

Phonon

Mitsuaki Kawamura

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1 Single harmonic Oscillator

The hamiltonian operator is

$$\hat{H} = \frac{\hat{p}^2}{2M} + \frac{C\hat{u}^2}{2}, \quad (1)$$

where \hat{u} and \hat{p} are the position and the momentum operator. These operators satisfies the following commutation relation:

$$[\hat{u}, \hat{p}] \equiv \hat{u}\hat{p} - \hat{p}\hat{u} = i \quad (2)$$

Then we introduce the creation- and anihilation- operator (\hat{b}^\dagger and \hat{b}) as follows

$$\hat{u} \equiv \frac{1}{(4MC)^{1/4}}(\hat{b} + \hat{b}^\dagger), \quad (3)$$

$$\hat{p} \equiv \left(\frac{MC}{4}\right)^{1/4}(-i\hat{b} + i\hat{b}^\dagger). \quad (4)$$

The commutation relation of \hat{b}^\dagger and \hat{b}

$$[\hat{b}, \hat{b}] = 0, [\hat{b}, \hat{b}^\dagger] = 1 \quad (5)$$

lead to the original commutation relation of \hat{u} and \hat{p} as

$$[\hat{u}, \hat{p}] = \frac{i}{2}(-[\hat{b}, \hat{b}] + [\hat{b}, \hat{b}^\dagger] - [\hat{b}^\dagger, \hat{b}] + [\hat{b}^\dagger, \hat{b}^\dagger]) = i, \quad (6)$$

and the hamiltonian becomes

$$\begin{aligned} \hat{H} &= \frac{1}{4} \left(\frac{(MC)^{1/2}}{M} (-i\hat{b} + i\hat{b}^\dagger)(-i\hat{b} + i\hat{b}^\dagger) + \frac{C}{(MC)^{1/2}} (\hat{b} + \hat{b}^\dagger)(\hat{b} + \hat{b}^\dagger) \right) \\ &= \frac{1}{2} \left(\frac{C}{M} \right)^{1/2} (\hat{b}\hat{b}^\dagger + \hat{b}^\dagger\hat{b}) = \omega \left(\hat{b}^\dagger\hat{b} + \frac{1}{2} \right), \end{aligned} \quad (7)$$

where $\omega \equiv (C/M)^{1/2}$

2 Coupled Harmonic Oscillator

The hamiltonian operator is

$$\hat{H} = \frac{1}{2} \sum_s \frac{\hat{p}_s^2}{M_s} + \frac{1}{2} \sum_{ss'} \hat{u}_s C_{ss'} \hat{u}_{s'}, \quad (8)$$

where \hat{u}_s and \hat{p}_s are the position and the momentum operator. These operators satisfies the following commutation relation:

$$[\hat{u}_s, \hat{p}_{s'}] \equiv i\delta_{ss'}. \quad (9)$$

Then, we introduce the creation- and anihilation- operator (\hat{b}_ν^\dagger and \hat{b}_ν) as follows

$$\hat{u}_s \equiv \sum_\nu \frac{v_{s\nu}}{(M_s \omega_\nu)^{1/2}} (\hat{b}_\nu + \hat{b}_\nu^\dagger), \quad (10)$$

$$\hat{p}_s \equiv \sum_\nu (M_s \omega_\nu)^{1/2} v_{s\nu} (-i\hat{b}_\nu + i\hat{b}_\nu^\dagger), \quad (11)$$

where $v_{s\nu}$ and ω_ν^2 are eigenvectors and eigenvalues of rescaled force constant as

$$\sum_{s'} \frac{C_{ss'}}{(M_s M_{s'})^{1/2}} v_{s'\nu} = \omega_\nu^2 v_{s\nu} \quad (12)$$

