# Phonons and field theory (continued)

## Summary of previous notes

In the previous set of notes we discussed how to diagonalize the Hamiltonian of a 1D harmonic chain

$$H = \frac{1}{2}\sum_{i=1}^{N}\left(p_i^2 + \omega^2 q_i^2\right) + \frac{g}{2}\sum_{i=1}^{N}\left(q_i - q_{i+1}\right)^2 \qquad (1)$$

we learned that the whole task reduced to finding the eigenvalues and eigenvectors of a cyclic matrix

$$A = \begin{pmatrix} \omega^2+2g & -g & 0 & 0 & -g \\ -g & \omega^2+2g & -g & 0 & 0 \\ 0 & -g & \omega^2+2g & -g & 0 \\ 0 & 0 & -g & \omega^2+2g & -g \\ -g & 0 & 0 & -g & \omega^2+2g \end{pmatrix} \qquad (2)$$

we learned that this matrix is diagonalized by a Fourier transform

$$A = U \Lambda U^{\dagger} \qquad (3)$$

where $\Lambda$ is a diagonal matrix with entries

$$\lambda_k = \omega^2 + 2g(1-\cos k) \qquad (4)$$

and

$$U_{ik} = \frac{1}{\sqrt{N}} e^{ikx_i} \qquad x_i = i \qquad (5)$$

$$k = \frac{2\pi l}{N}, \quad l = 0, \pm 1, \pm 2, \dots, \pm N/2$$

As a consequence of $UU^{\dagger}=1$ and $U^{\dagger}U=1$, we get

$$\frac{1}{N}\sum_i e^{i(k-k')x_i} = \delta_{kk'}, \qquad \frac{1}{N}\sum_k e^{ik(x_i-x_j)} = \delta_{ij} \qquad (6)$$

If we now define a new set of operators

$$Q_k = \sum_i v_{ik} q_i = \frac{1}{\sqrt{N}} \sum_i e^{ikx_i} q_i \tag{7}$$

$$P_k = \sum_i v_{ik}^* p_i = \frac{1}{\sqrt{N}} \sum_i e^{-ikx_i} p_i \tag{8}$$

then Eq (1) becomes, with $\Omega_k = \sqrt{\lambda_k}$,

$$H = \frac{1}{2} \sum_k \left( P_k^\dagger P_k + \Omega_k^2 \, Q_k^\dagger Q_k \right) \tag{9}$$

The operators $Q_k$ and $P_k$ still satisfy the canonical algebra

$$[Q_k, P_k] = i \, \delta_{kk'} \tag{10}$$

But they are not Hermitian and $Q_k^\dagger = Q_{-k}$, $P_k^\dagger = P_{-k}$.

To put (9) in the standard form we then define creation and annihilation operators

$$a_k = \sqrt{\frac{\Omega_k}{2}} \left( Q_k + \frac{i P_k^\dagger}{\Omega_k} \right) \qquad\qquad Q_k = \frac{1}{\sqrt{2\Omega_k}} \left( a_k + a_{-k}^\dagger \right)$$

$$\text{or} \tag{11}$$

$$a_k^\dagger = \sqrt{\frac{\Omega_k}{2}} \left( Q_k^\dagger - \frac{i P_k}{\Omega_k} \right) \qquad\qquad P_k = i \sqrt{\frac{\Omega_k}{2}} \left( a_k^\dagger - a_{-k} \right)$$

Then

$$[a_k, a_{k'}^\dagger] = \delta_{kk'}$$

$$[a_k, a_{k'}] = 0 \tag{12}$$

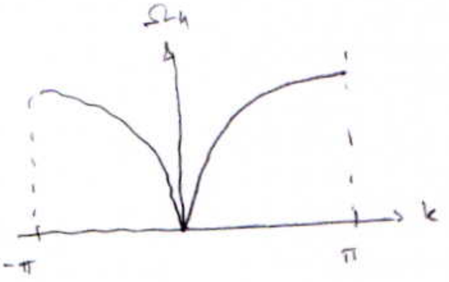
and the Hamiltonian becomes

$$\boxed{H = \sum_k \Omega_k \left( a_k^\dagger a_k + 1/2 \right)} \tag{13}$$

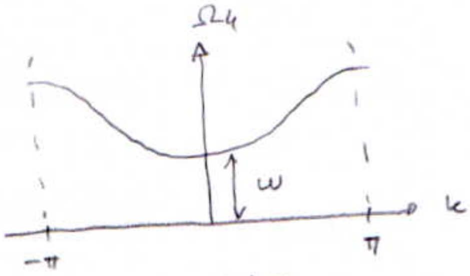
with

$$\Omega_k = \sqrt{\omega^2 + 2g(1-\cos k)} \tag{14}$$

From all this we emerged with the following interpretation: the operator $a_k^\dagger$ creates a quasi-particle, which we call a phonon, that has momentum $k$ and energy $\Omega_k$. The relation between $\Omega_k$ and $k$ is called the <u>dispersion</u> <u>relation</u>. It looks like this




