tr}\left[e^{-\gamma a^\dagger a}\, e^{\frac12 z'\circ z}\, D(z+z')\right]$$

$$= e^{\frac12 z'\circ z}\, e^{-|z+z'|^2(\bar n+1/2)}$$

$$= e^{\frac12(z'\bar z-\bar z' z)-(\bar n+1/2)(|z|^2+z'\bar z-\bar z' z+|z'|^2)}$$

$$= \underbrace{e^{-(\bar n+1/2)(|z|^2+|z'|^2)}}_{e^{-2W_k}}\; e^{-\bar n z'\bar z}\; e^{-(\bar n+1)\bar z' z}$$

$$-\bar z' z = \underbrace{\frac{(\vec q\cdot\vec\varepsilon_k)^2\hbar}{2M}}_{\lambda_k}\,\frac{1}{N}\, e^{+i\vec k\cdot(\vec R_i^0-\vec R_j^0)}\, e^{-i\omega_k t}$$

$$f_{ij}(t) = e^{-2W}\exp\left[\frac1N\sum_k\lambda_k\left\{(\langle\bar n_k\rangle+1)\, e^{i\vec k\cdot(\vec R_i^0-\vec R_j^0)}e^{-i\omega_k t}+\bar n_k\, e^{-i\vec k\cdot(\vec R_i^0-\vec R_j^0)}e^{+i\omega_k t}\right\}\right]$$

Razvoj do 1. reda: $f_{ij}(t) = e^{-2W}\prod_k\left[1+\frac{\lambda_k}{N}[\dots]\right]$

a) Ničfononski procesi: $S^{(0)}(\vec q,\omega) = e^{-2W} N\sum_{\vec G}\delta_{\vec q,\vec G}\,\delta(\omega)$

b) Enofononski procesi:

Emisija fonona

$V^e = e^{-2W}\lambda_k(\bar n_k+1)$

$\vec q = \vec k+\vec G$

$\omega = \omega_{\vec k}$

Absorpcija fonona

$V^a = e^{-2W}\lambda_k\bar n_k$

$\vec q = -\vec k+\vec G$

$\omega = -\omega_{\vec k}$

Do h

12. 3. 2024