Now we can quantize crystal displacement waves using the following formal rules:

1) Replace a variable x_ξ with an operator $\hat{x}_\xi$ $\quad (\hat{x}_\xi = x)$ (29)

2) Replace a variable p_ξ with an operator $\hat{p}_\xi$ $\quad \left(\hat{p}_\xi = -i\hbar \frac{\partial}{\partial x_\xi}\right)$ (30)

3) Replace Poisson's bracket $\{p, x\}$ with a commutator

$$[\hat{p}_{\xi_1}, \hat{x}_\xi] = \hat{p}_{\xi_1}\hat{x}_\xi - \hat{x}_\xi \hat{p}_{\xi_1} = -i\hbar \delta_{\xi\xi_1}$$ ← because oscillators are independent. (31)

Thus: $$E = \sum_\xi \left(\frac{\omega_\xi^2 x_\xi^2}{2} + \frac{p_\xi^2}{2}\right) = \sum_\xi \mathcal{E}_\xi$$

becomes $$\hat{H} = \sum_\xi \left(\frac{\omega_\xi^2 \hat{x}_\xi^2}{2} + \frac{\hat{p}_\xi^2}{2}\right) = \sum_\xi \hat{H}_\xi .$$

The oscillators are independent, so let us first consider a single oscillator (i.e. ξ is fixed). The energy levels $\mathcal{E}_\xi$ for this oscillator can be found from the Schrödinger equation:

$$\hat{H}_\xi \psi_{n_\xi}(x_\xi) = \mathcal{E}_{n_\xi} \cdot \psi_{n_\xi}(x_\xi) \qquad (32)$$

The eigenvalues $\mathcal{E}_{n_\xi}$ and eigenfunctions $\psi_{n_\xi}(x_\xi)$ are known from Q.M.

$$\mathcal{E}_{n_\xi} = \hbar\omega_\xi \left(n_\xi + \tfrac{1}{2}\right) \qquad (33)$$

$$\psi_{n_\xi}(x_\xi) = \frac{1}{\sqrt{2^n n! \sqrt{\pi} \cdot x_{0_\xi}}} \cdot e^{-\frac{1}{2}\left(\frac{x}{x_{0_\xi}}\right)^2} \cdot H_n\left(\frac{x}{x_{0_\xi}}\right),$$

where $H_n(z)$ are the Hermite polynomials $\left(H_n(z) = (-1)^n e^{z^2} \frac{d^n}{dz^n}\left(e^{-z^2}\right)\right)$

$$x_{0_\xi} = \sqrt{\frac{\hbar}{1 \cdot \omega_\xi}}$$

$$n_\xi = 0, 1, 2, \dots$$

However, it is instructive to obtain the quantisation of energy (33) using the second quantisation approach.

Let us introduce new operators:

$$\begin{cases} \hat{b}_3 = \dfrac{1}{\sqrt{2}}\left(\dfrac{\hat{x}_3}{x_{0_3}} + \dfrac{i}{\hbar}x_{0_3}\hat{p}_3\right) \\ \hat{b}_3^+ = \dfrac{1}{\sqrt{2}}\left(\dfrac{\hat{x}_3}{x_{0_3}} - \dfrac{i}{\hbar}x_{0_3}\hat{p}_3\right) \end{cases} \quad (34) \quad \text{or} \quad \begin{cases} \hat{x}_3 = \dfrac{x_{0_3}}{\sqrt{2}}\left(\hat{b}_3 + \hat{b}_3^+\right) \\ \hat{p}_3 = -\dfrac{i\hbar}{x_{0_3}\sqrt{2}}\left(\hat{b}_3 - \hat{b}_3^+\right) \end{cases} \quad (35)$$

