Grüneisenov parameter

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1 Definicija Grüneisenovega parametra

Poglejmo najprej, kaj sploh je Grüneisenov parameter. Koeficient temperaturnega raztezka lahko zapišem kot

$$\alpha = \frac{1}{L}\left(\frac{\partial L}{\partial T}\right)_p,$$

pri čemer se zavedam, da računam v 1D, zato volumen V povsod nadomestim z dolžino L. Izračunati moram torej $(\frac{\partial L}{\partial T})_p$, zato se poslužim sledečega trika:

$$\left(\frac{\partial L}{\partial T}\right)_p = -\frac{\left(\frac{\partial p}{\partial T}\right)_L}{\left(\frac{\partial p}{\partial L}\right)_T} \tag{1}$$

Elastnični modul E smo definirali kot

$$\left(\frac{\partial p}{\partial L}\right)_T = -EL,$$

torej se (1) zapiše kot

$$\left(\frac{\partial L}{\partial T}\right)_p = -\frac{1}{EL}\left(\frac{\partial p}{\partial T}\right)_L \tag{2}$$

Poiskati je torej treba $(\frac{\partial p}{\partial T})_L$. Spomnim se termodinamike in proste energije F:

$$F = U - TS$$

$$dF = dU - dTS - TdS$$

$$dU = -pdL + TdS$$

$$dF = -pdL - SdT$$

$$p = -\left(\frac{\partial F}{\partial L}\right)_T$$

$$\left(\frac{\partial U}{\partial T}\right)_L = T\left(\frac{\partial S}{\partial T}\right)_L$$

$$F = U - T\int_0^T \frac{dT'}{T'}\left(\frac{\partial U}{\partial T}\right)_L$$

Energijo U lahko zapišem kot člen brez fononov + prispevek fononov:

$$U = U^{eq} + \frac{1}{2}\sum_k \hbar\omega_k + \sum_k \hbar\omega_k n_k \tag{3}$$

$$n_k = \frac{1}{e^{\beta\hbar\omega_k} - 1}$$

V (3) ostane le 3. člen, saj je samo ta odvisen od T in zato edini preživi odvajanje po T . Tako dobim iskani odvod:

$$\left(\frac{\partial p}{\partial T}\right)_L = \sum_k -\frac{\partial \hbar\omega_k}{\partial L}\frac{\partial n_k}{\partial T}$$

Velja še:

$$c_v = \sum_k \frac{\hbar\omega_k}{L} + \frac{\partial}{\partial T} n_k \tag{4}$$

Koeficient temperaturnega raztezka α je torej

$$\alpha = \frac{1}{LE}\sum_k -\frac{\partial \hbar\omega_k}{\partial L}\frac{\partial n_k}{\partial T}$$
$$= \frac{1}{LE}\sum_k -\frac{\partial \hbar\omega_k}{\partial L}\frac{L}{\hbar\omega_k}\frac{\hbar\omega_k}{L}\partial L\frac{\partial n_k}{\partial T}$$
$$= \frac{1}{LE}\sum_k \gamma_k c_{vk},$$

kjer smo vpeljali Grüneisenov parameter kot

$$\gamma = \sum_k -\frac{L}{\omega_k}\frac{\partial \omega_k}{\partial L}. \tag{5}$$

2 Grüneisenov parameter - upoštevam le najbližja soseda (Ashcroft, stran 508, problem 3)

Izračunaj γ za 1-D verigo atomov z dolžino $L = Na$, kjer je N število atomov, ki so razmaknjeni za a. Atomi delujejo drug na drugega s potencialom $\phi(r)$.

Najprej moram izračunati ω.

$$T = \frac{m}{2}\sum_n \dot{u}_n^2$$

$$V = \sum_n \phi(u_{n+1} - u_n) = \sum_n \phi(a) + \phi'(a)(u_{n+1} - u_n) + \phi''(a)(u_{n+1} - u_n)^2 + \ldots,$$

$$\phi'(a)(u_{n+1} - u_n) = 0, \text{ sicer nimam mirovne lege}$$

$$L = T - V$$

$$0 = \frac{\partial}{\partial t}\frac{\partial L}{\partial \dot{u}_n} - \frac{\partial L}{\partial u_n}$$

$$0 = m\dot{u}_n + \phi''(a)(2u_n - u_{n+1} - u_{n-1}) \tag{6}$$

Enačbo (6) rešim z nastavkom:

