Ben Sauerwine
Quantum Mechanics 3 Homework 4

1) **Phonons in a One Dimensional Linear Chain: Consider**

$$H = \sum_{l=1}^{N} \frac{p_i^{\ 2}}{2m} + \frac{1}{2} m\omega^2 \left(q_{l+1} - q_l\right)^2$$

a) **Solve the equations of motion and find the dispersion relation ω_k by proposing that $q_l = \alpha_k e^{ikla} e^{-i\omega_k t}$ with a the equilibrium spacing.**

Hamilton's equations of motion are given by $\frac{\partial H}{\partial p_l} = \dot{q}_l \quad \frac{\partial H}{\partial q_l} = -\dot{p}_l$.

Then, I have:

$$\frac{\partial H}{\partial p_l} = \frac{p_l}{m} = \dot{q}_l \quad , \frac{\partial H}{\partial q_l} = -m\omega^2\left(q_{l+1} - q_l\right) + m\omega^2\left(q_l - q_{l-1}\right) = -\dot{p}_l$$

$$\dot{p}_i = m.\ddot{q}_i$$

$$-m\omega^2\left(q_{l+1} - q_l\right) + m\omega^2\left(q_l - q_{l-1}\right) = -m.\ddot{q}_i$$

$$\ddot{q}_l = -\omega^2\left(q_{l+1} + q_{l-1} - 2q_l\right).$$

$$Substitute \quad q_l = \alpha_k e^{ikla} e^{-i\omega_k t}$$

$$\omega_k^{\ 2} \alpha_k e^{ikla} e^{-i\omega_k t} = \omega^2\left(-\alpha_k e^{ik(l+1)a} e^{-i\omega_k t} - \alpha_k e^{ik(l-1)a} e^{-i\omega_k t} + 2\alpha_k e^{ikla} e^{-i\omega_k t}\right).$$

$$\omega_k^{\ 2} = \omega^2\left(-e^{-ika} - e^{ika} + 2\right) = \omega^2\left(2 - 2\cos ka\right) = \omega^2\left(4\sin^2\frac{ka}{2}\right)$$

b) **Impose periodic boundary conditions $q_l = q_{l+N}$ and find the allowed values of k, namely the Brillouin zone.**

$$q_l = \alpha_k e^{ikla} e^{-i\omega_k t} = q_N = \alpha_k e^{ik(l+N)a} e^{-i\omega_k t}$$

$$\therefore 1 = e^{ikNa}$$

$$k = n\frac{2\pi}{Na}$$

However, with N sites in the periodic boundary, there should be N solutions, corresponding to:

$$n \in \left\{ -\left\lfloor \frac{N-1}{2} \right\rfloor, -\left\lfloor \frac{N-1}{2} \right\rfloor + 1, \ldots, 0, \ldots, \left\lceil \frac{N-1}{2} \right\rceil - 1, \left\lceil \frac{N-1}{2} \right\rceil \right\}.$$

c) **Write $q_l = \frac{1}{\sqrt{N}} \frac{1}{\sqrt{2}} \sum_k \alpha_k e^{ikla} e^{-i\omega_k t} + \alpha_k^{\ *} e^{-ikla} e^{i\omega_k t}$ and write the Hamiltonian in terms of α, α^*.**

Then: $\frac{p_l}{m} = \dot{q}_l = \frac{1}{\sqrt{N}} \frac{i}{\sqrt{2}} \sum_k \omega_k \left[-\alpha_k e^{ikla} e^{-i\omega_k t} + \alpha_k^* e^{-ikla} e^{i\omega_k t} \right]$

Further, I will need this identity, the "Lattice Sum" identity:

$$\frac{1}{N}\sum_{l=1}^{N} e^{i(q-k)la} = \begin{cases} 1 & q = k \\ 0 & q \neq k \end{cases}$$

$$\frac{1}{N}\sum_{l=1}^{N} e^{i(q+k)la} = \begin{cases} 1 & q = -k : 2 \quad solutions! \\ 0 & \qquad q \neq -k \end{cases} ***$$

*** Technical point: Two solutions exist here; however, because of the "wrap around", whereby it is ambiguous as to which "side" of the loop from 1 to N is included, each must get a ½ factor: this is absolutely critical to getting the factors correct in the calculation below.

Now going through my Hamiltonian piece by piece I have:

Further,

$$(q_{l+1} - q_l)^2 = q_{l+1}{}^2 + q_l{}^2 - 2q_{l+1}q_l$$

Here, I have already assumed that differently-indexed coordinates commute.

Evaluating the components of this, then, I have:

$$\sum_{l=1}^{N} q_l{}^2 = \frac{1}{2N}\left(\sum_k \alpha_k e^{ikla} e^{-i\omega_k t} + \alpha_k{}^* e^{-ikla} e^{i\omega_k t}\right)^2$$

$$= \sum_{l=1}^{N} \frac{1}{2N} \sum_{k,k'} \begin{pmatrix} \alpha_k \alpha_{k'} e^{i(k+k')la} e^{-i(\omega_k + \omega_{k'})t} \\ + \alpha_k \alpha_{k'}{}^* e^{i(k-k')la} e^{-i(\omega_k - \omega_{k'})t} \\ + \alpha_{k'}{}^* \alpha_k e^{i(k-k')la} e^{-i(\omega_k - \omega_{k'})t} \\ + \alpha_k{}^* \alpha_{k'}{}^* e^{-i(k+k')la} e^{i(\omega_k + \omega_{k'})t} \end{pmatrix}$$

$$= \frac{1}{2}\sum_k \left[\frac{1}{2}(\alpha_k \alpha_{-k} + \alpha_{-k}\alpha_k) e^{-i(\omega_k + \omega_{-k})t} + \frac{1}{2}(\alpha_k{}^* \alpha_{-k}{}^* + \alpha_{-k}{}^* \alpha_k{}^*) e^{i(\omega_k + \omega_{-k})t} + \alpha_k \alpha_k{}^* + \alpha_k{}^* \alpha_k \right]$$

and:

$$q_{l+1}q_l = \frac{1}{2N}\left(\sum_k \alpha_k e^{ik(l+1)a}e^{-i\omega_k t} + \alpha_k{}^* e^{-ik(l+1)a}e^{i\omega_k t}\right)\left(\sum_k \alpha_k e^{ikla}e^{-i\omega_k t} + \alpha_k{}^* e^{-ikla}e^{i\omega_k t}\right)$$