$\omega = 0$




$\omega \neq 0$

For small $k$ we may expand (14) in a Taylor series to get

$$\Omega_k \simeq \sqrt{\omega^2 + g k^2} \tag{15}$$

which is just like the relativistic dispersion relation

$$E = \sqrt{m^2c^4 + p^2c^2} \tag{16}$$

(recall that $E = \hbar\Omega$ and $p = \hbar k$). Thus, the pinning frequency $\omega$ plays the role of a <u>"mass"</u> <u>term</u>, whereas the spring constant $g$ represents the <u>speed</u> of <u>sound</u>.

Phonons are not particles. They are excitations of the vibrational modes of a chain. However, for all stands and purposes, they do behave like particles, with definite momentum and energy

Finally, we discussed how the Hamiltonian (13) is already diagonal in the Fock basis

$$|n\rangle = |n_{k_1}\rangle \otimes |n_{k_2}\rangle \otimes \cdots \qquad (17)$$

where $k_1, k_2, \ldots,$ are all the allowed values of $k$. We have

$$H\,|n\rangle = E(n)\,|n\rangle \qquad (18)$$

where

$$E(n) = \sum_k \Omega_k (n_k + 1/2) \quad , \quad n_k = 0, 1, 2, \ldots \qquad (19)$$

With have therefore $N$ quantum numbers $n_k$, each of which can be in any value $0, 1, 2, \ldots$. Each $n_k$ represents the <u>number</u> of phonons in mode $k$.

## Phonon - phonon interactions

The Hamiltonian (13) of a harmonic chain represents non-interacting phonons. The reason is that the Fock states are eigen-states of H, so if we create one phonon in the chain, it simply stays there

Phonon interactions appear if we consider anharmonic terms. For instance

$$H = \frac{1}{2} \sum_i \left(p_i^2 + \omega^2 q_i^2\right) + \frac{g}{2} \sum_i (q_i - q_{i+1})^2 + \tag{20}$$

$$+ \frac{\chi}{3} \sum_i (q_i - q_{i+1})^3 + \frac{\lambda}{4} \sum_i (q_i - q_{i+1})^4$$

we will not study these anharmonic terms in detail at this point, but there are some messages that I wanted to convey. First, note that the quadratic part (the first line) is already diagonal (it is given by (13)). As for the other terms, we use (7) and (11) to write

$$q_i = \frac{1}{\sqrt{N}} \sum_k e^{-ikx_i} Q_k = \frac{1}{N} \sum_k \frac{e^{-ikx_i}}{\sqrt{2\Omega_k}} \left(a_k + a_{-k}^+\right) \tag{21}$$

In the last term we can change $k \to -k$ in the sum, to obtain the more symmetric form

$$\boxed{q_i = \frac{1}{N} \sum_k \frac{1}{\sqrt{2\Omega_k}} \left(a_k e^{-ikx_i} + a_k^+ e^{ikx_i}\right)} \tag{22}$$

Both (21) and (22) can be useful.

Let's now work out the cubic term

$$(q_i - q_{i+1}) = \frac{1}{N} \sum_k e^{-ikx_i}(1-e^{-ik})(a_k + a_{-k}^{\dagger})$$

$$(q_i - q_{i+1})^3 = \frac{1}{N} \sum_{kk'k''} e^{-i(k+k'+k'')x_i} (1-e^{-ik})(1-e^{-ik'})(1-e^{-ik''})$$
$$(a_k + a_{-k}^{\dagger})(a_{k'} + a_{-k'}^{\dagger})(a_{k''} + a_{-k''}^{\dagger}) \quad (23)$$

we now carry out the sum over $i$ and use (6). then

$$\frac{1}{N} \sum_i e^{-i(k+k'+k'')x_i} = \delta(k+k'+k''=0) \quad (24)$$

where $\delta(a=b)$ is just the Kronecker $\delta$ written a bit differently

Eq (23) thus becomes

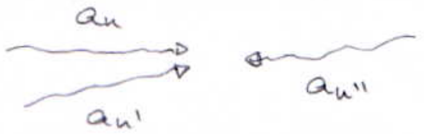
$$\sum_{i=1}^{N} (q_i - q_{i+1})^3 = \sum_{k,k'k''} \delta(k+k'+k''=0)(1-e^{-ik})(1-e^{-ik'})(1-e^{-ik''})$$
$$(a_k + a_{-k}^{\dagger})(a_{k'} + a_{-k'}^{\dagger})(a_{k''} + a_{-k''}^{\dagger}) \quad (25)$$

this is still very complicated, but we can now start to have an idea of what kinds of <u>processes</u> are generated by a cubic term. what is really important is that these processes <u>conserve momentum</u>