$$u_n = Ae^{-i\omega t}e^{ikna}, \tag{7}$$

dobim:

$$\omega^2 m = \phi''(a)(e^{ika} + e^{-ika} - 2)$$

$$\omega^2 = \frac{4\phi''(a)}{m}\sin^2\left(\frac{ka}{2}\right) \tag{8}$$

Odvod $\frac{\partial \omega}{\partial L}$ izrazimo z odvodom $\frac{\partial \omega^2}{\partial a}$:

$$\frac{\partial \omega}{\partial L} = \frac{1}{2\omega N}\frac{\partial \omega^2}{\partial a}$$

$$\gamma_k = -\frac{a}{2\omega^2}\frac{\partial \omega^2}{\partial a}$$

Torej (upoštevam, da je produkt ka neodvisen od a):

$$\frac{\partial \omega^2}{\partial a} = \frac{4\phi'''(a)}{m}\sin^2\left(\frac{ka}{2}\right) = \omega^2\frac{\phi'''(a)}{\phi''(a)} \tag{9}$$

Grüneisenov parameter je - v primeru, da upoštevam le najbližje sosede - očitno neodvisen od k:

$$\gamma = \gamma_k = -\frac{a}{2}\frac{\phi'''(a)}{\phi''(a)}$$

3 Grüneisenov parameter - upoštevam 2 najbližja soseda

Pokaži, da je, v primeru, da upoštevaš še naslednja najbližja soseda, Grüneisenov parameter odvisen od valovnega vektorja.

V tem primeru lahko zapišem:

$$T = \frac{m}{2}\sum_n \dot{u}_n^2$$

$$V = \sum_n \phi(u_{n+1} - u_n) + \sum_n \phi(u_{n+2} - u_n) = \sum_n \phi(a) + \phi'(a)(u_{n+1} - u_n) + \phi''(a)(u_{n+1} - u_n)^2 + \dots$$

$$+ \sum_n \phi(2a) + \phi'(2a)(u_{n+2} - u_n) + \phi''(2a)(u_{n+2} - u_n)^2 + \dots,$$

$$\phi'(a)(u_{n+1} - u_n) = \phi'(2a)(u_{n+2} - u_n) = 0$$

$$L = T - V$$

$$0 = \frac{\partial}{\partial t}\frac{\partial L}{\partial \dot{u}_n} - \frac{\partial L}{\partial u_n}$$

$$0 = m\dot{u}_n + \phi''(a)(2u_n - u_{n+1} - u_{n-1}) + \phi''(2a)(2u_n - u_{n+2} - u_{n-2}) \tag{10}$$

Zopet uporabim nastavek (7) in dobim:

$$\omega^2 m = \phi''(a)(e^{ika} + e^{-ika} - 2) + \phi''(2a)(e^{2ika} + e^{-2ika} - 2)$$

$$\omega^2 = \frac{4\phi''(a)}{m}\sin^2\left(\frac{ka}{2}\right) + \frac{4\phi''(2a)}{m}\sin^2(ka)$$

$$\frac{\partial \omega^2}{\partial a} = \frac{4\phi'''(a)}{m}\sin^2\left(\frac{ka}{2}\right) + \frac{8\phi'''(2a)}{m}\sin^2(ka)$$

Opazim, da je v tem primeru γ_k res odvisen od valovnega vektorja in zato $\gamma \neq \gamma_k$.

4 Enostavnejša rešitev naloge 2

Nalogo Poglavja 2 lahko rešim na enostavnejši način:
vem, da je v 3D:

$$\gamma = -\frac{\partial \ln \omega}{\partial \ln V} \to \text{v 1 D: } \gamma = -\frac{\partial \ln \omega}{\partial \ln L} = -\frac{L}{\omega}\frac{\partial \omega}{\partial L}.$$

Dolžina verige je $L = Na$, potencial pa je odvisen le od razdalje: $\phi(\vec{r})$=$\phi(r)$. Velja:

$$\kappa = \frac{\partial^2 \phi(a)}{\partial a^2} = \phi'',$$

$$\omega \propto \sqrt{\kappa},$$

$$L = Na,$$

$$dL = d(Na) = adN + Nda = Nda,$$

$$\gamma = -\frac{L}{\omega}\frac{\partial\omega}{\partial L} = -\frac{Na}{\sqrt{\phi''}}\frac{\partial(\sqrt{\phi''(a)}\ )}{N\partial L} = -\frac{a}{2}\frac{\phi'''(a)}{\phi''(a)}.$$