Približek tesne vezi: p-pasovi v kubičnih kristalih

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1.) **Naloga** (Ashcroft, 2.naloga v 10.poglavju, str.189)

V kubičnem kristalu imajo funkcije, ki opisujejo trojno degeneracijo p-pasov obliko $x\phi(r)$, $y\phi(r)$ in $z\phi(r)$, kjer je funkcija $\phi(r)$ odvisna le od velikosti vektorja $\vec{r}$.
Energijo treh p-pasov dobimo iz

$$\left(\varepsilon(\vec{k}) - E_p\right)\delta_{ij} + \beta_{ij} + \tilde{\gamma}_{ij}(\vec{k}) = 0,$$

kjer je

$$\tilde{\gamma}_{ij}(\vec{k}) = \sum_{\vec{R}} e^{i\vec{k}\cdot\vec{R}}\gamma_{ij}(\vec{R}),$$

$$\gamma_{ij}(\vec{R}) = -\int d\vec{r}\,\psi_i^*(\vec{r})\psi_j(\vec{r}-\vec{R})\Delta U(\vec{r}),$$

$$\beta_{ij} = \gamma_{ij}(\vec{R}=0)$$

in $\varepsilon(\vec{k})$ Blochova energija.

a) Pokaži, da zaradi kubične simetrije velja

$$\beta_{xx} = \beta_{yy} = \beta_{zz} = \beta,$$

$$\beta_{xy} = 0.$$

b) Privzamimo ,da je $\gamma_{ij}(\vec{R})$ zanemarljiv razen za najbližje sosede $\vec{R}$. Pokaži,da je za preprosto kubično mrežo $\tilde{\gamma}_{ij}(\vec{k})$ diagonalen, tako da $x\phi(r)$, $y\phi(r)$ in $z\phi(r)$ generirajo neodvisne pasove.

c) Za fcc Bravaisovo mrežo, kjer v $\gamma_{ij}(\vec{R})$ upoštevamo le prvega najbližjega soseda, pokaži, da so energijski pasovi koreni spodnje enačbe

$$\begin{bmatrix} \varepsilon(\vec{k})-\varepsilon^0(\vec{k})+4\gamma_0\cos(\tfrac{1}{2}k_ya)\cos\left(\tfrac{1}{2}k_za\right) & -4\gamma_1\sin(\tfrac{1}{2}k_xa)\sin(\tfrac{1}{2}k_ya) & -4\gamma_1\sin(\tfrac{1}{2}k_xa)\sin(\tfrac{1}{2}k_za) \\ -4\gamma_1\sin(\tfrac{1}{2}k_ya)\sin(\tfrac{1}{2}k_xa) & \varepsilon(\vec{k})-\varepsilon^0(\vec{k})+4\gamma_0\cos(\tfrac{1}{2}k_ya)\cos\left(\tfrac{1}{2}k_za\right) & -4\gamma_1\sin(\tfrac{1}{2}k_ya)\sin(\tfrac{1}{2}k_za) \\ -4\gamma_1\sin(\tfrac{1}{2}k_za)\sin(\tfrac{1}{2}k_xa) & -4\gamma_1\sin(\tfrac{1}{2}k_za)\sin(\tfrac{1}{2}k_ya) & \varepsilon(\vec{k})-\varepsilon^0(\vec{k})+4\gamma_0\cos(\tfrac{1}{2}k_xa)\cos\left(\tfrac{1}{2}k_ya\right) \end{bmatrix}$$

$$= 0$$

Vpeljali smo

$$\varepsilon^0(\vec{k}) = E_p - \beta - 4\gamma_2[\cos(\tfrac{1}{2}k_xa)\cos(\tfrac{1}{2}k_za) + \cos(\tfrac{1}{2}k_xa)\cos(\tfrac{1}{2}k_ya) + \cos(\tfrac{1}{2}k_ya)\cos(\tfrac{1}{2}k_za)],$$

$$\gamma_0 = -\int d\vec{r}\left[x^2 - y\left(y - \tfrac{1}{2}a\right)\right]\phi(r)\phi([x^2 + (y - \tfrac{1}{2}a)^2 + \left(z - \tfrac{1}{2}a\right)^2]^{1/2})\Delta U(\vec{r}) \;,$$