$$= \frac{1}{2N}\left(\sum_k \alpha_k e^{ik(l+1)a}e^{-i\omega_k t} + \alpha_k{}^* e^{-ik(l+1)a}e^{i\omega_k t}\right)\left(\sum_k \alpha_k e^{ikla}e^{-i\omega_k t} + \alpha_k{}^* e^{-ikla}e^{i\omega_k t}\right)$$

$$= \frac{1}{2N}\sum_{k,k'}\begin{bmatrix} \alpha_k\alpha_{k'}e^{ika}e^{i(k+k')la}e^{-i(\omega_k+\omega_{k'})t} \\ +\alpha_k\alpha_{k'}{}^* e^{ika}e^{i(k-k')la}e^{-i(\omega_k-\omega_{k'})t} \\ +\alpha_k{}^*\alpha_{k'}e^{-ika}e^{-i(k-k')la}e^{i(\omega_k-\omega_{k'})t} \\ +\alpha_k{}^*\alpha_{k'}{}^* e^{-ika}e^{-i(k+k')la}e^{i(\omega_k+\omega_{k'})t} \end{bmatrix}$$

$$= \frac{1}{2}\sum_k\left[\frac{1}{2}(\alpha_k\alpha_{-k} + \alpha_{-k}\alpha_k)e^{ika}e^{-i(\omega_k+\omega_{-k})t} + \frac{1}{2}\left(\alpha_k{}^*\alpha_{-k}{}^* + \alpha_{-k}{}^*\alpha_k{}^*\right)e^{-ika}e^{i(\omega_k+\omega_{-k})t} + \alpha_k\alpha_k{}^* + \alpha_k{}^*\alpha_k\right]$$

Then:

$$\sum_{l=1}^N (q_{l+1}-q_l)^2 = \sum_{l=1}^N q_{l+1}{}^2 + q_l{}^2 - 2q_{l+1}q_l$$

$$= \sum_k\left[\frac{1}{2}(\alpha_k\alpha_{-k} + \alpha_{-k}\alpha_k)e^{-i(\omega_k+\omega_{-k})t} + \frac{1}{2}\left(\alpha_k{}^*\alpha_{-k}{}^* + \alpha_{-k}{}^*\alpha_k{}^*\right)e^{i(\omega_k+\omega_{-k})t} + \alpha_k\alpha_k{}^* + \alpha_k{}^*\alpha_k\right]$$

$$-\sum_k\left[\frac{1}{2}(\alpha_k\alpha_{-k} + \alpha_{-k}\alpha_k)e^{ika}e^{-i(\omega_k+\omega_{-k})t} + \frac{1}{2}\left(\alpha_k{}^*\alpha_{-k}{}^* + \alpha_{-k}{}^*\alpha_k{}^*\right)e^{-ika}e^{i(\omega_k+\omega_{-k})t} + \alpha_k\alpha_{k'}{}^* + \alpha_k{}^*\alpha_{k'}\right]$$

$$= \sum_k\left[\frac{1}{2}(\alpha_k\alpha_{-k} + \alpha_{-k}\alpha_k)\left(1-e^{ika}\right)e^{-i(\omega_k+\omega_{-k})t} + \frac{1}{2}\left(\alpha_k{}^*\alpha_{-k}{}^* + \alpha_{-k}{}^*\alpha_k{}^*\right)\left(1-e^{-ika}\right)e^{i(\omega_k+\omega_{-k})t}\right]$$

Now I take the Momentum term:

$$\sum_{l=1}^N \frac{p_l}{m}^2 = \frac{m}{2N}\sum_{l=1}^N\left(\sum_k i\omega_k\left(-\alpha_k e^{ikla}e^{-i\omega_k t} + \alpha_k{}^* e^{-ikla}e^{i\omega_k t}\right)\right)^2$$

$$= \frac{-m}{2N}\sum_{l=1}^N\sum_{k,k'}\begin{pmatrix} \alpha_k\alpha_{k'}\omega_k\omega_{k'}e^{i(k+k')la}e^{-i(\omega_k+\omega_{k'})t} \\ -\alpha_k\alpha_{k'}{}^*\omega_k\omega_{k'}e^{i(k-k')la}e^{-i(\omega_k-\omega_{k'})t} \\ -\alpha_{k'}{}^*\alpha_k\omega_k\omega_{k'}e^{i(k-k')la}e^{-i(\omega_k-\omega_{k'})t} \\ +\alpha_k{}^*\alpha_{k'}{}^*\omega_k\omega_{k'}e^{-i(k+k')la}e^{i(\omega_k+\omega_{k'})t} \end{pmatrix}$$

$$= -\frac{m}{2}\sum_k\left[\frac{1}{2}(\alpha_k\alpha_{-k} + \alpha_{-k}\alpha_k)\omega_k\omega_{-k}e^{-i(\omega_k+\omega_{-k})t} + \frac{1}{2}\left(\alpha_k{}^*\alpha_{-k}{}^* + \alpha_{-k}{}^*\alpha_k{}^*\right)\omega_k\omega_{-k}e^{i(\omega_k+\omega_{-k})t} - \omega_k{}^2\left(\alpha_k\alpha_k{}^* + \alpha_k{}^*\alpha_k\right)\right]$$

From part a, I recall:

$\omega_k = 2\omega\sin\frac{ka}{2} \therefore \omega_k\omega_{-k} = -\omega^2\left[\left(1-e^{ika}\right)+\left(1-e^{-ika}\right)\right] = -\omega_k{}^2$.

Further, I identify: $\alpha_{-k} = \alpha_k^*$

This allows me to make a final simplification:

$$\frac{1}{2}\sum_{l=1}^{N}\frac{p_l}{m}^2 = -\frac{1}{2}\frac{m}{2}\sum_k\left[-\frac{1}{2}\left(\alpha_k\alpha_k^* + \alpha_k^*\alpha_k\right)\omega_k^2 - \frac{1}{2}\left(\alpha_k^*\alpha_k + \alpha_k\alpha_k^*\right)\omega_k^2 - \omega_k^2\left(\alpha_k\alpha_k^* + \alpha_k^*\alpha_k\right)\right]$$
$$= \frac{m}{4}\sum_k\left(\alpha_k\alpha_k^* + \alpha_k^*\alpha_k\right)\omega_k^2$$

and also

$$\frac{1}{2}m\omega^2\sum_{l=1}^{N}\left(q_{l+1} - q_l\right)^2 = \sum_{l=1}^{N} q_{l+1}^2 + q_l^2 - 2q_{l+1}q_l$$
$$= \frac{1}{2}m\omega^2\sum_k\left[\frac{1}{2}\left(\alpha_k\alpha_k^* + \alpha_k^*\alpha_k\right)\left(1 - e^{ika}\right) + \frac{1}{2}\left(\alpha_k^*\alpha_k + \alpha_k\alpha_k^*\right)\left(1 - e^{-ika}\right)\right] = \frac{1}{4}m\sum_k\left(\alpha_k\alpha_k^* + \alpha_k^*\alpha_k\right)\omega_k^2$$

