COUPLED OSCILLATORS IN TERMS OF CREATION AND ANNIHILATION OPERATORS; PHONONS

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References: Tom Lancaster and Stephen J. Blundell, *Quantum Field Theory for the Gifted Amateur*, (Oxford University Press, 2014) - Problem 2.3.

Suppose we have a one-dimensional chain of N equal masses m connected by identical springs of rest length a and spring constant k, so that mass j has a rest position of ja, $j=0\ldots N-1$. The masses can move only in the x direction, and moving one mass extends the spring on one side while compressing the spring on the other side. The total energy of the system is the sum of the kinetic energies of the masses and the potential energies of the springs. The kinetic energy of mass j is just $\frac{1}{2}mv_j^2$ or, in terms of the momentum operator

$$T_j=\frac{\hat{p}_j^2}{2m} \tag{1}$$

The potential energy of the spring connecting masses j and $j+1$ is $\frac{1}{2}k\left(\Delta x\right)^2$ where Δx is the amount the spring is stretched (or compressed). Δx is the difference between the amounts that the two masses on either end have moved from their equilibrium positions, so if we call x_j the amount by which mass j has moved from position ja, then

$$\Delta x_{j,j+1} = x_{j+1}-x_j \tag{2}$$

$$V_j = \frac{1}{2}K\left(\hat{x}_{j+1}-\hat{x}_j\right)^2 \tag{3}$$

where we've added hats to show that $\hat{x}_j$ is an operator. Therefore the hamiltonian of the system is

$$\hat{H}=\sum_j\frac{\hat{p}_j^2}{2m}+\sum_j\frac{1}{2}K\left(\hat{x}_{j+1}-\hat{x}_j\right)^2 \tag{4}$$

As it stands, the hamiltonian contains terms such as $k\hat{x}_j\hat{x}_{j+1}$ in which the spatial terms of two masses occur in a product, that is, it contains coupled terms. We can convert the hamiltonian to an uncoupled system in which it consists of a sum of terms where each term refers to only a single index. This is done by using discrete Fourier transforms. A discrete Fourier transform assumes that the raw data (the values of x_j and p_j) are samples at equally spaced intervals and that the behaviour outside the observed range (that is, for $j<0$ and $j\ge N$) is periodic, so that it repeats the observed behaviour with a period of Na. This is equivalent to imposing periodic boundary conditions so that

$$x_{j+N} = x_j \quad (5)$$
$$p_{j+N} = p_j \quad (6)$$

The discrete Fourier transform is then

$$x_j = \frac{1}{\sqrt{N}}\sum_k \tilde{x}_k e^{ikja} \quad (7)$$
$$p_j = \frac{1}{\sqrt{N}}\sum_k \tilde{p}_k e^{ikja} \quad (8)$$

[This transform differs from the one in the earlier reference in that it has a factor of $1/\sqrt{N}$ in front. All that matters is that the product of this factor with the corresponding factor in front of the inverse transform is $1/N$.] The index k is the frequency and because of the periodic boundary conditions, we must have

$$e^{ikja} = e^{ik(j+N)a} \quad (9)$$
$$e^{ikNa} = 1 \quad (10)$$
$$k = \frac{2\pi m}{Na} \quad (11)$$

for an integer m which is in a range such that ka varies over 2π. Any range of m that satisfies this condition would do, but it turns out to be most convenient to choose $-\frac{N}{2}<m\le\frac{N}{2}$. This gives $-\pi<ka\le\pi$.

We can now work out the hamiltonian 4 using the Fourier transformed variables $\tilde{x}_k$ and $\tilde{p}_k$. First, the kinetic energy term:

$$\sum_j p_j^2 = \sum_j\left(\frac{1}{\sqrt{N}}\sum_k \tilde{p}_k e^{ikja}\right)\left(\frac{1}{\sqrt{N}}\sum_{k'} \tilde{p}_{k'} e^{ik'ja}\right) \quad (12)$$
$$= \frac{1}{N}\sum_j\sum_k\sum_{k'}\tilde{p}_k\tilde{p}_{k'}e^{i(k+k')ja} \quad (13)$$