The Hamiltonian can be expressed using $\hat{b}_3$ and $\hat{b}_3^+$:

$$\hat{H}_3 = \frac{\hat{p}^2}{2} + \frac{\omega_3^2\hat{x}_3^2}{2} = -\frac{\hbar^2}{4x_{0_3}^2}(\hat{b}_3 - \hat{b}_3^+)(\hat{b}_3 - \hat{b}_3^+) + \frac{\omega_3^2 x_{0_3}^2}{4}(\hat{b}_3 + \hat{b}_3^+)(\hat{b}_3 + \hat{b}_3^+)$$

$$\frac{\hbar^2}{4x_{0_3}^2} = \frac{\hbar^2}{4}\cdot\frac{\omega_3}{\hbar} = \frac{\hbar\omega_3}{4} \quad ; \quad \frac{\omega_3^2 x_{0_3}^2}{4} = \frac{\omega_3^2\cdot\hbar}{4\omega_3} = \frac{\hbar\omega_3}{4}$$

$$\hat{H}_3 = \frac{\hbar\omega_3}{4}\left[-\hat{b}_3\hat{b}_3 + \hat{b}_3\hat{b}_3^+ + \hat{b}_3^+\hat{b}_3 - \hat{b}_3^+\hat{b}_3^+ + \hat{b}_3\hat{b}_3 + \hat{b}_3\hat{b}_3^+ + \hat{b}_3^+\hat{b}_3 + \hat{b}_3^+\hat{b}_3^+\right]$$

$$= \frac{\hbar\omega_3}{2}\left[\hat{b}_3\hat{b}_3^+ + \hat{b}_3^+\hat{b}_3\right] \quad (36)$$

Let us find a commutator $[\hat{b}_3\hat{b}_3^+]$:

$$[\hat{b}_3\hat{b}_3^+] = \hat{b}_3\hat{b}_3^+ - \hat{b}_3^+\hat{b}_3 \underset{(34)}{=} \frac{1}{2}\left(\frac{\hat{x}_3}{x_{0_3}} + \frac{i}{\hbar}x_{0_3}\hat{p}_3\right)\left(\frac{\hat{x}_3}{x_{0_3}} - \frac{i}{\hbar}x_{0_3}\hat{p}_3\right) - \frac{1}{2}\left(\frac{\hat{x}_3}{x_{0_3}} - \frac{i}{\hbar}x_{0_3}\hat{p}_3\right)\left(\frac{\hat{x}_3}{x_{0_3}} + \frac{i}{\hbar}x_{0_3}\hat{p}_3\right)$$

$$= -\frac{1}{2}\frac{i}{\hbar}\hat{x}_3\hat{p}_3 + \frac{1}{2}\frac{i}{\hbar}\hat{p}_3\hat{x}_3 - \frac{1}{2}\frac{i}{\hbar}\hat{x}_3\hat{p}_3 + \frac{1}{2}\frac{i}{\hbar}\hat{p}_3\hat{x}_3$$

$$= \frac{i}{\hbar}\left(\hat{p}_3\hat{x}_3 - \hat{x}_3\hat{p}_3\right) = \frac{i}{\hbar}[\hat{p}_3, \hat{x}_3] = \frac{i}{\hbar}(-i\hbar) = 1 \quad (37)$$

Eq. (36): $$\hat{H}_3 = \frac{\hbar\omega_3}{2}\Big(\underbrace{\hat{b}_3\hat{b}_3^+}_{1+b^+b} + \hat{b}_3^+\hat{b}_3\Big) = \frac{\hbar\omega_3}{2}\left(1 + \hat{b}_3^+\hat{b}_3 + \hat{b}_3^+\hat{b}_3\right) = \hbar\omega_3\left(\hat{b}_3^+\hat{b}_3 + \frac{1}{2}\right) \quad (38)$$

Let us find how $\hat{b}_\xi$ and $\hat{b}_\xi^+$ act on the wavefunction φ_{n_ξ}.

a) $\hat{H}_\xi \varphi_{n_\xi} = E_{n_\xi}\varphi_{n_\xi} \Rightarrow \hat{b}_\xi \hat{H}_\xi \varphi_{n_\xi} = E_{n_\xi}\hat{b}_\xi \varphi_{n_\xi} \underset{(38)}{\Rightarrow} \hbar\omega_\xi(\underbrace{\hat{b}_\xi \hat{b}_\xi^+}_{\hat{b}_\xi^+\hat{b}_\xi+1}\hat{b}_\xi + \hat{b}_\xi\cdot\frac{1}{2})\varphi_{n_\xi} = E_{n_\xi}\hat{b}_\xi\varphi_{n_\xi}$

