

Energy profile of lattice vibration at presence of a local drive

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Assuming the normal modes of system to be labeled by (α, q) , with which the equation of motion is written as

$$[\partial_t^2 + K_\alpha(q)]r_\alpha(q, t) = 0 \quad (1)$$

The Green's function in these modes becomes

$$\tilde{G}_\alpha(q, \omega) = \frac{1}{-\omega^2 + K_\alpha(q)}, \quad (2)$$

which satisfies

$$[-\omega^2 + K_\alpha(q)]\tilde{G}_\alpha(q, \omega) = 1 \quad (3)$$

Next, the ω_0 driving force acting on the center mass at site $j = 0$ is

$$\vec{F}_{ext}(j, \omega) = 2\pi\delta(\omega - \omega_0)\delta_{j,0}(c_x\hat{R}_x + c_y\hat{R}_y) \quad (4)$$

where (R_x, R_y) is the degree of freedom for the atom at the center of a unit cell. In the eigen-basis, the force can be represented as

$$\begin{aligned} \vec{F}_{ext}(j, \omega) &= 2\pi\delta(\omega - \omega_0) \int \frac{dq}{2\pi} \sum_\alpha c_\alpha(q) \hat{\alpha}(q) e^{iqR_j} \\ &\rightarrow F_{ext,\alpha}(q, \omega) = 2\pi\delta(\omega - \omega_0) c_\alpha(q) \end{aligned} \quad (5)$$

where $c_\alpha(q) \equiv (c_x\hat{R}_x + c_y\hat{R}_y) \cdot \hat{\alpha}(q)$. Therefore, letting $\hat{\alpha}(q) = \alpha_\lambda(q)\hat{r}_\lambda$, where λ represents the coordinates of atoms (i, x) or (i, y)

$$r_\lambda(q, \omega) = 2\pi\delta(\omega - \omega_0) \sum_\alpha \frac{c_\alpha(q)\alpha_\lambda(q)}{-\omega_0^2 + K_\alpha(q)} \quad (6)$$

transforming back to real space,

$$r_\lambda(j, t) = \int \frac{d^2q}{(2\pi)^2} \sum_\alpha \frac{c_\alpha(q)\alpha_\lambda(q)}{-\omega_0^2 + K_\alpha(q)} e^{i(qj - \omega_0 t)} \quad (7)$$

Assuming the elastic energy on site j can be written as

$$U(j) = \sum_{\lambda, \lambda'} r_{\lambda}(j, t) \tilde{K}_{\lambda, \lambda'} r_{\lambda'}(j, t) \quad (8)$$

the time-averaged energy is

$$\langle U(j) \rangle = \frac{1}{2} \sum_{\lambda, \lambda'} r_{\lambda}(j, 0) \tilde{K}_{\lambda, \lambda'} r_{\lambda'}(j, 0) \quad (9)$$