We can now make use of the sum (derived from a geometric series):

$$\sum_j e^{i2\pi mj/N} = N\delta_{m,0} \tag{14}$$

This means that

$$\sum_j e^{i(k+k')ja} = N\delta_{k,-k'} \tag{15}$$

so

$$\sum_j p_j^2 = \sum_k \tilde{p}_k \tilde{p}_{-k} \tag{16}$$

For the potential energy term we have

$$\sum_j (\hat{x}_{j+1} - \hat{x}_j)^2 = \frac{1}{N}\sum_j \left(\sum_k \tilde{x}_k e^{ik(j+1)a} - \sum_k \tilde{x}_k e^{ikja}\right)\left(\sum_{k'} \tilde{x}_{k'} e^{ik'(j+1)a} - \sum_{k'} \tilde{x}_{k'} e^{ik'ja}\right) \tag{17}$$

$$= \frac{1}{N}\sum_j \left(\sum_k \tilde{x}_k e^{ikja}\left(e^{ika}-1\right)\right)\left(\sum_{k'} \tilde{x}_{k'} e^{ik'ja}\left(e^{ik'a}-1\right)\right) \tag{18}$$

$$= \frac{1}{N}\sum_j \sum_k \sum_{k'} \tilde{x}_k \tilde{x}_{k'} e^{i(k+k')ja}\left(e^{ika}-1\right)\left(e^{ik'a}-1\right) \tag{19}$$

$$= \sum_k \tilde{x}_k \tilde{x}_{-k}\left(e^{ika}-1\right)\left(e^{-ika}-1\right) \tag{20}$$

$$= \sum_k \tilde{x}_k \tilde{x}_{-k}\left(2-\left(e^{ika}+e^{-ika}\right)\right) \tag{21}$$

$$= 2\sum_k \tilde{x}_k \tilde{x}_{-k}\left(1-\cos(ka)\right) \tag{22}$$

$$= 4\sum_k \tilde{x}_k \tilde{x}_{-k}\sin^2\frac{ka}{2} \tag{23}$$

It might not seem that we've made much progress, since now both the kinetic and potential energy terms appear to be coupled, involving products of $+k$ and $-k$ modes. However, the inverses of 7 and 8 are

$$\tilde{x}_k = \frac{1}{\sqrt{N}}\sum_j x_j e^{-ikja} \tag{24}$$

$$\tilde{p}_k = \frac{1}{\sqrt{N}}\sum_j p_j e^{-ikja} \tag{25}$$

Since x_j and p_j are observables, they must be hermitian operators, so $x_j^\dagger = x_j$ and $p_j^\dagger = p_j$ so

$$\tilde{x}_k^\dagger = \frac{1}{\sqrt{N}}\sum_j x_j e^{ikja} = \tilde{x}_{-k} \tag{26}$$

$$\tilde{p}_k^\dagger = \frac{1}{\sqrt{N}}\sum_j p_j e^{ikja} = \tilde{p}_{-k} \tag{27}$$

Therefore

$$\sum_j p_j^2 = \sum_k \tilde{p}_k \tilde{p}_{-k} \tag{28}$$

$$= \sum_k \tilde{p}_k \tilde{p}_k^\dagger \tag{29}$$

$$\sum_j \left(\hat{x}_{j+1} - \hat{x}_j\right)^2 = 4\sum_k \tilde{x}_k \tilde{x}_{-k} \sin^2 \frac{ka}{2} \tag{30}$$

$$= 4\sum_k \tilde{x}_k \tilde{x}_k^\dagger \sin^2 \frac{ka}{2} \tag{31}$$

$$\hat{H} = \frac{1}{2m}\sum_k \tilde{p}_k \tilde{p}_k^\dagger + 2K\sum_k \tilde{x}_k \tilde{x}_k^\dagger \sin^2 \frac{ka}{2} \tag{32}$$

$$= \frac{1}{2m}\sum_k \tilde{p}_k \tilde{p}_k^\dagger + \frac{1}{2}m\sum_k \omega_k^2 \tilde{x}_k \tilde{x}_k^\dagger \tag{33}$$

$$= \frac{1}{2m}\sum_k \tilde{p}_k \tilde{p}_{-k} + \frac{1}{2}m\sum_k \omega_k^2 \tilde{x}_k \tilde{x}_{-k} \tag{34}$$

where

$$\omega_k^2 \equiv 4\frac{K}{m}\sin^2 \frac{ka}{2} \tag{35}$$

That is, we've managed to write the hamiltonian as the sum over *uncoupled* oscillators, where oscillator k has frequency ω_k. The catch is that the operators $\tilde{p}_k$ and $\tilde{x}_k$ are in frequency space, not 'normal' space, so they are the 'momentum' and 'position' operators for the modes of oscillation of the coupled set of oscillators.

