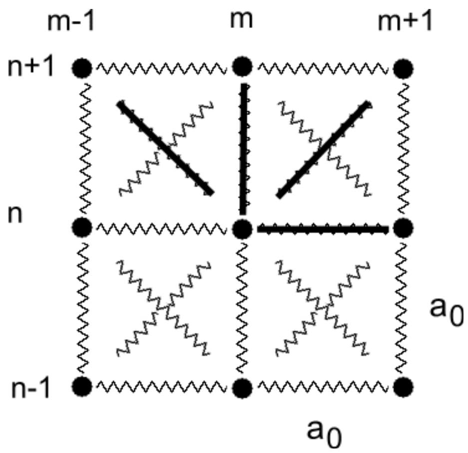
Disperzija fononov na dvodimenzionalni mreži

Martin Strojnik
FMF, vaje iz fizike trdne snovi, 26.3.2008

Predstavimo kristal kot dvodimenzionalno mrežo atomov, kjer je vsak atom povezan z vzmetmi z osmimi sosednjimi atomi.



Z m in n označimo koordinate v x in y smeri. $\mathbf{R}_{mn}$ naj bodo Bravaisovi vektorji do mrežnih koordinat, $\mathbf{u}_{mn}$ pa odmiki atomov iz teh 'ravnovesnih' leg. Tako zapišemo koordinato atoma $\mathbf{r}_{mn} = \mathbf{R}_{mn} + \mathbf{u}_{mn}$. Zapišimo posebej kinetični in potencialni del energije (kjer predstavlja $r = |\mathbf{r}|$)

$$T = \frac{M}{2}\sum_{m,n}\dot{\mathbf{r}}^2_{mn} = \frac{M}{2}\sum_{mn}\dot{\mathbf{u}}^2_{mn}, \tag{1}$$

$$V = \frac{K}{2}\sum_{\substack{m,n\\ \Delta m,\Delta n}}\left(|\mathbf{r}_{mn} - \mathbf{r}_{m+\Delta m,n+\Delta n}| - R_{\Delta m,\Delta n}\right)^2. \tag{2}$$

Pri potencialem delu pri vsakem atomu seštevamo še po njegovih neposrednih sosedih. Kjer pa zato, da upoštevamo vse vezi samo enkrat, seštevamo zgolj po sosedih

$$(\Delta m, \Delta n) = (-1,1)\,,(0,1)\,,(1,0)\,,(1,1)$$

$$\mathbf{R}_{\Delta m,\Delta n} = \begin{bmatrix}\Delta m\\ \Delta n\end{bmatrix} a_0$$

Najprej nekoliko preuredimo izraz za V :

$$\begin{aligned}
|\mathbf{r}_{mn} - \mathbf{r}_{m+\Delta m,n+\Delta n}| &= |\mathbf{R}_{mn} + \mathbf{u}_{mn} - \mathbf{R}_{m+\Delta m,n+\Delta n} - \mathbf{u}_{m+\Delta m,n+\Delta n}| \\
&= |-\mathbf{R}_{\Delta m,\Delta n} + (\mathbf{u}_{mn} - \mathbf{u}_{m+\Delta m,n+\Delta n})| \\
&= \sqrt{R^2_{\Delta m,\Delta n} - 2\mathbf{R}_{\Delta m,\Delta n}\cdot(\mathbf{u}_{mn} - \mathbf{u}_{m+\Delta m,n+\Delta n}) + (\mathbf{u}_{mn} - \mathbf{u}_{m+\Delta m,n+\Delta n})^2} \\
&\approx R_{\Delta m,\Delta n}\sqrt{1 - \frac{2\mathbf{R}_{\Delta m,\Delta n}\cdot(\mathbf{u}_{mn} - \mathbf{u}_{m+\Delta m,n+\Delta n})}{R^2_{\Delta m,\Delta n}}} \\
&\approx R_{\Delta m,\Delta n}\left(1 - \frac{\mathbf{R}_{\Delta m,\Delta n}(\mathbf{u}_{mn} - \mathbf{u}_{m+\Delta m,n+\Delta n})}{R^2_{\Delta m,\Delta n}}\right)
\end{aligned}$$

Sedaj lahko prepišemo potencialni del kot

$$\begin{aligned}
V &= \frac{K}{2}\sum_{\substack{m,n\\ \Delta m,\Delta n}}\left(-\frac{\mathbf{R}_{\Delta m,\Delta n}\cdot(\mathbf{u}_{mn} - \mathbf{u}_{m+\Delta m,n+\Delta n})}{R_{\Delta m,\Delta n}}\right)^2 \\
&= \frac{K}{2}\sum_{\substack{m,n\\ \Delta m,\Delta n}}\left(\mathbf{e}_{\Delta m,\Delta n}\cdot(\mathbf{u}_{mn} - \mathbf{u}_{m+\Delta m,n+\Delta n})\right)^2 \quad ; \quad \mathbf{e}_{\Delta m,\Delta n} = \frac{\mathbf{R}_{\Delta m,\Delta n}}{R_{\Delta m,\Delta n}} \qquad (3)
\end{aligned}$$

