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Lattice Normal Modes and Phonons via Quantum Mechanics

The Hamiltonian for the 1-D monatomic chain is a sum of coupled harmonic oscillators:

$$H = \sum_j \Big(\frac{p_j^2}{2m} + \frac{m\omega_0^2}{2}(x_{j+1} - x_j)^2 \Big) \tag{1}$$

Show that the following Fourier decomposition decouples them;

$$x_j = N^{-1/2} \sum_k e^{-ikja} X_k \qquad p_j = N^{-1/2} \sum_k e^{ikja} P_k \tag{2}$$

into the from:

$$H = \sum_k \Big(\frac{P_{-k} P_k}{2m} + \frac{m\omega_0^2}{2}(4\sin^2(ka/2)) X_{-k} X_k \Big) \tag{3}$$

where N is the number of atoms in the chain and a is the equilibrium atomic spacing.
Hint: use the identity $\sum_j exp(i(k' + k)ja) = N\delta_{k,-k'}$. What are the allowed values of k?

To do this part we simply substitute in the new operators as given to us. Be careful with your indeces!

$$H = N^{-1} \sum_{j,k,l} \left(\frac{P_k P_l e^{i(k+l)ja}}{2m} + \frac{m\omega_0^2}{2} \left(e^{-ika} - 1\right) e^{-ikja} X_k \left(e^{-ila} - 1\right) e^{-ikla} X_l \right). \tag{4}$$

If we perform the j summation first, we can use the identity provided in the hint:

$$H = \sum_{k,l} \left(\frac{P_k P_l}{2m} \delta_{k,-l} + \frac{m\omega_0^2}{2} \left(e^{-ika} - 1\right) \left(e^{-ila} - 1\right) X_k X_l \delta_{k,-l} \right), \tag{5}$$

$$\Longrightarrow H = \sum_k \left(\frac{P_k P_{-k}}{2m} + \frac{m\omega_0^2}{2} \left(e^{-ika} - 1\right) \left(e^{ika} - 1\right) X_k X_{-k} \right), \tag{6}$$

$$\Longrightarrow H = \sum_k \left(\frac{P_k P_{-k}}{2m} + \frac{m\omega_0^2}{2} \left(2 - 2\cos(ka)\right) X_k X_{-k} \right), \tag{7}$$

$$\Longrightarrow H = \sum_k \left(\frac{P_k P_{-k}}{2m} + \frac{m\omega_0^2}{2} \left(4\sin^2(ka/2)\right) X_k X_{-k} \right). \tag{8}$$

We are perfectly at liberty to change the dummy index k to $-k$, obtaining exactly the form in Eqn. 3. In defining our Fourier transforms (Eqn. 2), our k values are exactly the the values of k within the first Brillouin zone which are allowed by periodic boundary conditions: i.e., $k = \frac{2\pi m}{Na}$. This is to provide the correct periodicity of x_j.

So far we have made no assumptions about whether we are dealing with a quantum or a classical system. In the classical case, we could use this form of H to derive the same dispersion as in question 2 (don't worry about the details of how to do this - the easiest way is with Hamiltonian mechanics). In the quantum case, we need to explicitly consider the observables a operators.

1. *Show that* $[X_k, P_q] = i\hbar\delta_{k,q}$*, and that* $X_k^\dagger = X_{-k}$ *(and similarly for* $P_k^\dagger$*). To do this you will need to use the hermitian property of* x_j*:* $x_j^\dagger = x_j$*.*

2. *Define the operator* a_k *by:*

$$a_k = \left(\frac{m\omega_k}{2\hbar}\right)^{1/2}(X_k + \frac{i}{m\omega_k}P_k^\dagger), \tag{9}$$

where $\omega_k = 2\omega_0|\sin(ka/2)|$*. Show that* $[a_k, a_q^\dagger] = \delta_{k,q}$*, and hence that the Hamiltonian simplifies to the form:*

$$H = \sum_k \hbar\omega_k(a_k^\dagger a_k + 1/2) \tag{10}$$

1. To do the commutator, we again just substitute in. To do this, first invert Eqn. 2, which is reasonably simple.

$$[X_k, P_q] = \left[N^{-1/2}\sum_j e^{ikja}x_j, N^{-1/2}\sum_l e^{-iqla}p_l\right], \tag{11}$$

$$\implies [X_k, P_q] = N^{-1}\sum_{j,l} e^{ikja}e^{-iqla}\left[x_j, p_l\right]. \tag{12}$$