$\Rightarrow \hbar\omega_\xi(\hat{b}_\xi^+\hat{b}_\xi + 1 + \frac{1}{2})\cdot\hat{b}_\xi\varphi_{n_\xi} = E_{n_\xi}\hat{b}_\xi\varphi_{n_\xi} \Rightarrow (\hat{H}_\xi + \hbar\omega_\xi)\hat{b}_\xi\varphi_{n_\xi} = E_{n_\xi}\cdot\hat{b}_\xi\varphi_{n_\xi}$

$\Rightarrow \hat{H}_\xi\cdot(\hat{b}_\xi\varphi_{n_\xi}) = (E_{n_\xi} - \hbar\omega)\cdot(\hat{b}_\xi\varphi_{n_\xi})$

If φ_{n_ξ} is the eigenfunction corresponding to E_{n_ξ}, then $\hat{b}_\xi\varphi_{n_\xi}$ is also an eigenfunction corresponding to $(E_{n_\xi} - \hbar\omega_\xi)$.

Therefore, $\hat{b}_\xi$ is an operator of annihilation of a phonon in state ξ,

Let us consider a state with the lowest energy ($n_\xi = 0$)

$\hat{H}_\xi\cdot\varphi_0 = E_0\cdot\varphi_0.$

The energy cannot be lowered anymore, thus $\hat{b}_\xi\varphi_0 = 0$

$\Rightarrow \hat{b}_\xi^+\hat{b}_\xi\varphi_0 = \hat{b}_\xi^+\cdot 0 = 0 \Rightarrow \underbrace{\hbar\omega_\xi(\hat{b}_\xi^+\cdot\hat{b}_\xi + \frac{1}{2})}_{\hat{H}_\xi}\varphi_0 = \hbar\omega_\xi\cdot\frac{1}{2}\varphi_0 \Rightarrow \hat{H}_\xi\cdot\varphi_0 = \frac{1}{2}\hbar\omega_\xi\cdot\varphi_0$

$\Rightarrow E_0 = \frac{1}{2}\hbar\omega_\xi$ ← we have found the lowest energy.

b) $\hat{H}_\xi\varphi_{n_\xi} = E_{n_\xi}\varphi_{n_\xi} \Rightarrow \hat{b}_\xi^+\hat{H}_\xi\varphi_{n_\xi} = E_{n_\xi}\hat{b}_\xi^+\varphi_{n_\xi} \underset{(38)}{\Rightarrow} \hbar\omega_\xi(\hat{b}_\xi^+\underbrace{\hat{b}_\xi^+\hat{b}_\xi}_{\hat{b}_\xi\hat{b}_\xi^+-1} + \hat{b}_\xi^+\cdot\frac{1}{2})\varphi_{n_\xi} = E_{n_\xi}\hat{b}_\xi^+\varphi_{n_\xi}$

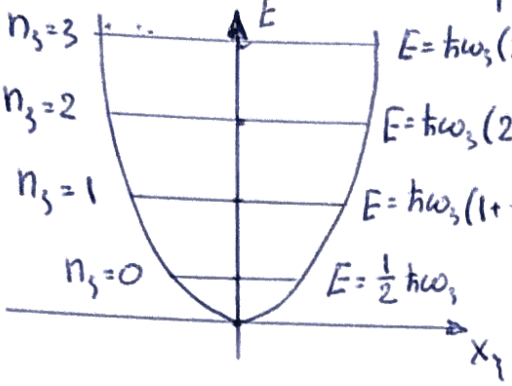
$\Rightarrow \hbar\omega_\xi(\hat{b}_\xi^+\hat{b}_\xi\hat{b}_\xi^+ - \hat{b}_\xi^+\cdot\frac{1}{2})\cdot\varphi_{n_\xi} = E_{n_\xi}\hat{b}_\xi^+\varphi_{n_\xi} \Rightarrow \hbar\omega_\xi(\hat{b}_\xi^+\hat{b}_\xi - \frac{1}{2})\cdot\hat{b}_\xi^+\varphi_{n_\xi} = E_{n_\xi}\hat{b}_\xi^+\varphi_{n_\xi}$