Then at long last I have:

$$H = \sum_{l=1}^{N}\frac{p_i^2}{2m} + \frac{1}{2}m\omega^2\left(q_{l+1} - q_l\right)^2$$
$$= \frac{m}{4}\sum_k\left(\alpha_k\alpha_k^* + \alpha_k^*\alpha_k\right)\omega_k^2 + \frac{m}{4}\sum_k\left(\alpha_k\alpha_k^* + \alpha_k^*\alpha_k\right)\omega_k^2$$
$$= \frac{m}{2}\sum_k\left(\alpha_k\alpha_k^* + \alpha_k^*\alpha_k\right)\omega_k^2$$

d) Quantize: Consider α_k, α_k^* to be operators and define $a_k = \sqrt{\frac{m\omega_k}{\hbar}}\alpha_k$. Write H in terms of a_k^+ and a_k by imposing bosonic commutation relations.

$$\left[a_k, a_{k'}^+\right] = \delta_{k,k'}$$
$$\left[a_k, a_{k'}\right] = \left[a_k^+, a_{k'}^+\right] = 0$$
$$H = \frac{m}{2}\sum_k\left(\alpha_k\alpha_k^* + \alpha_k^*\alpha_k\right)\omega_k^2 = \frac{\hbar}{2}\sum_k\left(a_k a_k^+ + a_k^+ a_k\right)$$
$$= \frac{\hbar}{2}\sum_k\left(a_k^+ a_k + 1 + a_k^+ a_k\right) = \frac{\hbar}{2}\sum_k\left(2a_k^+ a_k + 1\right) = \hbar\sum_k\left(a_k^+ a_k + \frac{1}{2}\right)$$

2) With the results of problem 1: Consider a Fock state $\left|n_{k_1}, n_{k_2}, n_{k_3}, ...\right\rangle$, with n_k the number of phonons of momentum k. In this state, compute:

a) $\left\langle n_{k_1}, n_{k_2}, n_{k_3}, ...\right| q_l(t) \left| n_{k_1}, n_{k_2}, n_{k_3}, ...\right\rangle$

$$q_l(t) = \frac{1}{\sqrt{N}} \frac{1}{\sqrt{2}} \sum_k \hat{\alpha}_k e^{ikla} e^{-i\omega_k t} + \hat{\alpha}_k{}^+ e^{-ikla} e^{i\omega_k t}$$

$$= \frac{1}{\sqrt{N}} \frac{1}{\sqrt{2}} \sum_k \sqrt{\frac{\hbar}{m\omega_k}} \left[a_k e^{ikla} e^{-i\omega_k t} + a_k{}^+ e^{-ikla} e^{i\omega_k t} \right]$$

Note that in order for $\langle n_{k_1}, n_{k_2}, n_{k_3}, ... | q_l(t) | n_{k_1}, n_{k_2}, n_{k_3}, ... \rangle$ to be non-zero, there needs to be terms like $a_k^+ a_k$ or $a_k a_k^+$, otherwise the Fock state will always be changed to a state not identical to the original state. Since the creation and annihilation operators here only appear separately,

$$\langle n_{k_1}, n_{k_2}, n_{k_3}, ... | q_l(t) | n_{k_1}, n_{k_2}, n_{k_3}, ... \rangle = 0 .$$

b) $\langle n_{k_1}, n_{k_2}, n_{k_3}, ... | p_l(t) | n_{k_1}, n_{k_2}, n_{k_3}, ... \rangle$

$$p_l(t) = \frac{m}{\sqrt{N}} \frac{i}{\sqrt{2}} \sum_k \omega_k \left[-\hat{\alpha}_k e^{ikla} e^{-i\omega_k t} + \hat{\alpha}_k{}^+ e^{-ikla} e^{i\omega_k t} \right]$$

Again, the creation and annihilation operators only appear separately here: then,

$$\langle n_{k_1}, n_{k_2}, n_{k_3}, ... | p_l(t) | n_{k_1}, n_{k_2}, n_{k_3}, ... \rangle = 0 .$$

c) $\langle n_{k_1}, n_{k_2}, n_{k_3}, ... | q_l{}^2(t) | n_{k_1}, n_{k_2}, n_{k_3}, ... \rangle$

$$q_l(t)^2 = \left[\frac{1}{\sqrt{N}} \frac{1}{\sqrt{2}} \sum_k \hat{\alpha}_k e^{ikla} e^{-i\omega_k t} + \hat{\alpha}_k{}^+ e^{-ikla} e^{i\omega_k t} \right]^2$$

$$= \frac{\hbar}{2Nm} \sum_k \sum_{k'} \frac{1}{\sqrt{\omega_k \omega_{k'}}} \left[a_k e^{ikla} e^{-i\omega_k t} + a_k{}^+ e^{-ikla} e^{i\omega_k t} \right] \left[a_{k'} e^{ik'la} e^{-i\omega_{k'} t} + a_{k'}{}^+ e^{-ik'la} e^{i\omega_{k'} t} \right]$$

