Phonon

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1 Single harmonic Oscillator

The hamiltonian operator is

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

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

$$[\hat{u}, \hat{p}] \equiv \hat{u}\hat{p} - \hat{p}\hat{u} = i \tag{2}$$

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

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

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

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

$$[\hat{b}, \hat{b}] = 0, [\hat{b}, \hat{b}^\dagger] = 1 \tag{5}$$

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

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

and the hamiltonian becomes

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

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

2 Coupled Harmonic Oscillator

The hamiltonian operator is

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

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

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

Then, we introduce the creation- and anihiration- operator ($\hat{b}^\dagger_\nu$ and $\hat{b}_\nu$) as follows

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

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

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

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

The commutation relation of $\hat{b}^\dagger_\nu$ and $\hat{b}_\nu$

$$[\hat{b}_\nu, \hat{b}_{\nu'}] = 0, [\hat{b}_\nu, \hat{b}^\dagger_{\nu'}] = \delta_{\nu\nu'} \tag{13}$$

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

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

and the hamiltonian becomes

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

3 Periodic Coupled Harmonic Oscillator

The hamiltonian operator is

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

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:

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

The Fourier-transformed operators are defined as follows:

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

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

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

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

$$= i\delta_{\mathbf{q}\mathbf{q}'}\delta_{ss'}\delta_{\alpha\alpha'}. \tag{21}$$

The hamiltonian becomes

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

where

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

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

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

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

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

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

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

4 Electron-phonon vertex

Electron-nuclear Hamiltonian in 2nd quantization representation

$$\hat{H}_{en} = \sum_{\sigma} \int d^3r \hat{\psi}_\sigma(\mathbf{r})^\dagger \hat{\psi}_\sigma(\mathbf{r}) V(\mathbf{r}; \{\hat{R}_{\mathbf{T}s\alpha}\}), \tag{29}$$

where $\hat{R}_{\mathbf{T}s\alpha}$ is the position operator of nuclear as

$$\hat{R}_{\mathbf{T}s\alpha} = R^0_{\mathbf{T}s\alpha} + \hat{u}_{\mathbf{T}s\alpha}, \tag{30}$$

$R^0_{\mathbf{T}s\alpha}$ is equiribrium position.

We expand $V(\mathbf{r};\{\hat{R}_{\mathbf{T}s\alpha}\})$ arround $R^0_{\mathbf{T}s\alpha}$ and obtain

$$\hat{H}_{en} = \sum_{\sigma}\int d^3r\hat{\psi}_\sigma(\mathbf{r})^\dagger\hat{\psi}_\sigma(\mathbf{r})V(\mathbf{r};\{R^0_{\mathbf{T}s\alpha}\}) + \sum_{\sigma}\int d^3r\hat{\psi}_\sigma(\mathbf{r})^\dagger\hat{\psi}_\sigma(\mathbf{r})\sum_{\mathbf{T}s\alpha}\frac{\partial V(\mathbf{r};\{R^0\})}{\partial R^0_{\mathbf{T}s\alpha}}\hat{u}_{\mathbf{T}s\alpha}. \tag{31}$$

The first term is the electron-fixed nuclear interaction term, and the second term is the electron-phonon interaction term $\hat{H}_{ep}$. By expanding $\hat{\psi}_\sigma$ with Bloch orbitals $\varphi_{n\mathbf{k}}$

$$\hat{\psi}_\sigma(\mathbf{r}) = \sum n\mathbf{k}\varphi_{n\mathbf{k}}(\mathbf{r})\hat{c}_{n\mathbf{k}\sigma}, \tag{32}$$

we obtain

$$\hat{H}_{ep} = \sum_{\sigma nn'\mathbf{k}\mathbf{k}'\mathbf{T}s\alpha}\hat{c}^\dagger_{n\mathbf{k}\sigma}\hat{c}_{n'\mathbf{k}'\sigma}\hat{u}_{\mathbf{T}s\alpha}\int d^3r\varphi^*_{n\mathbf{k}}(\mathbf{r})\varphi_{n'\mathbf{k}'}(\mathbf{r})\frac{\partial V(\mathbf{r};\{R^0\})}{\partial R^0_{\mathbf{T}s\alpha}}. \tag{33}$$