Now we can use the good old commutation relations of second year, $[x_j, p_l] = i\hbar\delta_{j,l}$,

$$[X_k, P_q] = \frac{i\hbar}{N}\sum_j e^{i(k-q)ja} = i\hbar\delta_{i,j}. \tag{13}$$

The conjugation property is not too hard to show:

$$X_k^\dagger = \left(N^{-1/2}\sum_j e^{ikja}x_j\right)^\dagger = N^{-1/2}\sum_j e^{-ikja}x_j^\dagger = N^{-1/2}\sum_j e^{-ikja}x_j = X_{-k} \tag{14}$$

2. We now have everything we need to evaluate the second commutator:

$$[a_k, a_q^\dagger] = \frac{i}{2\hbar}\left(-(\omega_k/\omega_q)^{1/2}[X_k, P_q] + (\omega_q/\omega_k)^{1/2}[P_k^\dagger, X_q^\dagger]\right) = \delta_{k,q}. \tag{15}$$

To prove that we can rewrite the Hamiltonian, it is easiest to expand $\hbar\omega_k(a_k^\dagger a_k + 1/2)$:

$$\hbar\omega_k(a_k^\dagger a_k + 1/2) = \left(\frac{\hbar m w_k^2}{2\hbar}\right)\left(X_k X_k^\dagger + \left(\frac{-i}{m\omega_k}\right)X_k P_k + \left(\frac{i}{m\omega_k}\right)P_k^\dagger X_k^\dagger + \frac{1}{(m\omega_k)^2}P_k^\dagger P_k\right) + \frac{\hbar\omega_k}{2}. \tag{16}$$

We now commute $P_k^\dagger$ and $X_k^\dagger$, and use the conjugation relation derived earlier:

$$\hbar\omega_k(a_k^\dagger a_k + 1/2) = \left(\frac{m w_k^2}{2}\right)\left(X_k X_{-k} + \frac{1}{(m\omega_k)^2}P_k P_{-k} + \left(\frac{-i}{m\omega_k}\right)X_k P_k + \left(\frac{i}{m\omega_k}\right)X_{-k}P_{-k} - \frac{\hbar}{m\omega_k}\right) + \frac{\hbar\omega_k}{2}. \tag{17}$$

$$\implies \hbar\omega_k(a_k^\dagger a_k + 1/2) = \left(\frac{m w_k^2}{2}\right)\left(X_k X_{-k} + \frac{1}{(m\omega_k)^2}P_k P_{-k} + \left(\frac{-i}{m\omega_k}\right)X_k P_k + \left(\frac{i}{m\omega_k}\right)X_{-k}P_{-k})\right). \tag{18}$$

If we sum over all k, the third and fourth terms will cancel each other.

$$\implies \sum_k \hbar\omega_k(a_k^\dagger a_k + 1/2) = \sum_k \left(\frac{m w_k^2}{2}\right)\left(X_k X_{-k} + \frac{1}{(m\omega_k)^2}P_k P_{-k}\right). \tag{19}$$

Which is the Hamiltonian!

We have now decoupled the system into independent quantum oscillators. What is the energy spectrum? Explain what each of the new operators means physically. Referring to your answer, or otherwise, explain what a phonon is.

$E = \sum_k \hbar\omega_k n_k$

$a_k^\dagger$ increases the energy of the kth normal mode by $\hbar w_k$, and a_k decreases it by the same amount. These quantized excitations of the normal modes can be interpreted as bosons, which we call phonons.