By the same argument as in part a, however, I may throw out terms where $k \neq k'$ and where the number of creation and annihilation operators is unequal:

$$\langle n_{k_1}, n_{k_2}, n_{k_3}, \ldots | q_l{}^2(t) | n_{k_1}, n_{k_2}, n_{k_3}, \ldots \rangle$$

$$= \langle n_{k_1}, n_{k_2}, n_{k_3}, \ldots | \frac{\hbar}{2Nm} \sum_k \frac{1}{\omega_k} \left[a_k a_k{}^+ + a_k{}^+ a_k \right] n_{k_1}, n_{k_2}, n_{k_3}, \ldots \rangle$$

$$= \langle n_{k_1}, n_{k_2}, n_{k_3}, \ldots | \frac{\hbar}{2Nm} \sum_k \frac{1}{\omega_k} \left[1 + 2a_k{}^+ a_k \right] n_{k_1}, n_{k_2}, n_{k_3}, \ldots \rangle$$

$$Note: a_k{}^+ a_k = \hat{N}_k$$

$$= \langle n_{k_1}, n_{k_2}, n_{k_3}, \ldots | \frac{\hbar}{2Nm} \sum_k \frac{1}{\omega_k} \left[1 + 2n_k \right] n_{k_1}, n_{k_2}, n_{k_3}, \ldots \rangle$$

$$= \frac{\hbar}{2Nm} \sum_k \frac{1 + 2n_k}{\omega_k}$$

d) $\langle n_{k_1}, n_{k_2}, n_{k_3}, \ldots | p_l{}^2(t) | n_{k_1}, n_{k_2}, n_{k_3}, \ldots \rangle$

$$p_l{}^2(t) = -\frac{m^2}{2N} \sum_k \sum_{k'} \omega_k \omega_{k'} \left[-\hat{\alpha}_k e^{ikla} e^{-i\omega_k t} + \hat{\alpha}_k{}^+ e^{-ikla} e^{i\omega_k t} \right] \left[-\hat{\alpha}_{k'} e^{ik'la} e^{-i\omega_{k'} t} + \hat{\alpha}_{k'}{}^+ e^{-ik'la} e^{i\omega_{k'} t} \right]$$

$$p_l{}^2(t) = -\frac{m\hbar}{2N} \sum_k \sum_{k'} \frac{\omega_k \omega_{k'}}{\sqrt{\omega_k \omega_{k'}}} \left[-a_k e^{ikla} e^{-i\omega_k t} + a_k{}^+ e^{-ikla} e^{i\omega_k t} \right] \left[-a_{k'} e^{ik'la} e^{-i\omega_{k'} t} + a_{k'}{}^+ e^{-ik'la} e^{i\omega_{k'} t} \right]$$

Again, I may throw out terms where $k \neq k'$ and where the number of creation and annihilation operators is unequal:

$$\langle n_{k_1}, n_{k_2}, n_{k_3}, \ldots | p_l{}^2(t) | n_{k_1}, n_{k_2}, n_{k_3}, \ldots \rangle$$

$$= \langle n_{k_1}, n_{k_2}, n_{k_3}, \ldots | \frac{-m\hbar}{2N} \sum_k \omega_k \left[-a_k a_k{}^+ - a_k{}^+ a_k \right] n_{k_1}, n_{k_2}, n_{k_3}, \ldots \rangle$$

$$= \langle n_{k_1}, n_{k_2}, n_{k_3}, \ldots | \frac{m\hbar}{2N} \sum_k \omega_k \left[1 + 2a_k{}^+ a_k \right] n_{k_1}, n_{k_2}, n_{k_3}, \ldots \rangle$$

$$Note: a_k{}^+ a_k = \hat{N}_k$$

$$= \langle n_{k_1}, n_{k_2}, n_{k_3}, \ldots | \frac{m\hbar}{2N} \sum_k \omega_k \left[1 + 2n_k \right] n_{k_1}, n_{k_2}, n_{k_3}, \ldots \rangle$$

$$= \frac{m\hbar}{2N} \sum_k \omega_k \left[1 + 2n_k \right]$$

e) Now consider a coherent state $|\alpha_{k_1}, \alpha_{k_2}, \alpha_{k_3}, \ldots\rangle$ **such that** $a_{k_i} |\alpha_{k_1}, \alpha_{k_2}, \alpha_{k_3}, \ldots\rangle = \alpha_{k_i} |\alpha_{k_1}, \alpha_{k_2}, \alpha_{k_3}, \ldots\rangle$ **(*Beware! These are distinct from the alpha operators and simply represent eigenvalues of the annihilation operator on a coherent state!*). Compute parts a – d (above) for this coherent state of phonons.**

Note that similarly, $\langle \alpha_{k_1}, \alpha_{k_2}, \alpha_{k_3}, \ldots | a_{k_i}{}^+ = \langle \alpha_{k_1}, \alpha_{k_2}, \alpha_{k_3}, \ldots | \alpha_{k_i}{}^*$.

$$\left\langle \alpha_{k_1}, \alpha_{k_2}, \alpha_{k_3}, \ldots \middle| q_l(t) \middle| \alpha_{k_1}, \alpha_{k_2}, \alpha_{k_3}, \ldots \right\rangle$$

$$= \left\langle \alpha_{k_1}, \alpha_{k_2}, \alpha_{k_3}, \ldots \middle| \frac{1}{\sqrt{N}} \frac{1}{\sqrt{2}} \sum_k \sqrt{\frac{\hbar}{m\omega_k}} \left[a_k e^{ikla} e^{-i\omega_k t} + a_k^{+} e^{-ikla} e^{i\omega_k t} \right] \middle| \alpha_{k_1}, \alpha_{k_2}, \alpha_{k_3}, \ldots \right\rangle$$

$$= \left\langle \alpha_{k_1}, \alpha_{k_2}, \alpha_{k_3}, \ldots \middle| \frac{1}{\sqrt{N}} \frac{1}{\sqrt{2}} \sum_k \sqrt{\frac{\hbar}{m\omega_k}} \left[\alpha_k^{*} e^{ikla} e^{-i\omega_k t} + \alpha_k e^{-ikla} e^{i\omega_k t} \right] \middle| \alpha_{k_1}, \alpha_{k_2}, \alpha_{k_3}, \ldots \right\rangle$$

$$= \sqrt{\frac{\hbar}{2Nm}} \sum_k \sqrt{\frac{1}{\omega_k}} \left[\alpha_k^{*} e^{ikla} e^{-i\omega_k t} + \alpha_k e^{-ikla} e^{i\omega_k t} \right]$$