The commutation relation of \hat{b}_ν^\dagger and \hat{b}_ν

$$[\hat{b}_\nu, \hat{b}_{\nu'}] = 0, [\hat{b}_\nu, \hat{b}_{\nu'}^\dagger] = \delta_{\nu\nu'} \quad (13)$$

lead to the original commutation relation of \hat{u}_s and \hat{p}_s as

$$[\hat{u}_s, \hat{p}_{s'}] = \sum_{\nu\nu'} v_{s\nu} v_{s'\nu'} \frac{i}{2} (-[\hat{b}_\nu, \hat{b}_{\nu'}] + [\hat{b}_\nu, \hat{b}_{\nu'}^\dagger] - [\hat{b}_\nu^\dagger, \hat{b}_{\nu'}] + [\hat{b}_\nu^\dagger, \hat{b}_{\nu'}^\dagger]) = i \sum_\nu v_{s\nu} v_{s'\nu} = i\delta_{ss'}, \quad (14)$$

and the hamiltonian becomes

$$\begin{aligned} \hat{H} &= \frac{1}{2} \sum_{\nu\nu'} (\omega_\nu \omega_{\nu'})^{1/2} (-i\hat{b}_\nu + i\hat{b}_\nu^\dagger) (-i\hat{b}_{\nu'} + i\hat{b}_{\nu'}^\dagger) \sum_s \frac{M_s}{M_s} v_{s\nu} v_{s\nu'} \\ &+ \frac{1}{2} \sum_{\nu\nu'} (\hat{b}_\nu + \hat{b}_\nu^\dagger) (\hat{b}_{\nu'} + \hat{b}_{\nu'}^\dagger) \frac{1}{(\omega_\nu \omega_{\nu'})^{1/2}} \sum_{ss'} v_{s\nu} \frac{C_{ss'}}{(M_s M_{s'})^{1/2}} v_{s'\nu'} \\ &= \frac{1}{2} \sum_{\nu\nu'} (\omega_\nu \omega_{\nu'})^{1/2} (-\hat{b}_\nu \hat{b}_{\nu'} + \hat{b}_\nu \hat{b}_{\nu'}^\dagger + \hat{b}_\nu^\dagger \hat{b}_{\nu'} - \hat{b}_\nu^\dagger \hat{b}_{\nu'}^\dagger) \sum_s v_{s\nu} v_{s\nu'} \\ &+ \frac{1}{2} \sum_{\nu\nu'} (\hat{b}_\nu \hat{b}_{\nu'} + \hat{b}_\nu \hat{b}_{\nu'}^\dagger + \hat{b}_\nu^\dagger \hat{b}_{\nu'} + \hat{b}_\nu^\dagger \hat{b}_{\nu'}^\dagger) \frac{\omega_{\nu'}^2}{(\omega_\nu \omega_{\nu'})^{1/2}} \sum_s v_{s\nu} v_{s\nu'} \\ &= \frac{1}{2} \sum_\nu \omega_\nu (\hat{b}_\nu \hat{b}_\nu^\dagger + \hat{b}_\nu^\dagger \hat{b}_\nu) = \sum_\nu \omega_\nu \left(\hat{b}_\nu^\dagger \hat{b}_\nu + \frac{1}{2} \right), \end{aligned} \quad (15)$$

3 Periodic Coupled Harmonic Oscillator

The hamiltonian operator is

$$\hat{H} = \frac{1}{2} \sum_{\mathbf{T}s\alpha} \frac{\hat{p}_{\mathbf{T}s\alpha}^2}{M_s} + \frac{1}{2} \sum_{\mathbf{T}s\alpha \mathbf{T}'s'\alpha'} \hat{u}_{\mathbf{T}s\alpha} C_{\mathbf{T}s\alpha \mathbf{T}'s'\alpha'} \hat{u}_{\mathbf{T}'s'\alpha'}, \quad (16)$$

where $\hat{u}_{\mathbf{T}s\alpha}$ and $\hat{p}_{\mathbf{T}s\alpha}$ are the position and the momentum operator. These operators satisfies the following commutation relation:

$$[\hat{u}_{\mathbf{T}s\alpha}, \hat{p}_{\mathbf{T}'s'\alpha'}] \equiv i\delta_{\mathbf{T}\mathbf{T}'} \delta_{ss'} \delta_{\alpha\alpha'}. \quad (17)$$