$\Rightarrow \hbar\omega_\xi(\hat{b}_\xi^+\hat{b}_\xi + \frac{1}{2})\hat{b}_\xi^+\varphi_{n_\xi} = (E_{n_\xi} + \hbar\omega_\xi)\cdot\hat{b}_\xi^+\varphi_{n_\xi} \Rightarrow \hat{H}_\xi\cdot(\hat{b}_\xi^+\varphi_{n_\xi}) = (E_{n_\xi} + \hbar\omega_\xi)\cdot(\hat{b}_\xi^+\varphi_{n_\xi})$

If φ_{n_ξ} is the eigenfunction corresponding to E_{n_ξ}, then $\hat{b}_\xi^+\varphi_{n_\xi}$ is also an eigenfunction corresponding to $(E_{n_\xi} + \hbar\omega_\xi)$.

Therefore, $\hat{b}_\xi^+$ is an operator of creation of a phonon in state ξ.

From this it follows that the energy levels of a harmonic quantum oscillator are separated by $\hbar\omega_\xi$



$$E_{n_\xi} = \hbar\omega_\xi\left(n_\xi + \frac{1}{2}\right) \qquad (39)$$

$$\hat{b}_\xi \varphi_{n_\xi} \propto \varphi_{n_\xi - 1} \qquad (40)$$

$$\hat{b}_\xi^{+} \varphi_{n_\xi} \propto \varphi_{n_\xi + 1} \qquad (41)$$

$$\hat{n}_\xi = \hat{b}_\xi^{+}\hat{b}_\xi \leftarrow \text{number of phonons} \qquad (42)$$

Let us find normalization of $\hat{b}_\xi\varphi_{n_\xi}$ and $\hat{b}_\xi^{+}\varphi_{n_\xi}$ (to determine the constants in eqs. (40) and (41)):

a) $$\langle \hat{b}_\xi\varphi_{n_\xi} | \hat{b}_\xi\varphi_{n_\xi}\rangle = \int (\hat{b}_\xi\varphi_{n_\xi})^{*}\cdot \hat{b}_\xi\varphi_{n_\xi}\cdot dx_\xi = \int \varphi_{n_\xi}^{*}\cdot \underbrace{\hat{b}_\xi^{+}\hat{b}_\xi}_{\frac{\hat{H}_\xi}{\hbar\omega_\xi}-\frac{1}{2}}\cdot\varphi_{n_\xi}\,dx_\xi =$$

$$= \int \varphi_{n_\xi}^{*}\left(\frac{E_{n_\xi}}{\hbar\omega_\xi}-\frac{1}{2}\right)\cdot\varphi_{n_\xi}\cdot dx_\xi = \left(\frac{E_{n_\xi}}{\hbar\omega_\xi}-\frac{1}{2}\right)\underbrace{\langle\varphi_{n_\xi}|\varphi_{n_\xi}\rangle}_{1} = n_\xi$$

Therefore, $$\hat{b}_\xi\varphi_{n_\xi} = \sqrt{n_\xi}\cdot\varphi_{n_\xi-1} \quad \text{or} \quad \hat{b}_\xi|n_\xi\rangle = \sqrt{n_\xi}\cdot|n_\xi-1\rangle \qquad (43)$$