Next,

$$p_l(t) = \frac{i}{\sqrt{2N}} \sum_k \sqrt{m\hbar\omega_k} \left[-a_k e^{ikla} e^{-i\omega_k t} + a_k^{+} e^{-ikla} e^{i\omega_k t} \right]$$

$$\left\langle \alpha_{k_1}, \alpha_{k_2}, \alpha_{k_3}, \ldots \middle| p_l(t) \middle| \alpha_{k_1}, \alpha_{k_2}, \alpha_{k_3}, \ldots \right\rangle$$

$$= \left\langle \alpha_{k_1}, \alpha_{k_2}, \alpha_{k_3}, \ldots \middle| \frac{i}{\sqrt{2N}} \sum_k \sqrt{m\hbar\omega_k} \left[-a_k e^{ikla} e^{-i\omega_k t} + a_k^{+} e^{-ikla} e^{i\omega_k t} \right] \middle| \alpha_{k_1}, \alpha_{k_2}, \alpha_{k_3}, \ldots \right\rangle$$

$$= i\sqrt{\frac{m\hbar}{2N}} \left\langle \alpha_{k_1}, \alpha_{k_2}, \alpha_{k_3}, \ldots \middle| \sum_k \sqrt{\omega_k} \left[-\alpha_k^{*} e^{ikla} e^{-i\omega_k t} + \alpha_k e^{-ikla} e^{i\omega_k t} \right] \middle| \alpha_{k_1}, \alpha_{k_2}, \alpha_{k_3}, \ldots \right\rangle$$

$$= i\sqrt{\frac{m\hbar}{2N}} \sum_k \sqrt{\omega_k} \left[-\alpha_k^{*} e^{ikla} e^{-i\omega_k t} + \alpha_k e^{-ikla} e^{i\omega_k t} \right]$$

Next,

$$\left\langle \alpha \ldots \middle| q_l(t)^2 \middle| \alpha \ldots \right\rangle$$

$$= \frac{\hbar}{2Nm} \left\langle \alpha \ldots \middle| \sum_k \sum_{k'} \frac{1}{\sqrt{\omega_k \omega_{k'}}} \left[a_k e^{ikla} e^{-i\omega_k t} + a_k^{+} e^{-ikla} e^{i\omega_k t} \right] \left[a_{k'} e^{ik'la} e^{-i\omega_{k'} t} + a_{k'}^{+} e^{-ik'la} e^{i\omega_{k'} t} \right] \middle| \alpha \ldots \right\rangle$$

$$= \frac{\hbar}{2Nm} \left\langle \alpha \ldots \middle| \sum_k \sum_{k'} \frac{1}{\sqrt{\omega_k \omega_{k'}}} \left[a_k e^{ikla} e^{-i\omega_k t} + \alpha_k^{*} e^{-ikla} e^{i\omega_k t} \right] \left[\alpha_{k'} e^{ik'la} e^{-i\omega_{k'} t} + a_{k'}^{+} e^{-ik'la} e^{i\omega_{k'} t} \right] \middle| \alpha \ldots \right\rangle$$

Commute :

$$= \frac{\hbar}{2Nm} \left\langle \alpha \ldots \middle| \sum_k \sum_{k'} \frac{1}{\sqrt{\omega_k \omega_{k'}}} \begin{pmatrix} e^{ikla} e^{-i\omega_k t} e^{-ik'la} e^{i\omega_{k'} t} \delta_{k,k'} \\ + \left[\alpha_{k'} e^{ik'la} e^{-i\omega_{k'} t} + a_{k'}^{+} e^{-ik'la} e^{i\omega_{k'} t} \right] \left[a_k e^{ikla} e^{-i\omega_k t} + \alpha_k^{*} e^{-ikla} e^{i\omega_k t} \right] \end{pmatrix} \middle| \alpha \ldots \right\rangle$$

$$= \frac{\hbar}{2Nm} \left\langle \alpha \ldots \middle| \sum_k \sum_{k'} \frac{1}{\sqrt{\omega_k \omega_{k'}}} \left(\delta_{k,k'} + \left[\alpha_{k'} e^{ik'la} e^{-i\omega_{k'} t} + \alpha_{k'}^{*} e^{-ik'la} e^{i\omega_{k'} t} \right] \left[\alpha_k e^{ikla} e^{-i\omega_k t} + \alpha_k^{*} e^{-ikla} e^{i\omega_k t} \right] \right) \middle| \alpha \ldots \right\rangle$$

$$= \frac{\hbar}{2Nm} \left[\left(\sum_k \frac{\alpha_k e^{ikla} e^{-i\omega_k t} + \alpha_k^{*} e^{-ikla} e^{i\omega_k t}}{\sqrt{\omega_k}} \right)^2 + \sum_k \frac{1}{\omega_k} \right]$$

Next,

$\langle \alpha ...| p_l(t)^2 | \alpha ... \rangle$

$= \langle \alpha ...| \left[\frac{i}{\sqrt{2N}} \sum_k \sqrt{m\hbar\omega_k} \left[-a_k e^{ikla} e^{-i\omega_k t} + a_k^+ e^{-ikla} e^{i\omega_k t} \right] \right]^2 | \alpha ... \rangle$

$= \frac{-m\hbar}{2N} \langle \alpha ...| \sum_k \sum_{k'} \sqrt{\omega_k \omega_{k'}} \left[-a_k e^{ikla} e^{-i\omega_k t} + a_k^+ e^{-ikla} e^{i\omega_k t} \right] \left[-a_{k'} e^{ik'la} e^{-i\omega_{k'} t} + a_k^+ e^{-ik'la} e^{i\omega_{k'} t} \right] \alpha ... \rangle$

$= \frac{-m\hbar}{2N} \langle \alpha ...| \sum_k \sum_{k'} \sqrt{\omega_k \omega_{k'}} \left[-a_k e^{ikla} e^{-i\omega_k t} + \alpha_k^* e^{-ikla} e^{i\omega_k t} \right] \left[-\alpha_{k'} e^{ik'la} e^{-i\omega_{k'} t} + a_k^+ e^{-ik'la} e^{i\omega_{k'} t} \right] \alpha ... \rangle$

$Commute:$

$= \frac{-m\hbar}{2N} \langle \alpha ...| \sum_k \sum_{k'} \sqrt{\omega_k \omega_{k'}} \begin{pmatrix} -e^{ikla} e^{-i\omega_k t} e^{-ik'la} e^{i\omega_{k'} t} \delta_{k,k'} \\ + \left[-\alpha_{k'} e^{ik'la} e^{-i\omega_{k'} t} + a_k^+ e^{-ik'la} e^{i\omega_{k'} t} \right] \left[-a_k e^{ikla} e^{-i\omega_k t} + \alpha_k^* e^{-ikla} e^{i\omega_k t} \right] \end{pmatrix} | \alpha ... \rangle$

$= \frac{-m\hbar}{2N} \langle \alpha ...| \sum_k \sum_{k'} \sqrt{\omega_k \omega_{k'}} \left(-\delta_{k,k'} + \left[-\alpha_{k'} e^{ik'la} e^{-i\omega_{k'} t} + \alpha_k^+ e^{-ik'la} e^{i\omega_{k'} t} \right] \left[-\alpha_k e^{ikla} e^{-i\omega_k t} + \alpha_k^* e^{-ikla} e^{i\omega_k t} \right] \right) | \alpha ... \rangle$