The Fourier-transformed operators are defined as follows:

$$\hat{U}_{\mathbf{q}s\alpha} \equiv \frac{1}{N_C^{1/2}} \sum_{\mathbf{T}} \hat{u}_{\mathbf{T}s\alpha} e^{i\mathbf{q}\cdot\mathbf{T}}, \hat{P}_{\mathbf{q}s\alpha} \equiv \frac{1}{N_C^{1/2}} \sum_{\mathbf{T}} \hat{p}_{\mathbf{T}s\alpha} e^{i\mathbf{q}\cdot\mathbf{T}} \quad (18)$$

$$\hat{u}_{\mathbf{T}s\alpha} = \frac{1}{N_C^{1/2}} \sum_{\mathbf{q}} \hat{U}_{\mathbf{q}s\alpha} e^{-i\mathbf{q}\cdot\mathbf{T}}, \hat{p}_{\mathbf{T}s\alpha} = \frac{1}{N_C^{1/2}} \sum_{\mathbf{q}} \hat{P}_{\mathbf{q}s\alpha} e^{-i\mathbf{q}\cdot\mathbf{T}}, \quad (19)$$

where N_C is the number of cells within the Born-von Karman boundary condition. They also satisfy the commutation relation.

$$[\hat{U}_{\mathbf{q}s\alpha}, \hat{P}_{\mathbf{q}'s'\alpha'}^\dagger] = \frac{1}{N_C} \sum_{\mathbf{T}\mathbf{T}'} e^{i\mathbf{q}\cdot\mathbf{T}} e^{-i\mathbf{q}'\cdot\mathbf{T}'} [\hat{u}_{\mathbf{T}s\alpha}, \hat{p}_{\mathbf{T}'s'\alpha'}] = i \frac{1}{N_C} \sum_{\mathbf{T}} e^{i(\mathbf{q}-\mathbf{q}')\cdot\mathbf{T}} \delta_{ss'} \delta_{\alpha\alpha'} \quad (20)$$

$$= i \delta_{\mathbf{q}\mathbf{q}'} \delta_{ss'} \delta_{\alpha\alpha'}. \quad (21)$$

The hamiltonian becomes

$$\begin{aligned} \hat{H} &= \frac{1}{2N_C} \sum_{\mathbf{q}\mathbf{q}'\mathbf{T}s\alpha} \frac{\hat{P}_{\mathbf{q}s\alpha} \hat{P}_{\mathbf{q}'s'\alpha'} e^{i(\mathbf{q}+\mathbf{q}')\cdot\mathbf{T}}}{M_s} + \frac{1}{2N_C} \sum_{\mathbf{q}\mathbf{q}'s\alpha s'\alpha'} \hat{U}_{\mathbf{q}s\alpha} \hat{U}_{\mathbf{q}'s'\alpha'} \sum_{\mathbf{T}\mathbf{T}'} C_{\mathbf{T}s\alpha\mathbf{T}'s'\alpha'} e^{i\mathbf{q}\cdot\mathbf{T}} e^{i\mathbf{q}'\cdot\mathbf{T}'} \\ &= \frac{1}{2} \sum_{\mathbf{q}\mathbf{q}'\mathbf{T}s\alpha} \frac{\hat{P}_{\mathbf{q}s\alpha}^\dagger \hat{P}_{\mathbf{q}s\alpha}}{M_s} + \frac{1}{2N_C} \sum_{\mathbf{q}\mathbf{q}'s\alpha s'\alpha'} \hat{U}_{\mathbf{q}s\alpha} \hat{U}_{\mathbf{q}'s'\alpha'} \sum_{\mathbf{T}\mathbf{T}'} C_{\mathbf{0}s\alpha(\mathbf{T}'-\mathbf{T})s'\alpha'} e^{i\mathbf{q}'\cdot(\mathbf{T}'-\mathbf{T})} e^{i(\mathbf{q}+\mathbf{q}')\cdot\mathbf{T}} \\ &= \sum_{\mathbf{q}} \left(\frac{1}{2} \sum_{s\alpha} \frac{\hat{P}_{\mathbf{q}s\alpha}^\dagger \hat{P}_{\mathbf{q}s\alpha}}{M_s} + \frac{1}{2} \sum_{s\alpha s'\alpha'} \hat{U}_{\mathbf{q}s\alpha}^\dagger \tilde{C}_{\mathbf{q}s\alpha s'\alpha'} \hat{U}_{\mathbf{q}s'\alpha'} \right), \end{aligned} \quad (22)$$

