The Quantum Linear Chain

Following the usual quantization procedure

$$q_n(t) \longrightarrow \hat{q}_n(t)$$

$$p_n(t) \longrightarrow \hat{p}_n(t)$$

where $\hat{q}_n(t)$ and $\hat{p}_n(t)$ are now operators satisfying the commutation relation

$$[\hat{q}_n(t), \hat{p}_{n'}(t)] = i\hbar\,\delta_{nn'}$$

$$[\hat{q}_n(t), \hat{q}_{n'}(t)] = 0$$

$$[\hat{p}_n(t), \hat{p}_{n'}(t)] = 0$$

– i.e., the Poisson brackets have been replaced by commutators.

Focusing on $\hat{q}_n(t)$:

$ka = \frac{2\pi l}{N}$

$$\hat{q}_n(t) = \sum_l (\hat{a}_l(t)\, u_{n,l} + \hat{a}_l^\dagger u_{n,l}^*)$$

where $\hat{a}_l(t)$ are now operators whose meaning is to be determined.

Similarly,

$$\hat{p}_n(t) = m\dot{\hat{q}}(t) = im \sum_l \omega_l (\hat{a}_l(t)\, u_{n,l} - \hat{a}_l^\dagger u_{n,l}^*)$$

Let's invert the relationships

$$\hat{q}_n(t) = \sum_l \left(\hat{a}_l(t) u_{n,l} + \hat{a}_l^{+} u_{n,l}^{*} \right) \qquad (1)$$

$$\hat{p}_n(t) = i m \sum_l \omega_l \left(\hat{a}_l(t) u_{n,l} - a_l^{+} u_{n,l}^{*} \right) \qquad (2)$$

Multiply (1) and (2) by $u^{*}_{n,l'}$, and sum over n

$$\sum_{n=1}^{N} u^{*}_{n,l'} \hat{q}_n(t) =$$

$$= \sum_l \left\{ \hat{a}_l(t) \underbrace{\sum_{n=1}^{N} u^{*}_{n,l'} u_{n,l}}_{\delta_{ll'}} + \hat{a}_l^{+} \underbrace{\sum_{n=1}^{N} u^{*}_{n,l'} u^{*}_{n,l}}_{\delta_{l,-l'}} \right\}$$

$$= \hat{a}_{l'}(t) + \hat{a}^{+}_{-l'}(t) \qquad (3)$$

$$\sum_{n=1}^{N} u^{*}_{n,l'} \hat{p}_n(t)$$

$$= i m \sum_l \omega_l \left\{ \hat{a}_l(t) \sum_{n=1}^{N} u^{*}_{n,l'} u_{n,l} - \hat{a}_l^{+}(t) \sum_{n=1}^{N} u^{*}_{n,l'} u^{*}_{n,l} \right\}$$

$$= i m \omega_{l'} \left[\hat{a}_{l'}(t) - \hat{a}^{+}_{-l'}(t) \right] \qquad (4)$$

Then, from (3) and (4)

$$\hat{a}_{\ell'}(t) + \hat{a}^{\dagger}_{-\ell'}(t) = \sum_{n=1}^{N} u^{*}_{n,\ell'} \hat{q}_{n}(t) \qquad (5)$$

$$\hat{a}_{\ell'}(t) - \hat{a}^{\dagger}_{-\ell'}(t) = \sum_{n=1}^{N} \frac{1}{im\omega_{\ell'}} u^{*}_{n,\ell'} \hat{p}_{n}(t) \qquad (6)$$

Adding (5) and (6),

$$\hat{a}_{\ell'}(t) = \frac{1}{2} \sum_{n=1}^{N} u^{*}_{n,\ell'} \left[\hat{q}_{n}(t) + \frac{1}{im\omega_{\ell'}} \hat{p}_{n}(t) \right] \qquad (7)$$

Since

$$\hat{q}_{n}(t) = \left[\hat{q}_{n}(t) \right]^{\dagger}$$

$$\hat{p}_{n}(t) = \left[\hat{p}_{n}(t) \right]^{\dagger}$$

we have

$$\hat{a}^{\dagger}_{\ell'}(t) = \frac{1}{2} \sum_{n=1}^{N} u_{n,\ell'} \left[\hat{q}_{n}(t) - \frac{1}{im\omega_{\ell'}} \hat{p}_{n}(t) \right]$$

The relationship we derived between $a_\ell(t)$ and $(q_n(t), p_n(t))$ now becomes the operator relation

$$\hat{a}_\ell(t) = \frac{1}{2}\sum_{n=1}^{N} u^*_{n,\ell}\left[\hat{q}_n(t) + \frac{i}{m\omega_\ell}\hat{p}_n(t)\right]$$