$= \frac{-m\hbar}{2N} \left[\left(\sum_k \omega_k \left[-\alpha_{k'} e^{ikla} e^{-i\omega_k t} + \alpha_k^+ e^{-ikla} e^{i\omega_k t} \right] \right)^2 - \sum_k \omega_k \right]$

3) Consider a linear chain with two types of atoms (at even and odd sites), all joined together with springs with the same constant κ.

a) Obtain the equations of motion and propose that $q_{even} = Q_k^{(e)} e^{ik2na} e^{-i\omega_k t}$, $q_{odd} = Q_k^{(o)} e^{ik(2n+1)a} e^{-i\omega_k t}$.

$$H = \sum_{i=2n} \frac{p_i^2}{2m} + \sum_{j=2n+1} \frac{p_j^2}{2M} + \frac{1}{2}\kappa (q_{l+1} - q_l)^2$$

Then using:

$$\frac{\partial H}{\partial p_l} = \dot{q}_l \quad \frac{\partial H}{\partial q_l} = -\dot{p}_l$$

I obtain four kinds of relation: two for each equation above, one per lattice site.

$$\frac{\partial H}{\partial p_{2l}} = \frac{p_{2l}}{m} = \dot{q}_{2l} \quad \frac{\partial H}{\partial q_{2l+1}} = \frac{p_{2l+1}}{M} = \dot{q}_{2l+1}$$

$$\frac{\partial H}{\partial q_{2l}} = \kappa(2q_{2l} - q_{2l-1} - q_{2l+1}) = -m\dot{p}_{2l} = -m\ddot{q}_{2l} \quad \frac{\partial H}{\partial q_{2l+1}} = \kappa\left(2q_{2l+1} - q_{2l} - q_{2(l+1)}\right) = -M\dot{p}_{2l+1} = -M\ddot{q}_{2l+1}$$

Proposing that $q_{even} = Q_k^{(e)} e^{ik2na} e^{-i\omega_k t}$, $q_{odd} = Q_k^{(o)} e^{ik(2n+1)a} e^{-i\omega_k t}$, these yield:

$$\kappa\left(2q_{2l}-q_{2l-1}-q_{2l+1}\right)=-m\ddot{q}_{2l}$$
$$\kappa\left(2Q_k^{(e)}e^{ik2la}e^{-i\omega_k t}-Q_k^{(o)}e^{ik(2l-1)a}e^{-i\omega_k t}-Q_k^{(o)}e^{ik(2l+1)a}e^{-i\omega_k t}\right)=m\omega_k^2Q_k^{(e)}e^{ik2la}e^{-i\omega_k t}$$
$$\kappa\left(2Q_k^{(e)}-Q_k^{(o)}e^{-ika}-Q_k^{(o)}e^{ika}\right)=m\omega_k^2Q_k^{(e)}$$
and
$$\kappa\left(2q_{2l+1}-q_{2l}-q_{2(l+1)}\right)=-M\ddot{q}_{2l+1}$$
$$\kappa\left(2Q_k^{(o)}e^{ik(2l+1)a}e^{-i\omega_k t}-Q_k^{(e)}e^{ik2la}e^{-i\omega_k t}-Q_k^{(e)}e^{ik2(l+1)a}e^{-i\omega_k t}\right)=M\omega_k^2Q_k^{(o)}e^{ik(2l+1)a}e^{-i\omega_k t}$$
$$\kappa\left(2Q_k^{(o)}-Q_k^{(e)}e^{-ika}-Q_k^{(e)}e^{ika}\right)=M\omega_k^2Q_k^{(o)}$$

In the next step, I will eliminate the Q coefficients in order to obtain my dispersion relations.

b) Find the dispersion relations ω_k and show that there are two branches. Obtain the $k\to 0$ and $k\to\frac{\pi}{2a}$ for both.

$$\kappa\left(2Q_k^{(e)}-Q_k^{(o)}e^{-ika}-Q_k^{(o)}e^{ika}\right)=m\omega_k^2Q_k^{(e)}$$
$$-2\kappa Q_k^{(o)}\cos(ka)=\left(m\omega_k^2-2\kappa\right)Q_k^{(e)}$$
$$\kappa\left(2Q_k^{(o)}-Q_k^{(e)}e^{-ika}-Q_k^{(e)}e^{ika}\right)=M\omega_k^2Q_k^{(o)}$$
$$-2\kappa Q_k^{(e)}\cos(ka)=\left(M\omega_k^2-2\kappa\right)Q_k^{(o)}$$
e.g.:
$$-2\kappa\left[\frac{-2\kappa\cos(ka)}{M\omega_k^2-2\kappa}\right]\cos(ka)=\left(m\omega_k^2-2\kappa\right)$$
$$\left(m\omega_k^2-2\kappa\right)\left(M\omega_k^2-2\kappa\right)-4\kappa^2\cos^2(ka)=0$$
$$mM\omega_k^4-2\kappa(m+M)\omega_k^2+4\kappa^2-4\kappa^2\cos^2(ka)=0$$
$$\omega_k^2=\frac{2\kappa(m+M)\pm\sqrt{4\kappa^2(m+M)^2-4mM\left(4\kappa^2-4\kappa^2\cos^2(ka)\right)}}{2mM}$$
$$=\frac{\kappa(m+M)\pm\kappa\sqrt{m^2+M^2-2mM+4mM\cos^2(ka)}}{mM}$$
$$=\frac{\kappa(m+M)\pm\kappa\sqrt{m^2+M^2-2mM+4mM\frac{1}{2}(1+\cos(2ka))}}{mM}=\frac{\kappa(m+M)\pm\kappa\sqrt{m^2+M^2+2mM\cos(2ka)}}{mM}$$

So I see that there are two branches, corresponding to the plus and minus choice.

$$\frac{\kappa(m+M)\pm\kappa\sqrt{m^2+M^2+2mM\cos(2ka)}}{mM}$$

$$\omega_{k+}^2(k\to 0)=\frac{\kappa(m+M)+\kappa\sqrt{m^2+M^2+2mM}}{mM}=\frac{2\kappa(m+M)}{mM}$$

$$\omega_{k+}^2\left(k\to\frac{\pi}{2a}\right)=\frac{\kappa(m+M)+\kappa\sqrt{m^2+M^2-2mM}}{mM}=\frac{\kappa(m+M)+\kappa|M-m|}{mM}$$

$$\omega_{k-}^2(k\to 0)=\frac{\kappa(m+M)-\kappa\sqrt{m^2+M^2+2mM}}{mM}=0$$

$$\omega_{k-}^2\left(k\to\frac{\pi}{2a}\right)=\frac{\kappa(m+M)-\kappa\sqrt{m^2+M^2-2mM}}{mM}=\frac{\kappa(m+M)-\kappa|M-m|}{mM}$$