By using Eqs (19, 24) and $\varphi_{n\mathbf{k}}(\mathbf{r}) \equiv N_C^{-1/2}e^{i\mathbf{k}\cdot\mathbf{r}}\chi_{n\mathbf{k}}(\mathbf{r})$, we obtain

$$\hat{H}_{ep} = \sum_{\sigma nn'\mathbf{k}\mathbf{k}'\mathbf{q}\nu}\hat{c}^\dagger_{n\mathbf{k}\sigma}\hat{c}_{n'\mathbf{k}'\sigma}(\hat{b}_{\mathbf{q}\nu} + \hat{b}^\dagger_{\mathbf{q}\nu})g^{\mathbf{q}\nu}_{n\mathbf{k}n'\mathbf{k}'}, \tag{34}$$

where $g^{\mathbf{q}\nu}_{n\mathbf{k}n'\mathbf{k}'}$ is the electron-phonon vertex as

$$\begin{aligned}
g^{\mathbf{q}\nu}_{n\mathbf{k}n'\mathbf{k}'} &\equiv \sum_{\mathbf{T}s\alpha}e^{-i\mathbf{q}\cdot\mathbf{T}}\frac{v_{s\alpha\mathbf{q}\nu}}{(N_C^3M_s\omega_{\mathbf{q}\nu})^{1/2}}\int d^3re^{i(\mathbf{k}'-\mathbf{k})\cdot\mathbf{r}}\chi^*_{n\mathbf{k}}(\mathbf{r})\chi_{n'\mathbf{k}'}(\mathbf{r})\frac{\partial V(\mathbf{r};\{R^0\})}{\partial R^0_{\mathbf{T}s\alpha}} \\
&= \sum_{\mathbf{T}\mathbf{T}'s\alpha}e^{-i\mathbf{q}\cdot\mathbf{T}}\frac{v_{s\alpha\mathbf{q}\nu}}{(N_C^3M_s\omega_{\mathbf{q}\nu})^{1/2}}\int_{\text{cell}}d^3re^{i(\mathbf{k}'-\mathbf{k})\cdot(\mathbf{r}+\mathbf{T}')}\chi^*_{n\mathbf{k}}(\mathbf{r})\chi_{n'\mathbf{k}'}(\mathbf{r})\frac{\partial V(\mathbf{r}+\mathbf{T}';\{R^0\})}{\partial R^0_{\mathbf{T}s\alpha}} \\
&= \sum_{\mathbf{T}}e^{i(\mathbf{k}'-\mathbf{k}-\mathbf{q})\cdot\mathbf{T}}\sum_{\mathbf{T}'s\alpha}\frac{v_{s\alpha\mathbf{q}\nu}}{(N_C^3M_s\omega_{\mathbf{q}\nu})^{1/2}}\int_{\text{cell}}d^3re^{i(\mathbf{k}'-\mathbf{k})\cdot(\mathbf{r}+\mathbf{T}'-\mathbf{T})}\chi^*_{n\mathbf{k}}(\mathbf{r})\chi_{n'\mathbf{k}'}(\mathbf{r})\frac{\partial V(\mathbf{r};\{R^0\})}{\partial R^0_{(\mathbf{T}-\mathbf{T}')s\alpha}} \\
&= \delta_{\mathbf{k}',\mathbf{k}+\mathbf{q}}\sum_{s\alpha}\frac{v_{s\alpha\mathbf{q}\nu}}{(N_CM_s\omega_{\mathbf{q}\nu})^{1/2}}\int_{\text{cell}}d^3re^{i\mathbf{q}\cdot\mathbf{r}}\chi^*_{n\mathbf{k}}(\mathbf{r})\chi_{n'\mathbf{k}+\mathbf{q}}(\mathbf{r})\sum_{\mathbf{T}}e^{-i\mathbf{q}\cdot\mathbf{T}}\frac{\partial V(\mathbf{r};\{R^0\})}{\partial R^0_{\mathbf{T}s\alpha}}.
\end{aligned} \tag{35}$$

If we use V_{KS} alternative to V, we obtain the screened electron-phonon vertex.