Imamo vse komponente Lagrangeove funkcije $L = T - V$, in lahko zapišemo Eluer-Lagrangeov sistem

$$\frac{\partial L}{\partial \mathbf{u}_{mn}} - \frac{d}{dt}\frac{\partial L}{\partial \dot{\mathbf{u}}_{mn}} = 0,$$

kjer za $\mathbf{u}_{mn}$ vzamemo nastavek

$$\mathbf{u}_{mn} = \mathbf{A}(\mathbf{k})\, e^{i\mathbf{k}\mathbf{R}_{mn}} e^{-i\omega t}. \qquad (4)$$

Prvi del je tako enak

$$\begin{aligned}
\frac{\partial L}{\partial \mathbf{u}_{mn}} &= -\frac{\partial V}{\partial \mathbf{u}_{mn}} = -K\sum_{\Delta m,\Delta n}\left(\mathbf{e}_{\Delta m,\Delta n}\cdot(-\mathbf{u}_{m+\Delta m,n+\Delta n} + 2\mathbf{u}_{mn} - \mathbf{u}_{m-\Delta m,n-\Delta n})\right)\mathbf{e}_{\Delta m,\Delta n} \\
&= -K\sum_{\Delta m,\Delta n}\left(-e^{i\mathbf{k}\mathbf{R}_{m+\Delta m,n+\Delta n}} + 2e^{i\mathbf{k}\mathbf{R}_{mn}} - e^{i\mathbf{k}\mathbf{R}_{m-\Delta m,n-\Delta n}}\right)e^{-i\omega t}\left(\mathbf{e}_{\Delta m,\Delta n}\cdot\mathbf{A}(\mathbf{k})\right)\mathbf{e}_{\Delta m,\Delta n} \\
&= -K\sum_{\Delta m,\Delta n} e^{i\mathbf{k}\mathbf{R}_{mn}}e^{-i\omega t}\left(2 - \left(e^{i\mathbf{k}\mathbf{R}_{\Delta m,\Delta n}} + e^{i\mathbf{k}\mathbf{R}_{-\Delta m,-\Delta n}}\right)\right)\left(\mathbf{e}_{\Delta m,\Delta n}\cdot\mathbf{A}(\mathbf{k})\right)\mathbf{e}_{\Delta m,\Delta n} \\
&= -2K\sum_{\Delta m,\Delta n} e^{i\mathbf{k}\mathbf{R}_{mn}}e^{-i\omega t}\left(1 - \cos(\mathbf{k}\mathbf{R}_{\Delta m,\Delta n})\right)\left(\mathbf{e}_{\Delta m,\Delta n}\cdot\mathbf{A}(\mathbf{k})\right)\mathbf{e}_{\Delta m,\Delta n} \\
&= -4K\sum_{\Delta m,\Delta n} e^{i\mathbf{k}\mathbf{R}_{mn}}e^{-i\omega t}\sin^2\left(\frac{\mathbf{k}\mathbf{R}_{\Delta m,\Delta n}}{2}\right)\left(\mathbf{e}_{\Delta m,\Delta n}\cdot\mathbf{A}(\mathbf{k})\right)\mathbf{e}_{\Delta m,\Delta n} \qquad (5)
\end{aligned}$$

drugi pa

$$\frac{d}{dt}\frac{\partial L}{\partial \dot{\mathbf{u}}_{mn}} = \frac{d}{dt}\frac{\partial T}{\partial \dot{\mathbf{u}}_{mn}} = M\ddot{\mathbf{u}}_{mn} = -M\omega^2\mathbf{A}(\mathbf{k})\, e^{i\mathbf{k}\mathbf{R}_{mn}}e^{-i\omega t} \qquad (6)$$

Sestavimo ju v gibalno enačbo, pokrajšamo eksponentne valovne dele in dobimo

$$
\begin{aligned}
4K \sum_{\Delta m,\Delta n} \sin^2\left(\frac{\mathbf{kR}_{\Delta m,\Delta n}}{2}\right)\left(\mathbf{e}_{\Delta m,\Delta n}\cdot\mathbf{A}(\mathbf{k})\right)\mathbf{e}_{\Delta m,\Delta n} - M\omega^2\mathbf{A}(\mathbf{k}) &= 0 \\
4\omega_0^2 \sum_{\Delta m,\Delta n} \sin^2\left(\frac{\mathbf{kR}_{\Delta m,\Delta n}}{2}\right)\left(\mathbf{e}_{\Delta m,\Delta n}\cdot\mathbf{A}(\mathbf{k})\right)\mathbf{e}_{\Delta m,\Delta n} - \omega^2\mathbf{A}(\mathbf{k}) &= 0 \quad ; \quad \frac{K}{M} = \omega_0^2 \qquad (7)
\end{aligned}
$$