$$\gamma_1 = -\int d\vec{r}\left[x\left(y - \tfrac{1}{2}a\right)\right]\phi(r)\phi([\left(x - \tfrac{1}{2}a\right)^2 + (y - \tfrac{1}{2}a)^2 + z^2]^{1/2})\Delta U(\vec{r}),$$

$$\gamma_2 = -\int d\vec{r}\, x\left(x - \tfrac{1}{2}a\right)\phi(r)\phi([\left(x - \tfrac{1}{2}a\right)^2 + (y - \tfrac{1}{2}a)^2 + z^2]^{1/2})\Delta U(\vec{r}).$$

d) Pokaži, da so pri $\vec{k}=0$ vsi trije pasovi degenerirani, ko imamo $\vec{k}$ v smeri kubične osi (ΓX) ali diagonale (ΓL) pa imamo dvojno degeneracijo.

2.) **Rešitev**

a) Želimo pozati $\beta_{xx} = \beta_{yy} = \beta_{zz} = \beta$ in $\beta_{xy} = 0.$

Zapišemo

$$\beta_{xx} = -\int d\vec{r}\psi_x^*(\vec{r}) \cdot \psi_x \Delta U(\vec{r}) = -\int d\vec{r} \cdot x^2 \cdot |\phi(\vec{r})|^2 \cdot \Delta U(\vec{r})$$

in

$$\beta_{yy} = -\int d\vec{r}\psi_y^*(\vec{r}) \cdot \psi_x \Delta U(\vec{r}) = -\int d\vec{r} \cdot y^2 \cdot |\phi(\vec{r})|^2 \cdot \Delta U(\vec{r})$$

Sedaj enačbi odštejemo $0 = \beta_{xx} - \beta_{yy} = -\int d\vec{r} \cdot (x^2 - y^2) \cdot |\phi(\vec{r})|^2 \cdot \Delta U(\vec{r})$ ter uvedemo novi spremenljivki $x' = x - y$ in $y' = x + y$, kar je v bistvu rotacija v prostoru.

Dobimo

$$0 = \beta_{xx} - \beta_{yy} = -\int d\vec{r} \cdot (x' \cdot y') \cdot |\phi(\vec{r}')|^2 \cdot \Delta U(\vec{r}') = \beta_{xy} = 0.$$

b) Upoštevati moramo le najbljižje sosede $\vec{R}$. Teh sosedov je 6, in sicer

$$\vec{R} = a(\pm 1,0,0); a(0,0,\pm 1); a(0,\pm 1,0).$$

Pokazati želimo, da so izvendiagonalni elementi $\tilde{\gamma}_{\mathrm{ij}}(\vec{\mathrm{k}})$ enaki 0.

$$\begin{aligned}
\tilde{\gamma}_{\mathrm{xy}}(\vec{\mathrm{k}}) = -e^{ik_x a} \int d\vec{r} \cdot xy \cdot \phi(\vec{r}) \cdot \phi\left(((x-a)^2 + y^2 + z^2)^{\frac{1}{2}}\right) \Delta U(\vec{r}) \\
-e^{-ik_x a} \int d\vec{r} \cdot xy \cdot \phi(\vec{r}) \cdot \phi\left(((x+a)^2 + y^2 + z^2)^{\frac{1}{2}}\right) \Delta U(\vec{r}) \\
-e^{ik_y a} \int d\vec{r} \cdot x(y-a) \cdot \phi(\vec{r}) \cdot \phi\left((x^2 + (y-a)^2 + z^2)^{\frac{1}{2}}\right) \Delta U(\vec{r}) \\
-e^{-ik_y a} \int d\vec{r} \cdot x(y+a) \cdot \phi(\vec{r}) \cdot \phi\left((x^2 + (y+a)^2 + z^2)^{\frac{1}{2}}\right) \Delta U(\vec{r}) \\
-e^{ik_z a} \int d\vec{r} \cdot xy \cdot \phi(\vec{r}) \cdot \phi\left((x^2 + y^2 + (z-a)^2)^{\frac{1}{2}}\right) \Delta U(\vec{r}) \\
-e^{-ik_z a} \int d\vec{r} \cdot xy \cdot \phi(\vec{r}) \cdot \phi\left((x^2 + y^2 + (z+a)^2)^{\frac{1}{2}}\right) \Delta U(\vec{r}) = 0
\end{aligned}$$

saj zaradi rotacijske transformacije $x \to y$ in $y \to -x$ vsak integral zamenja predznak.