b) $$\langle \hat{b}_\xi^{+}\varphi_{n_\xi} | \hat{b}_\xi^{+}\varphi_{n_\xi}\rangle = \int (\hat{b}_\xi^{+}\varphi_{n_\xi})^{*}\cdot \hat{b}_\xi^{+}\varphi_{n_\xi}\cdot dx_\xi = \int \varphi_{n_\xi}^{*}\cdot \underbrace{\hat{b}_\xi\hat{b}_\xi^{+}}_{\frac{\hat{H}_\xi}{\hbar\omega_\xi}+\frac{1}{2}}\cdot\varphi_{n_\xi}\cdot dx_\xi$$

$$= \int \varphi_{n_\xi}^{*}\cdot\left(\frac{E_{n_\xi}}{\hbar\omega_\xi}+\frac{1}{2}\right)\cdot\varphi_{n_\xi}\cdot dx_\xi = \left(\frac{E_{n_\xi}}{\hbar\omega_\xi}+\frac{1}{2}\right)\cdot\underbrace{\langle\varphi_{n_\xi}|\varphi_{n_\xi}\rangle}_{1} = n_\xi + 1$$

Therefore, $$\hat{b}_\xi^{+}\varphi_{n_\xi} = \sqrt{n_\xi+1}\cdot\varphi_{n_\xi+1} \quad \text{or} \quad \hat{b}_\xi^{+}|n_\xi\rangle = \sqrt{n_\xi+1}\cdot|n_\xi+1\rangle \qquad (44)$$

So far, we had a displacement of any atom in a crystal, which now also can be quantized:

$$u^{\alpha}_{j\vec{n}} = \frac{1}{\sqrt{NM_j}} \sum_{s,\vec{f}} \left[Q_s(\vec{f})\, \ell^{\alpha}_{js}(\vec{f})\, e^{i\vec{f}\vec{n} - i\omega_s(\vec{f})t} + Q^*_s(\vec{f})\, \ell^{*\alpha}_{js}(\vec{f})\, e^{-i\vec{f}\vec{n} + i\omega_s(\vec{f})t} \right]$$

$$= \frac{1}{\sqrt{NM_j}} \sum_{\xi} \left[\ell^{\alpha}_{j\xi} e^{i\vec{f}\vec{n}} \cdot q_{\xi} + \ell^{*\alpha}_{j\xi} e^{-i\vec{f}\vec{n}} \cdot q^*_{\xi} \right].$$

Here $q_{\xi} \underset{(23)}{=} Q_s(\vec{f}) \cdot e^{-i\omega_s(\vec{f})t} \underset{(26)}{=} \frac{1}{2}\left(x_{\xi} - \frac{p_{\xi}}{i\omega_{\xi}}\right) \rightarrow \frac{1}{2}\left(\hat{x}_{\xi} - \frac{\hat{p}_{\xi}}{i\omega_{\xi}}\right)$

$$\underset{(35)}{=} \frac{1}{2}\left(\frac{x_{0\xi}}{\sqrt{2}}(\hat{b}_{\xi} + \hat{b}^+_{\xi}) - \frac{i\hbar}{x_{0\xi}\sqrt{2}} \frac{-1}{i\omega_{\xi}}(\hat{b}_{\xi} - \hat{b}^+_{\xi}) \right) \underset{x_{0\xi} = \sqrt{\frac{\hbar}{\omega_{\xi}}}}{=} \frac{1}{2}\sqrt{\frac{\hbar}{2\omega_{\xi}}} \left(\hat{b}_{\xi} + \hat{b}^+_{\xi} + \hat{b}_{\xi} - \hat{b}^+_{\xi} \right) = \sqrt{\frac{\hbar}{2\omega_{\xi}}}\, \hat{b}_{\xi}$$

$$q^*_{\xi} \underset{(23)}{=} Q_s(\vec{f}) \cdot e^{i\omega_s(\vec{f})t} \underset{(26)}{=} \frac{1}{2}\left(x_{\xi} + \frac{p_{\xi}}{i\omega_{\xi}}\right) \rightarrow \frac{1}{2}\left(\hat{x}_{\xi} + \frac{\hat{p}_{\xi}}{i\omega_{\xi}}\right)$$