Taylor expanding the term $\omega_{k-}^2(k\approx 0)$ gives:

$$\omega_{k-}^2(k\approx 0)=\frac{2a^2\kappa^2}{m+M}k^2+O(k^4)$$

And the region between $\omega_{k-}^2\left(k\to\frac{\pi}{2a}\right)$ and $\omega_{k+}^2\left(k\to\frac{\pi}{2a}\right)$ is identified as the band gap.

c) Analyze the behavior of the normal modes for $k\to 0$ for both branches.

$$\frac{-2\kappa\cos(ka)}{(M\omega_k^2-2\kappa)}=\frac{Q_k^{(o)}}{Q_k^{(e)}}$$

For the ω_{k-}^2 branch,

$$\frac{-2\kappa\cos(ka)}{(M\omega_{k-}^2-2\kappa)}=\frac{-2\kappa}{-2\kappa}=1=\frac{Q_k^{(o)}}{Q_k^{(e)}}$$

this indicates that the motion of the two types of particles are in-phase for the $\omega_{k-}^2(k\to 0)$ branch.

For the ω_{k+}^2 branch,

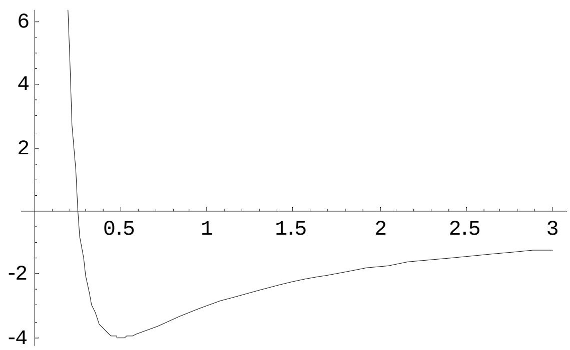
$$\frac{-2\kappa\cos(ka)}{(M\omega_{k+}^2-2\kappa)}=\frac{-2\kappa}{\left(M\frac{2\kappa(m+M)}{mM}-2\kappa\right)}=\frac{1}{1-\frac{M+m}{m}}=-\frac{m}{M}=\frac{Q_k^{(o)}}{Q_k^{(e)}}$$

$$M>0, m>0$$

$$\therefore\frac{Q_k^{(o)}}{Q_k^{(e)}}=-\frac{m}{M}<0$$

Since this is negative and real, it indicates that the motion of the two types of particles are 180 degrees out of phase for the $\omega^2_{k+}(k \to 0)$ branch.

4) **Consider a linear chain of N atoms** $H = \sum_{i=1}^{N} \frac{p_i^2}{2m} + V(|q_i - q_{i+1}|)$ **with** $V(x)$ **a potential of the form**



The equilibrium position of the atoms corresponds to $q_i^{(0)}$ **so that** $|q_i^{(0)} - q_{i+1}^{(0)}| = a$ **.**

a) **Expand the potential up to cubic terms around the equilibrium position and write** H **up to this order. The cubic term is an anharmonic perturbation.**

$$V(x) = V(a) + \left.\frac{\partial V}{\partial x}\right|_{x=a}(x-a) + \frac{1}{2}\left.\frac{\partial^2 V}{\partial x^2}\right|_{x=a}(x-a)^2 + \frac{1}{6}\left.\frac{\partial^3 V}{\partial x^3}\right|_{x=a}(x-a)^3 + \ldots$$

$$\to \frac{1}{2}\left.\frac{\partial^2 V}{\partial x^2}\right|_{x=a}(x-a)^2 + \frac{1}{6}\left.\frac{\partial^3 V}{\partial x^3}\right|_{x=a}(x-a)^3 + \ldots$$

Here I have dropped the zero-point energy and since this is a local minimum, the first-order term also.

$$define: m\omega^2 = \left.\frac{\partial^2 V}{\partial x^2}\right|_{x=a} \qquad \beta = \left.\frac{\partial^3 V}{\partial x^3}\right|_{x=a}$$

$$H = \sum_{i=1}^{N} \frac{p_i^2}{2m} + \frac{1}{2}m\omega^2(q_i - q_{i+1})^2 + \frac{1}{6}\beta|q_i - q_{i+1}|^3$$

b) **Write the Hamiltonian in terms of the phonon creation and annihilation operators of problem 1 and express the cubic perturbation term in** a_k^+, a_k **and interpret the processes described by the cubic term.**

Once again, let $q_l = \frac{1}{\sqrt{N}} \frac{1}{\sqrt{2}} \sum_k \alpha_k e^{ikla} e^{-i\omega_k t} + \alpha_k{}^* e^{-ikla} e^{i\omega_k t}$. I have already seen that under the definition $a_k = \sqrt{\frac{m\omega_k}{\hbar}} \alpha_k$ where $\omega_k{}^2 = \omega^2 \left(4\sin^2 \frac{ka}{2} \right)$ (as in problem 1),

$$define : m\omega^2 = \left. \frac{\partial^2 V}{\partial x^2} \right|_{x=a} \qquad \beta = \left. \frac{\partial^3 V}{\partial x^3} \right|_{x=a}$$

$$H = \hbar \sum_k \left(a_k^+ a_k + \frac{1}{2} \right) + \sum_{l=1}^{N} \frac{1}{6} \beta \left| q_i - q_{i+1} \right|^3$$

It is then left to write $\frac{1}{6} \beta \left| q_i - q_{i+1} \right|^3$ in terms of these operators.