c) Energijo dobimo, če postavimo determinant enako nič:

$$\left|\left(\varepsilon(\vec{k}) - E_p\right)\delta_{ij} + \beta_{ij} + \tilde{\gamma}_{ij}(\vec{k})\right| = 0$$

Najprej bomo pokazali, da velja

$$\varepsilon(\vec{k}) - E_p + \beta_{xx} + \tilde{\gamma}_{xx}(\vec{k}) = \varepsilon(\vec{\mathrm{k}}) - \varepsilon^0(\vec{\mathrm{k}}) + 4\gamma_0 \cos(\tfrac{1}{2}\mathrm{k_y a}) \cos\left(\tfrac{1}{2}\mathrm{k_z a}\right)$$

V približku tesnih vezi upoštevamo le najbližje sosede glede na izhodišče (teh je 12)

$$\vec{R} = a(\pm 1, \pm 1,0); a(\pm 1,0,\pm 1); a(0,\pm 1,\pm 1)$$

V tem približku bomo izračunali $\tilde{\gamma}_{xx}(\vec{k})$.

$$\tilde{\gamma}_{xx}(\vec{k}) = \sum_{R} e^{i\vec{k}\cdot\vec{R}} =$$

$$-e^{i\frac{a}{2}(k_x+k_y)}\int d\vec{r}\cdot x\left(x-\frac{a}{2}\right)\cdot\phi(\vec{r})\cdot\phi\left(\left[\left(x-\frac{a}{2}\right)^2+\left(y-\frac{a}{2}\right)^2+z^2\right]^{\frac{1}{2}}\right)\Delta U(\vec{r})$$

$$-e^{i\frac{a}{2}(k_x-k_y)}\int d\vec{r}\cdot x\left(x-\frac{a}{2}\right)\cdot\phi(\vec{r})\cdot\phi\left(\left[\left(x-\frac{a}{2}\right)^2+\left(y+\frac{a}{2}\right)^2+z^2\right]^{\frac{1}{2}}\right)\Delta U(\vec{r})$$

$$-e^{i\frac{a}{2}(-k_x+k_y)}\int d\vec{r}\cdot x\left(x+\frac{a}{2}\right)\cdot\phi(\vec{r})\cdot\phi\left(\left[\left(x+\frac{a}{2}\right)^2+\left(y-\frac{a}{2}\right)^2+z^2\right]^{\frac{1}{2}}\right)\Delta U(\vec{r})$$

$$-e^{i\frac{a}{2}(-k_x-k_y)}\int d\vec{r}\cdot x\left(x+\frac{a}{2}\right)\cdot\phi(\vec{r})\cdot\phi\left(\left[\left(x+\frac{a}{2}\right)^2+\left(y+\frac{a}{2}\right)^2+z^2\right]^{\frac{1}{2}}\right)\Delta U(\vec{r})$$

$$-e^{i\frac{a}{2}(k_x+k_z)}\int d\vec{r}\cdot x\left(x-\frac{a}{2}\right)\cdot\phi(\vec{r})\cdot\phi\left(\left[\left(x-\frac{a}{2}\right)^2+y^2+\left(z-\frac{a}{2}\right)^2\right]^{\frac{1}{2}}\right)\Delta U(\vec{r})$$

$$-e^{i\frac{a}{2}(k_x-k_z)}\int d\vec{r}\cdot x\left(x-\frac{a}{2}\right)\cdot\phi(\vec{r})\cdot\phi\left(\left[\left(x-\frac{a}{2}\right)^2+y^2+\left(z+\frac{a}{2}\right)^2\right]^{\frac{1}{2}}\right)\Delta U(\vec{r})$$

$$-e^{i\frac{a}{2}(-k_x+k_z)}\int d\vec{r}\cdot x\left(x+\frac{a}{2}\right)\cdot\phi(\vec{r})\cdot\phi\left(\left[\left(x+\frac{a}{2}\right)^2+y^2+\left(z-\frac{a}{2}\right)^2\right]^{\frac{1}{2}}\right)\Delta U(\vec{r})$$