$$\underset{(35)}{=} \frac{1}{2}\left(\frac{x_{0\xi}}{\sqrt{2}}(\hat{b}_{\xi} + \hat{b}^+_{\xi}) - \frac{i\hbar}{x_{0\xi}\sqrt{2}} \cdot \frac{1}{i\omega_{\xi}}(\hat{b}_{\xi} - \hat{b}^+_{\xi}) \right) \underset{x_{0\xi} = \sqrt{\frac{\hbar}{\omega_{\xi}}}}{=} \frac{1}{2}\sqrt{\frac{\hbar}{2\omega_{\xi}}} \left(\hat{b}_{\xi} + \hat{b}^+_{\xi} - \hat{b}_{\xi} + \hat{b}^+_{\xi} \right) = \sqrt{\frac{\hbar}{2\omega_{\xi}}}\, \hat{b}^+_{\xi}$$

Therefore,

$$\hat{u}^{\alpha}_{j\vec{n}} = \sum_{\xi} \sqrt{\frac{\hbar}{2M_j N\omega_{\xi}}} \left[\ell^{\alpha}_{j\xi} e^{i\vec{f}\vec{n}} \cdot \hat{b}_{\xi} + \ell^{*\alpha}_{j\xi} e^{-i\vec{f}\vec{n}} \cdot \hat{b}^+_{\xi} \right] = \sum_{\xi} \hat{u}^{\alpha}_{j\vec{n}\xi}$$

The total wavefunction of a crystal is $\Phi = \prod_{\xi} \psi_{n_{\xi}}(x_{\xi}) = \prod_{\xi} |n_{\xi}\rangle$

The total energy of a crystal is: $E = \sum_{\xi} E_{n_{\xi}}$, because

$$\hat{H}\Phi = \sum_{\xi} \hat{H}_{\xi} \cdot \prod_{\xi_1} |n_{\xi_1}\rangle = \sum_{\xi} \prod_{\xi_1} \hat{H}_{\xi} |n_{\xi_1}\rangle = \sum_{\xi} \prod_{\xi_1} E_{n_{\xi}} \cdot |n_{\xi_1}\rangle = \left(\sum_{\xi} E_{n_{\xi}}\right) \cdot \Phi$$

Let us calculate some matrix elements

a) $\langle \{S\} | \hat{u}^{\alpha}_{j\vec{n}} \{n\} \rangle \underset{(45)}{=} \sum_{\xi} \sqrt{\frac{\hbar}{2M_j N\omega_\xi}} \cdot \{ \ell^{\alpha}_{j\xi} e^{i\vec{f}\vec{n}} \langle \{S\} | \hat{b}_\xi | \{n\} \rangle + \overset{*}{\ell}{}^{\alpha}_{j\xi} e^{-i\vec{f}\vec{n}} \langle \{S\} | \hat{b}^{+}_\xi | \{n\} \rangle \}$

$\{S\}, \{n\}$ – two states of a crystal

$$\langle \{S\} | \hat{b}_\xi | \{n\} \rangle = \underbrace{\langle \{S\}^{(\xi)} | \{n\}^{(\xi)} \rangle}_{\prod_{\xi_1 \neq \xi} \delta_{S_{\xi_1}, n_{\xi_1}}} \cdot \underbrace{\langle S_\xi | \hat{b}_\xi | n_\xi \rangle}_{\sqrt{n_\xi} \cdot \delta_{S_\xi, n_\xi - 1}} \quad \text{(see (43))}$$

all wave functions except of ξ

$$\langle \{S\} | \hat{b}^{+}_\xi | \{n\} \rangle = \underbrace{\langle \{S\}^{(\xi)} | \{n\}^{(\xi)} \rangle}_{\prod_{\xi_1 \neq \xi} \delta_{S_{\xi_1}, n_{\xi_1}}} \cdot \underbrace{\langle S_\xi | \hat{b}^{+}_\xi | n_\xi \rangle}_{\sqrt{n_\xi + 1} \cdot \delta_{S_\xi, n_\xi + 1}} \quad \text{(see (44))}.$$