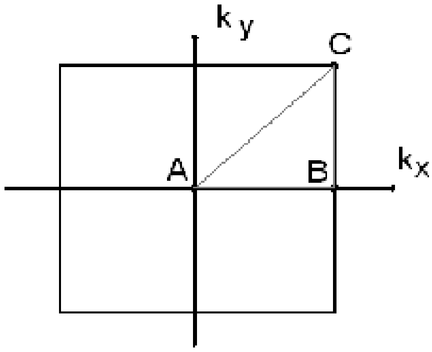
oz. v matrični obliki $\underline{E}\mathbf{A} = 0$, kjer je $\mathbf{A} = \begin{bmatrix} A_x \\ A_y \end{bmatrix}$, ob upoštevanju relacije

$$(\widehat{\mathbf{e}}\cdot\mathbf{A})\,\widehat{\mathbf{e}} = \begin{bmatrix} e_x e_x & e_y e_x \\ e_x e_y & e_y e_y \end{bmatrix}\mathbf{A}$$

pa dobimo matriko $\underline{E}$:

$$\begin{bmatrix} 2\omega_0^2\left(\sin^2\frac{\mathbf{kR}_{-1,1}}{2} + 2\sin^2\frac{\mathbf{kR}_{1,0}}{2} + \sin^2\frac{\mathbf{kR}_{1,1}}{2}\right) - \omega^2 & 2\omega_0^2\left(-\sin^2\frac{\mathbf{kR}_{-1,1}}{2} + \sin^2\frac{\mathbf{kR}_{1,1}}{2}\right) \\ 2\omega_0^2\left(-\sin^2\frac{\mathbf{kR}_{-1,1}}{2} + \sin^2\frac{\mathbf{kR}_{1,1}}{2}\right) & 2\omega_0^2\left(\sin^2\frac{\mathbf{kR}_{-1,1}}{2} + 2\sin^2\frac{\mathbf{kR}_{0,1}}{2} + \sin^2\frac{\mathbf{kR}_{1,1}}{2}\right) - \omega^2 \end{bmatrix} \qquad (8)$$

Sedaj lahko izračunamo energijske pasove v prvi Brillouinovi coni po poti A$(0,0)$-B$\left(\frac{\pi}{a_0},0\right)$-C$\left(\frac{\pi}{a_0},\frac{\pi}{a_0}\right)$-A$(0,0)$:



1) $k_x \in \left[0, \frac{\pi}{a_0}\right], k_y = 0$
Matrika E z lastnimi vrednostmi in vektorji je:

$$E = \begin{bmatrix} 8\omega_0^2\sin^2\frac{\mathbf{k_x a_0}}{2} - \omega^2 & 0 \\ 0 & 4\omega_0^2\sin^2\frac{\mathbf{k_x a_0}}{2} - \omega^2 \end{bmatrix} \qquad \begin{aligned} \omega_1^2 &= 4\omega_0^2\sin^2\left(\tfrac{1}{2}k_x a_0\right) & A_1 &= \begin{bmatrix} 0 \\ 1 \end{bmatrix} \\ \omega_2^2 &= 8\omega_0^2\sin^2\left(\tfrac{1}{2}k_x a_0\right) & A_2 &= \begin{bmatrix} 1 \\ 0 \end{bmatrix} \end{aligned}$$

2) $k_x = \frac{\pi}{a_0}, k_y \in \left[0, \frac{\pi}{a_0}\right]$
Matrika E z lastnimi vrednostmi in vektorji je:

$$E = \begin{bmatrix} 4\omega_0^2\left(1 + \cos^2\left(\frac{k_y a_0}{2}\right)\right) - \omega^2 & 0 \\ 0 & 4\omega_0^2 - \omega^2 \end{bmatrix} \qquad \begin{aligned} \omega_1^2 &= 4\omega_0^2 & A_1 &= \begin{bmatrix} 0 \\ 1 \end{bmatrix} \\ \omega_2^2 &= 4\omega_0^2\left(1 + \cos^2\left(\tfrac{1}{2}a_0 k_y\right)\right) & A_2 &= \begin{bmatrix} 1 \\ 0 \end{bmatrix} \end{aligned}$$

3) $k_x = k_y = k \in \left[0, \frac{\pi}{a_0}\right]$
Matrika E z lastnimi vrednostmi in vektorji je:

$$E = \begin{bmatrix} 2\omega_0^2\left(2\sin^2\frac{a_0k}{2} + \sin^2\frac{2a_0k}{2}\right) - \omega^2 & 2\omega_0^2\sin^2(a_0k) \\ 2\omega_0^2\sin^2(a_0k) & 2\omega_0^2\left(2\sin^2\frac{a_0k}{2} + \sin^2\frac{2a_0k}{2}\right) - \omega^2 \end{bmatrix}$$

$$\omega_1^2 = 4\omega_0^2\sin^2\left(\tfrac{1}{2}ka_0\right) \qquad A_1 = \begin{bmatrix} -1 \\ 1 \end{bmatrix}$$

$$\omega_2^2 = 4\omega_0^2\sin^2(ka_0) + 4\omega_0^2\sin^2\left(\tfrac{1}{2}ka_0\right) \qquad A_2 = \begin{bmatrix} 1 \\ 1 \end{bmatrix}$$

Disperzijska zveza po izbrani poti je narisana na spodnjem grafu, pri čemer ω_1 ustreza transverzalnemu, ω_2 pa longitudinalnemu nihanju atomov, glede na smer širitve vala.