$$-e^{i\frac{a}{2}(-k_x-k_z)}\int d\vec{r}\cdot x\left(x+\frac{a}{2}\right)\cdot\phi(\vec{r})\cdot\phi\left(\left[\left(x+\frac{a}{2}\right)^2+y^2+\left(z+\frac{a}{2}\right)^2\right]^{\frac{1}{2}}\right)\Delta U(\vec{r})$$

$$-e^{i\frac{a}{2}(k_y+k_z)}\int d\vec{r}\cdot x^2\cdot\phi(\vec{r})\cdot\phi\left(\left[x^2+\left(y-\frac{a}{2}\right)^2+\left(z-\frac{a}{2}\right)^2\right]^{\frac{1}{2}}\right)\Delta U(\vec{r})$$

$$-e^{i\frac{a}{2}(k_y-k_z)}\int d\vec{r}\cdot x^2\cdot\phi(\vec{r})\cdot\phi\left(\left[x^2+\left(y-\frac{a}{2}\right)^2+\left(z+\frac{a}{2}\right)^2\right]^{\frac{1}{2}}\right)\Delta U(\vec{r})$$

$$-e^{i\frac{a}{2}(-k_y+k_z)}\int d\vec{r}\cdot x^2\cdot\phi(\vec{r})\cdot\phi\left(\left[x^2+\left(y+\frac{a}{2}\right)^2+\left(z-\frac{a}{2}\right)^2\right]^{\frac{1}{2}}\right)\Delta U(\vec{r})$$

$$-e^{i\frac{a}{2}(-k_y-k_z)}\int d\vec{r}\cdot x^2\cdot\phi(\vec{r})\cdot\phi\left(\left[x^2+\left(y+\frac{a}{2}\right)^2+\left(z+\frac{a}{2}\right)^2\right]^{\frac{1}{2}}\right)\Delta U(\vec{r})$$

Opazimo

$$-\int d\vec{r}\cdot x\left(x-\frac{a}{2}\right)\cdot\phi(\vec{r})\cdot\phi\left(\left[\left(x-\frac{a}{2}\right)^2+\left(y-\frac{a}{2}\right)^2+z^2\right]^{\frac{1}{2}}\right)\Delta U(\vec{r})=\gamma_2$$

$$-\int d\vec{r}\cdot x^2\cdot\phi(\vec{r})\cdot\phi\left(\left[x^2+\left(y+\frac{a}{2}\right)^2+\left(z+\frac{a}{2}\right)^2\right]^{\frac{1}{2}}\right)\Delta U(\vec{r})=\gamma_0+\gamma_2$$

Torej lahko zgornjo enačbo prepišemo v

$$\tilde{\gamma}_{xx}(\vec{k})=\begin{pmatrix} e^{i\frac{a}{2}(k_x+k_y)}+e^{i\frac{a}{2}(k_x-k_y)}+e^{-i\frac{a}{2}(k_x+k_y)}+e^{-i\frac{a}{2}(k_x-k_y)}+ \\ +e^{i\frac{a}{2}(k_x+k_z)}+e^{i\frac{a}{2}(k_x-k_z)}+e^{-i\frac{a}{2}(k_x+k_z)}+e^{-i\frac{a}{2}(k_x-k_z)} \end{pmatrix}\gamma_2$$

$$+\left(e^{i\frac{a}{2}(k_y+k_z)}+e^{i\frac{a}{2}(k_y-k_z)}+e^{-i\frac{a}{2}(k_y+k_z)}+e^{-i\frac{a}{2}(k_y-k_z)}\right)(\gamma_0+\gamma_2)$$

oziroma

$$\tilde{\gamma}_{xx}(\vec{k})=\left(4\cos\left(\tfrac{1}{2}k_xa\right)\cos\left(\tfrac{1}{2}k_ya\right)+4\cos\left(\tfrac{1}{2}k_xa\right)\cos\left(\tfrac{1}{2}k_za\right)\right)\gamma_2$$
$$+4\cos\left(\tfrac{1}{2}k_ya\right)\cos\left(\tfrac{1}{2}k_za\right)(\gamma_0+\gamma_2)$$