Therefore $\langle \underbrace{\{n\}^{(\xi)}, n_\xi \pm 1}_{} | \hat{u}^{\alpha}_{j\vec{n}} | \{n\} \rangle = \sqrt{\frac{\hbar}{2M_j N\omega_\xi}} \cdot \begin{cases} \sqrt{n_\xi} \cdot \ell^{\alpha}_{j\xi} e^{i\vec{f}\vec{n}} \\ \sqrt{n_\xi + 1} \cdot \overset{*}{\ell}{}^{\alpha}_{j\xi} \cdot e^{-i\vec{f}\vec{n}} \end{cases}$

a new state, where a single photon in state „ξ" was created or annihilated

All other matrix elements are zero, e.g. $\overline{u^{\alpha}_{j\vec{n}}} = \langle \{n\} | \hat{u}^{\alpha}_{j\vec{n}} | \{n\} \rangle = 0$

Let us find mean squared displacement of an atom:

$$\overline{u^2_{j\vec{n}}} = \langle \{n\} | \hat{u}^{\alpha}_{j\vec{n}} \hat{u}^{\alpha}_{j\vec{n}} | \{n\} \rangle = \langle \{n\} | \sum_{\xi} \hat{u}^{\alpha}_{j\vec{n}\xi} \cdot \sum_{\xi_1} \hat{u}^{\alpha}_{j\vec{n}\xi_1} | \{n\} \rangle =$$

$$= \sum_{\xi \xi_1} \underbrace{\langle \{n\} | \hat{u}^{\alpha}_{j\vec{n}\xi} \hat{u}^{\alpha}_{j\vec{n}\xi_1} | \{n\} \rangle}_{\delta_{\xi\xi_1}} = \sum_{\xi} \langle \{n\} | \hat{u}^{\alpha}_{j\vec{n}\xi} \hat{u}^{\alpha}_{j\vec{n}\xi} | \{n\} \rangle$$

$$= \sum_{\xi} \frac{\hbar}{2M_j N\omega_\xi} \cdot \underbrace{\langle \{n\}^{(\xi)} | \{n\}^{(\xi)} \rangle}_{\prod_{\xi \neq \xi_1} 1 = 1} \cdot \langle n_\xi | (\ell^{\alpha}_{j\xi} e^{i\vec{f}\vec{n}} \hat{b}_\xi + \overset{*}{\ell}{}^{\alpha}_{j\xi} e^{-i\vec{f}\vec{n}} \hat{b}^{+}_\xi)(\ell^{\alpha}_{j\xi} e^{i\vec{f}\vec{n}} \hat{b}_\xi + \overset{*}{\ell}{}^{\alpha}_{j\xi} e^{-i\vec{f}\vec{n}} \hat{b}_\xi | n_\xi \rangle$$

$$= \sum_{\xi} \frac{\hbar}{2M_j N\omega_\xi} \cdot \langle n_\xi | \ell^{\alpha}_{j\xi} \hat{b}_\xi \cdot \overset{*}{\ell}{}^{\alpha}_{j\xi} \hat{b}^{+}_\xi + \overset{*}{\ell}{}^{\alpha}_{j\xi} \hat{b}^{+}_\xi \cdot \ell^{\alpha}_{j\xi} \cdot \hat{b}_\xi | n_\xi \rangle =$$

$$= \sum_{\xi} \frac{\hbar}{2M_j N\omega_\xi} |\ell^{\alpha}_{j\xi} \overset{*}{\ell}{}^{\alpha}_{j\xi}| \cdot \langle n_\xi | \underbrace{\hat{b}_\xi \hat{b}^{+}_\xi}_{\hat{n}_\xi + 1 \ (37)} + \underbrace{\hat{b}^{+}_\xi \hat{b}_\xi}_{\hat{n}_\xi \ (42)} | n_\xi \rangle = \sum_{\xi} \frac{\hbar}{2M_j N\omega_\xi} \cdot |\vec{\ell}_{j\xi}|^2 \cdot (2n_\xi + 1)$$