We can use this to determine the commutators associated with the operators $\hat{a}_\ell(t)$:

$$[\hat{a}_\ell(t), \hat{a}^\dagger_{\ell'}(t)]$$

$$= \frac{1}{4}\sum_n\sum_{n'} u^*_{n,\ell}\, u_{n',\ell'}\left\{\left[\hat{q}_n(t) + \frac{i}{m\omega_\ell}\hat{p}_n(t)\right]\left[\hat{q}_{n'}(t) - \frac{i}{m\omega_{\ell'}}\hat{p}_{n'}(t)\right] - \left[\hat{q}_{n'}(t) - \frac{i}{m\omega_\ell}\hat{p}_{n'}(t)\right]\left[\hat{q}_n(t) + \frac{i}{m\omega_\ell}\hat{p}_n(t)\right]\right\}$$

$$= \frac{1}{4}\sum_n\sum_{n'} u^*_{n,\ell}\, u_{n',\ell'}\left\{\hat{q}_n(t)\hat{q}_{n'}(t) - \hat{q}_{n'}(t)\hat{q}_n(t) - \frac{i}{m\omega_\ell}\left(\hat{q}_n(t)\hat{p}_{n'}(t) - p_{n'}(t)\hat{q}_n(t)\right) + \frac{i}{m\omega_\ell}\left(\hat{p}_n(t)\hat{q}_{n'}(t) - \hat{q}_{n'}(t)\hat{p}_n(t)\right) - \left(\frac{i}{m\omega_\ell}\right)^2\left(\hat{p}_n(t)\hat{p}_{n'}(t) - \hat{p}_{n'}(t)\hat{p}_n(t)\right)\right\}$$

$$= \frac{1}{4}\sum_n\sum_{n'} u^*_{n\ell}\, u_{n'\ell'}\left\{-\frac{i}{m\omega_\ell}\, i\delta_{nn'} + \frac{i}{m\omega_\ell}(-i\delta_{nn'})\right\}$$

$$= \frac{1}{2}\frac{1}{m}\frac{1}{\omega_\ell}\sum_n u^*_{n\ell}\, u_{n\ell'}$$

$$= \frac{1}{2m\omega_\ell} \delta_{\ell\ell'}$$

So

$$\left[\sqrt{2m\omega_\ell}\, \hat{a}_\ell(t), \sqrt{2m\omega_{\ell'}}\, \hat{a}^\dagger_{\ell'}(t) \right] = \delta_{\ell\ell'}$$

Define

$$\hat{b}_\ell(t) \equiv \sqrt{2m\omega_\ell}\; \hat{a}_\ell(t)$$

Then

$$\left[\hat{b}_\ell(t), \hat{b}^\dagger_{\ell'}(t) \right] = \delta_{\ell\ell'} \qquad \hat{b}\hat{b}^\dagger - \hat{b}^\dagger\hat{b} = 1$$

Let's now express the Hamiltonian in terms of $\hat{b}_\ell(t)$:

$$H = \sum_\ell m\omega_\ell^2 \left[\hat{a}^\dagger_\ell(t)\hat{a}_\ell(t) + \hat{a}_\ell(t)\hat{a}^\dagger_\ell(t) \right]$$

$$= \sum_\ell m\omega_\ell^2 \frac{1}{2m\omega_\ell} \left[\hat{b}^\dagger_\ell(t)\hat{b}_\ell(t) + \underbrace{\hat{b}_\ell(t)\hat{b}^\dagger_\ell(t)}_{1 + b^\dagger_\ell(t)b_\ell(t)} \right]$$

$$= \frac{1}{2} \sum_\ell \omega_\ell \left[2\hat{b}^\dagger_\ell(t)\hat{b}_\ell(t) + 1 \right]$$

$$= \sum_\ell \omega_\ell \left[\hat{b}^\dagger_\ell(t)\hat{b}_\ell(t) + \frac{1}{2} \right]$$

Using the creation and annihilation operators for each mode, $\hat{b}_l^+$ and $\hat{b}_l$, we can create the multiphonon state

$$|n_1, n_2, n_3, \ldots\rangle = \prod_l |n_l\rangle$$

product given the independence of the modes

where

$$|n_l\rangle = \frac{1}{\sqrt{n_l!}} (\hat{b}_l^+)^{n_l} |0_l\rangle \qquad \langle n_l | n_l \rangle = 1$$

The state $|0_l\rangle$ is the vacuum state for mode l.