Sedaj lahko $\tilde{\gamma}_{xx}(\vec{k})$ vstavimo v začetno enačbo in z malo računanja dobimo

$$\varepsilon(\vec{k})-E_p+\beta_{xx}+\tilde{\gamma}_{xx}(\vec{k})=\varepsilon(\vec{k})\text{-}\varepsilon^0(\vec{k})+4\gamma_0\cos(\tfrac{1}{2}k_ya)\cos\left(\tfrac{1}{2}k_za\right)$$

kar smo hoteli pokazati. Ostale elemente dobimo na podoben način.

d) Za $\vec{k}$=0 so vsi trije pasovi degenerirani

$$\varepsilon_0=E_p-\beta-12\gamma_2-4\gamma_0\ \rightarrow\ E_p-\beta=\varepsilon_0+12\gamma_2+4\gamma_0$$

Za $\vec{k}$ v smeri osi x dobimo $\Gamma X-\vec{k}=\left(\frac{2\pi\mu}{a},0{,}0\right)$, kjer $0\leq\mu\leq 1$.

$$\frac{e_1(\mu)}{e_0}=1+\frac{8\gamma_2}{e_0}(1-\cos(\pi\cdot\mu))$$

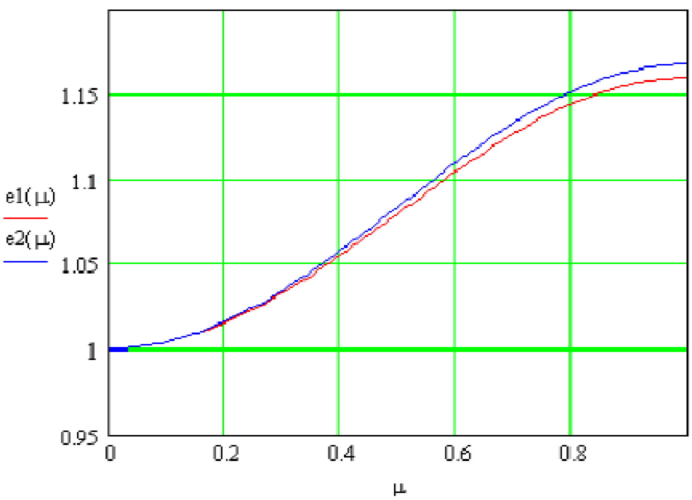
in

$$\frac{e_2(\mu)}{e_0}=1+\frac{8\gamma_2+4\gamma_0}{e_0}(1-\cos(\pi\cdot\mu))$$

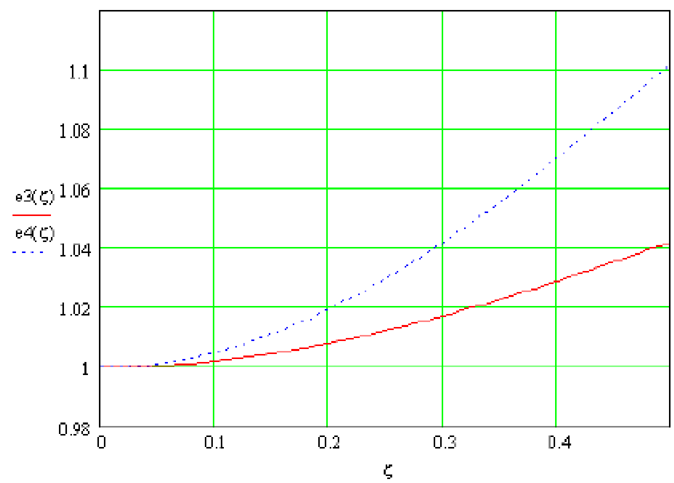
Za $\vec{k}$ v smeri diagonale : $\Gamma L - \vec{k} = \frac{2\pi}{a}(\xi, \xi, \xi)$, kjer $0 \leq \xi \leq \frac{1}{2}$.

$$\frac{e_1(\xi)}{e_0} = 1 + \frac{12\gamma_2 + 4\gamma_0 - 4\gamma_1}{e_0} sin^2(\pi \cdot \xi)$$

$$\frac{e_2(\xi)}{e_0} = 1 + \frac{12\gamma_2 + 4\gamma_0 + 8\gamma_1}{e_0} sin^2(\pi \cdot \xi)$$



Slika 1: Degeneracija; $\vec{k}$ v smeri osi x (ΓX)



Slika 2: Degeneracija, $\vec{k}$ v smeri diagonale