The formal equivalence of the hamiltonian in mode space with the hamiltonian for a single oscillator in normal space means we can define creation and annihilation operators in the same way. That is (reverting to 'hat' notation to indicate operators):

$$\hat{a}_k^\dagger = \frac{1}{\sqrt{2\hbar m\omega_k}}\left[-i\hat{p}_k^\dagger + m\omega_k\hat{x}_k^\dagger\right] \tag{36}$$
$$= \frac{1}{\sqrt{2\hbar m\omega_k}}\left[-i\hat{p}_{-k} + m\omega_k\hat{x}_{-k}\right] \tag{37}$$
$$\hat{a}_k = \frac{1}{\sqrt{2\hbar m\omega_k}}\left[i\hat{p}_k + m\omega_k\hat{x}_k\right] \tag{38}$$

Inverting these equations, we get (note that ω_k is always the positive square root of 35):

$$\hat{a}_{-k}^\dagger = \frac{1}{\sqrt{2\hbar m\omega_k}}\left[-i\hat{p}_k + m\omega_k\hat{x}_k\right] \tag{39}$$
$$\hat{a}_{-k}^\dagger + \hat{a}_k = \frac{2}{\sqrt{2\hbar m\omega_k}} m\omega_k\hat{x}_k \tag{40}$$
$$\hat{x}_k = \sqrt{\frac{\hbar}{2m\omega_k}}\left(\hat{a}_{-k}^\dagger + \hat{a}_k\right) \tag{41}$$
$$\hat{p}_k = i\sqrt{\frac{\hbar m\omega_k}{2}}\left(\hat{a}_{-k}^\dagger - \hat{a}_k\right) \tag{42}$$

Example. We can express the original space coordinate x_j in terms of the creation and annihilation operators. From 7

$$x_j = \frac{1}{\sqrt{N}}\sum_k \hat{x}_k e^{ikja} \tag{43}$$
$$= \sqrt{\frac{\hbar}{2mN}}\sum_k \frac{1}{\sqrt{\omega_k}}\left(\hat{a}_{-k}^\dagger + \hat{a}_k\right)e^{ikja} \tag{44}$$
$$= \sqrt{\frac{\hbar}{2mN}}\sum_k \frac{1}{\sqrt{\omega_k}}\left(\hat{a}_k^\dagger e^{-ikja} + \hat{a}_k e^{ikja}\right) \tag{45}$$

where the last line follows from the fact that we're summing over k over a range of values symmetric about $k = 0$ so we can replace k by $-k$ and get the same sum.

Inserting 41 and 42 into 34 we get

$$\hat{H} = -\frac{\hbar}{4}\sum_k \omega_k \left(\hat{a}^\dagger_{-k} - \hat{a}_k\right)\left(\hat{a}^\dagger_k - \hat{a}_{-k}\right) + \frac{\hbar}{4}\sum_k \omega_k \left(\hat{a}^\dagger_{-k} + \hat{a}_k\right)\left(\hat{a}^\dagger_k + \hat{a}_{-k}\right) \tag{46}$$

$$= \frac{\hbar}{2}\sum_k \omega_k \left(\hat{a}^\dagger_{-k}\hat{a}_{-k} + \hat{a}_k\hat{a}^\dagger_k\right) \tag{47}$$

Since the commutator is

$$\left[\hat{a}_k, \hat{a}^\dagger_k\right] = 1 \tag{48}$$

we get

$$\hat{H} = \frac{\hbar}{2}\sum_k \omega_k \left(\hat{a}^\dagger_{-k}\hat{a}_{-k} + 1 + \hat{a}^\dagger_{-k}\hat{a}_{-k}\right) \tag{49}$$

$$= \sum_k \hbar\omega_k \left(\hat{a}^\dagger_{-k}\hat{a}_{-k} + \frac{1}{2}\right) \tag{50}$$

$$= \sum_k \hbar\omega_k \left(\hat{a}^\dagger_k\hat{a}_k + \frac{1}{2}\right) \tag{51}$$

That is, the hamiltonian is the sum of the hamiltonians for individual oscillators in terms of creation and annihilation operators. The 'particles' that are created or annihilated are the modes of oscillation in the chain of 'real' oscillators; these modes are called *phonons*, since they are reminiscent of sound waves passing through a medium.