$$\sum_{l=1}^{N} \frac{1}{6} \beta \left| q_i - q_{i+1} \right|^3$$

$$= \frac{1}{6} \beta \left| \sum_{l=1}^{N} \sum_{k,k',k''} \left(\alpha_k e^{ikla} e^{-i\omega_k t} + \alpha_k{}^* e^{-ikla} e^{i\omega_k t} \right) \left(\alpha_{k'} e^{ik'la} e^{-i\omega_{k'} t} + \alpha_{k'}{}^* e^{-ik'la} e^{i\omega_{k'} t} \right) \left(\alpha_{k''} e^{ik''la} e^{-i\omega_{k''} t} + \alpha_{k''}{}^* e^{-ik''la} e^{i\omega_{k''} t} \right) \right|$$

$$= \frac{1}{6} \beta \frac{1}{(2N)^{\frac{3}{2}}} \left| \sum_{l=1}^{N} \sum_{k,k',k''} \begin{bmatrix} \alpha_k \alpha_{k'} \alpha_{k''} e^{i(k+k'+k'')la} e^{-i(\omega_k + \omega_{k'} + \omega_{k''})t} + \alpha_k{}^* \alpha_{k'} \alpha_{k''} e^{i(-k+k'+k'')la} e^{-i(\omega_k + \omega_{k'} + \omega_{k''})t} \\ + \alpha_k \alpha_{k'}{}^* \alpha_{k''} e^{i(k-k'+k'')la} e^{-i(\omega_k - \omega_{k'} + \omega_{k''})t} + \alpha_k{}^* \alpha_{k'}{}^* \alpha_{k''} e^{i(-k-k'+k'')la} e^{-i(-\omega_k - \omega_{k'} + \omega_{k''})t} \\ + \alpha_k \alpha_{k'} \alpha_{k''}{}^* e^{i(k+k'-k'')la} e^{-i(\omega_k + \omega_{k'} - \omega_{k''})t} + \alpha_k{}^* \alpha_{k'} \alpha_{k''}{}^* e^{i(-k+k'-k'')la} e^{-i(-\omega_k + \omega_{k'} - \omega_{k''})t} \\ + \alpha_k \alpha_{k'}{}^* \alpha_{k''}{}^* e^{i(k-k'-k'')la} e^{-i(\omega_k - \omega_{k'} - \omega_{k''})t} + \alpha_k{}^* \alpha_{k'}{}^* \alpha_{k''}{}^* e^{i(-k-k'-k'')la} e^{-i(-\omega_k - \omega_{k'} - \omega_{k''})t} \end{bmatrix} \right|$$

$$= \frac{1}{6} \beta \frac{1}{2\sqrt{N}} \left| \sum_{k,k',k''} \begin{bmatrix} \frac{1}{4} \alpha_k \alpha_{k'} \alpha_{k''} \delta^0_{k+k'+k''} e^{-i(\omega_k + \omega_{k'} + \omega_{k''})t} + \frac{1}{2} \alpha_k{}^* \alpha_{k'} \alpha_{k''} \delta^k_{k'+k''} e^{-i(\omega_k + \omega_{k'} + \omega_{k''})t} \\ + \frac{1}{2} \alpha_k \alpha_{k'}{}^* \alpha_{k''} \delta^{k'}_{k+k''} e^{-i(\omega_k - \omega_{k'} + \omega_{k''})t} + \frac{1}{2} \alpha_k{}^* \alpha_{k'}{}^* \alpha_{k''} \delta^{k''}_{k+k'} e^{-i(-\omega_k - \omega_{k'} + \omega_{k''})t} \\ + \frac{1}{2} \alpha_k \alpha_{k'} \alpha_{k''}{}^* \delta^{k''}_{k+k'} e^{-i(\omega_k + \omega_{k'} - \omega_{k''})t} + \frac{1}{2} \alpha_k{}^* \alpha_{k'} \alpha_{k''}{}^* \delta^{k'}_{k+k''} e^{-i(-\omega_k + \omega_{k'} - \omega_{k''})t} \\ + \frac{1}{2} \alpha_k \alpha_{k'}{}^* \alpha_{k''}{}^* \delta^{k}_{k'+k''} e^{-i(\omega_k - \omega_{k'} - \omega_{k''})t} + \frac{1}{4} \alpha_k{}^* \alpha_{k'}{}^* \alpha_{k''}{}^* \delta^0_{k+k'+k''} e^{-i(-\omega_k - \omega_{k'} - \omega_{k''})t} \end{bmatrix} \right|$$

In the fourth step here I have used the argument from problem (1) that the delta-functions with same-sign entries bring a factor of one-half for each repeated factor. Then:

$$\sum_{l=1}^{N}\frac{1}{6}\beta\left|q_i - q_{i+1}\right|^3$$

$$=\frac{1}{6}\beta\frac{1}{2\sqrt{N}}\left|\begin{array}{l}\frac{1}{2}\sum_{k,k'=0}^{\infty}\left[\begin{array}{l}\alpha_{-k-k'}{}^{*}\alpha_k\alpha_{k'}e^{-i\left(\omega_{-k-k'}+\omega_k+\omega_{k'}\right)t}+\alpha_k\alpha_{-k-k'}{}^{*}\alpha_{k'}e^{-i\left(\omega_k-\omega_{-k-k'}+\omega_{k'}\right)t}\\ +\alpha_k{}^{*}\alpha_{k'}{}^{*}\alpha_{-k-k'}e^{-i\left(-\omega_k-\omega_{k'}+\omega_{-k-k'}\right)t}+\alpha_k\alpha_{k'}\alpha_{-k-k'}{}^{*}e^{-i\left(\omega_k+\omega_{k'}-\omega_{-k-k'}\right)t}\\ +\alpha_k{}^{*}\alpha_{-k-k'}\alpha_{k'}{}^{*}e^{-i\left(-\omega_k+\omega_{-k-k'}-\omega_{k'}\right)t}+\alpha_{-k-k'}\alpha_k{}^{*}\alpha_{k'}{}^{*}e^{-i\left(\omega_{-k-k'}-\omega_k-\omega_{k'}\right)t}\end{array}\right]\\ +\frac{1}{4}\sum_{k=0}^{\infty}\sum_{k'=-\infty}^{\infty}\left[\alpha_k\alpha_{k'}\alpha_{-k-k'}e^{-i\left(\omega_k+\omega_{k'}+\omega_{k-k'}\right)t}+\alpha_k{}^{*}\alpha_{k'}{}^{*}\alpha_{-k-k'}{}^{*}e^{-i\left(-\omega_k-\omega_{k'}-\omega_{-k-k'}\right)t}\right]\end{array}\right|$$

and of course once could substitute $\sqrt{\frac{\hbar}{m\omega_k}}a_k = \alpha_k$ for each operator here.

I expect the time dependent version to vanish under the action of the absolute value operator, but the mechanism for this may be rather complex; so I see that the cubic perturbation is some combination of 3 of the phonon creation and destruction operators: Either 3 creators, 2 creators and 1 destructor, 2 destructors and 1 creator, or 3 destructors.