where

$$\tilde{C}_{\mathbf{q}s\alpha s'\alpha'} \equiv \sum_{\mathbf{T}} C_{\mathbf{0}s\alpha\mathbf{T}s'\alpha'} e^{i\mathbf{q}\cdot\mathbf{T}} \quad (23)$$

With the same discussion in the previous section, we obtain the following results:

$$\hat{U}_{\mathbf{q}s\alpha} \equiv \sum_{\nu} \frac{v_{s\alpha\mathbf{q}\nu}}{(M_s \omega_{\mathbf{q}\nu})^{1/2}} (\hat{b}_{\mathbf{q}\nu} + \hat{b}_{\mathbf{q}\nu}^\dagger), \quad (24)$$

$$\hat{P}_{\mathbf{q}s\alpha} \equiv \sum_{\nu} (M_s \omega_{\mathbf{q}\nu})^{1/2} v_{s\alpha\mathbf{q}\nu} (-i\hat{b}_{\mathbf{q}\nu} + i\hat{b}_{\mathbf{q}\nu}^\dagger), \quad (25)$$

$$\sum_{s'\alpha'} \frac{\tilde{C}_{\mathbf{q}s\alpha s'\alpha'}}{(M_s M_{s'})^{1/2}} v_{s'\alpha'\mathbf{q}\nu} = \omega_{\mathbf{q}\nu}^2 v_{s\alpha\mathbf{q}\nu} \quad (26)$$

$$\hat{H} = \sum_{\mathbf{q}\nu} \omega_{\mathbf{q}\nu} \left(\hat{b}_{\mathbf{q}\nu}^\dagger \hat{b}_{\mathbf{q}\nu} + \frac{1}{2} \right) \quad (27)$$

$$\begin{aligned} [\hat{U}_{\mathbf{q}s\alpha}, \hat{P}_{\mathbf{q}'s'\alpha'}^\dagger] &= \sum_{\nu\nu'} v_{s\alpha\mathbf{q}\nu} v_{s'\alpha'\mathbf{q}'\nu'}^* \frac{i}{2} (-[\hat{b}_{\mathbf{q}\nu}, \hat{b}_{\mathbf{q}'\nu'}] + [\hat{b}_{\mathbf{q}\nu}, \hat{b}_{\mathbf{q}'\nu'}^\dagger] - [\hat{b}_{\mathbf{q}\nu}^\dagger, \hat{b}_{\mathbf{q}'\nu'}] + [\hat{b}_{\mathbf{q}\nu}^\dagger, \hat{b}_{\mathbf{q}'\nu'}^\dagger]) \\ &= i \delta_{\mathbf{q}\mathbf{q}'} \sum_{\nu} v_{s\alpha\mathbf{q}\nu} v_{s'\alpha'\mathbf{q}'\nu}^* = i \delta_{\mathbf{q}\mathbf{q}'} \delta_{ss'} \delta_{\alpha\alpha'}, \end{aligned} \quad (28)$$