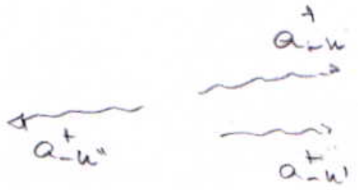
$$k + k' + k'' = 0 \quad (26)$$

this is a consequence of the translation invariance of our model

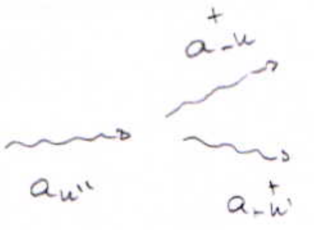
For instance, there will be a term in (25) which is of the form $a_k a_{k'} a_{k''}$. This is a triple annihilation




Two phonons collide with a third one and they are all annihilated, with momentum being conserved. Since H is Hermitian, we must also have triple creation processes $a^\dagger_{-k} a^\dagger_{-k'} a^\dagger_{-k''}$




And, of course, we have mixed processes, like $a^\dagger_{-k} a^\dagger_{-k'} a_{k''}$. This represents something like




Phonon $a_{k''}$ is annihilated and two other phonons are created, with momenta $k + k' = k''$.

Recall that H is the guy that drives Schrödinger's equation. Thus, if we start in an arbitrary state, as time goes on, we will start to see all these scattering events, leading to a extremely complicated dynamics.

So here are the messages I want you to take home

1) Any Hamiltonian which is quadratic in $a$ and $a^\dagger$, is easy to deal with: you only need to diagonalize a matrix.

$\boxed{\text{Quadratic = free particles}}$

2) Any term which is cubic or higher is usually really really complicated. Normally handled with perturbation theory.

$\boxed{\text{cubic, quartic = interactions / scattering processes}}$

3) Momentum is always conserved when your lattice is translationally invariant (homogeneous and periodic boundary conditions).

## Thermal properties

Let's go back to the start: I give you a 1D chain with Hamiltonian

$$H = \frac{1}{2} \sum_{i=1}^{N} (p_i^2 + \omega^2 q_i^2) + \frac{g}{2} \sum_{i=1}^{N} (q_i - q_{i+1})^2 \qquad (27)$$

and ask you to compute the thermal properties of this model. At first this seems like a very hard task: each oscillator lives in an infinite dimensional Hilbert space and there are N of them. How in the world will we be able to compute $e^{-\beta H}$?

Well, we first diagonalize this Hamiltonian, by writing it as

$$H = \sum_k \Omega_k (a_k^\dagger a_k + 1/2) \qquad (28)$$

this procedure may require some effort. But now that it's in diagonal form, we simply have N independent harmonic oscillators, so computing thermal properties is trivial. For instance

$$Z = \mathrm{tr}\, e^{-\beta H} = \mathrm{tr}\, e^{-\beta \sum_k \Omega_k (a_k^\dagger a_k + 1/2)} \qquad (29)$$

But the $a_k^\dagger a_k$ commute with each other so

$$Z = \mathrm{tr}\left[ \prod_k e^{-\beta \Omega_k (a_k^\dagger a_k + 1/2)} \right]$$

$$= \prod_k \mathrm{tr}_k \left( e^{-\beta \Omega_k (a_k^\dagger a_k + 1/2)} \right) \qquad (30)$$

We now have N independent traces, each identical to what we already found before in (26).

Thus

$$Z = \prod_k \frac{e^{-\beta\Omega_k/2}}{(1-e^{-\beta\Omega_k})} = \prod_k Z_k \tag{31}$$

Similarly, the Gibbs state becomes simply

$$\boxed{\rho = \prod_k \rho_k = \prod_k (1-e^{-\beta\Omega_k})\, e^{-\beta\Omega_k a_k^\dagger a_k}} \tag{32}$$

For instance, we know that for one harmonic oscillator

$$\Omega(\langle a^\dagger a\rangle + 1/2) = \Omega(\bar{n}+1/2) = \frac{\Omega}{2}\coth\left(\frac{\Omega}{2T}\right) \tag{33}$$

where

$$\bar{n} = \frac{1}{e^{\beta\Omega}-1}$$

Thus, since (87) is just a sum of independent oscillators, we get

$$\boxed{U = \langle H\rangle = \sum_k \Omega_k(\bar{n}_k + 1/2) = \sum_k \frac{\Omega_k}{2}\coth\left(\frac{\Omega_k}{2T}\right)} \tag{34}$$

A similar reasoning holds for all other thermodynamic quantities. For instance

$$\langle a_k^\dagger a_k\rangle = \bar{n}_k = \frac{1}{e^{\beta\Omega_k}-1} \tag{35}$$