

Phonons and field theory

In these notes we will talk about systems of coupled harmonic oscillators. These systems have collective excitations, called phonons, which behave a lot like actual particles. We call them quasi-particles. We will also learn how, in certain limits, the system of harmonic oscillators behave like a continuum. This will lead us to the concept of field theory.

We start with a single quantum harmonic oscillator

$$H = \frac{p^2}{2m} + \frac{1}{2} m \omega^2 q^2 \quad (1)$$

Here q and p are operators satisfying the canonical commutation relations

$$[q, p] = i\hbar \quad (2)$$

(I reintroduce \hbar for completeness. But I'll get rid of it again soon).

We now introduce the so-called creation and annihilation operators

$$\begin{aligned} q &= \sqrt{\frac{\hbar}{m\omega}} \frac{(a^\dagger + a)}{\sqrt{2}} & a &= \frac{1}{\sqrt{2}} \left(\sqrt{\frac{m\omega}{\hbar}} q + i \frac{p}{\sqrt{m\hbar\omega}} \right) \\ p &= i\sqrt{\hbar m\omega} \frac{(a^\dagger - a)}{\sqrt{2}} & a^\dagger &= \frac{1}{\sqrt{2}} \left(\sqrt{\frac{m\omega}{\hbar}} q - i \frac{p}{\sqrt{m\hbar\omega}} \right) \end{aligned} \quad (3)$$

Note that q and p are Hermitian, but a is not.

The constants are chosen so that a is dimensionless. Moreover, they are such that (2) implies

$$[a, a^\dagger] = 1$$

(4)

We now have

$$q^2 = \frac{\hbar}{2m\omega} (a^\dagger a + a a^\dagger + a a + a^\dagger a^\dagger)$$

(5)

$$p^2 = \frac{m\hbar\omega}{2} (a^\dagger a + a a^\dagger - a a - a^\dagger a^\dagger)$$

so

$$\frac{p^2}{2m} = \frac{\hbar\omega}{4} (a^\dagger a + a a^\dagger - a a - a^\dagger a^\dagger)$$

(6)

$$\frac{1}{2} m \omega^2 q^2 = \frac{\hbar\omega}{4} (a^\dagger a + a a^\dagger - a a - a^\dagger a^\dagger)$$

and then (1) becomes

$$H = \frac{\hbar\omega}{2} (a^\dagger a + a a^\dagger)$$

(7)

Finally, using (4) we can write

$$a a^\dagger = 1 + a^\dagger a$$

(8)

Hence

$$H = \hbar\omega (a^\dagger a + \frac{1}{2})$$

(9)

An algebraic problem

The whole treatment of the QHO has therefore been reduced to a mathematical problem.

"Given an operator a satisfying $[a, a^\dagger] = 1$, what are the eigenvalues and eigenvectors of $a^\dagger a$?"

Note that $a^\dagger a$ is Hermitian and so its eigenvalues will be real and the eigenvectors should form an orthonormal basis. It is quite cool that all we need is the algebra of the operators $[E_7(4)]$. Everything follows from the algebra.

Let us write

$$a^\dagger a |\lambda\rangle = \lambda |\lambda\rangle \quad (10)$$

we want to know λ and $|\lambda\rangle$. The first piece of information is that λ must be non-negative; multiplying (10) by $\langle\lambda|$ we get

$$\langle\lambda| a^\dagger a |\lambda\rangle = \lambda \langle\lambda|\lambda\rangle = \lambda$$

But if we let $|\psi\rangle = a |\lambda\rangle$ then $\langle\lambda| a^\dagger = \langle\psi|$ so

$$\langle\lambda| a^\dagger a |\lambda\rangle = \langle\psi|\psi\rangle \geq 0$$

Hence

$$\lambda \geq 0 \quad (11)$$

Any operator which can be decomposed as $A^\dagger A$ is by construction a positive semi-definite operator

Next consider the state $|\phi\rangle = a|\lambda\rangle$. Applying $a^\dagger a$ we get

$$a^\dagger a |\phi\rangle = a^\dagger a a |\lambda\rangle$$

we now use the algebra (4) to move things around. Recall that

$$[AB, C] = A[B, C] + [A, C]B$$

thus

$$[a^\dagger a, a] = a^\dagger \underbrace{[a, a]}_0 + \underbrace{[a^\dagger, a]}_{-1} a = -a$$

$$\therefore [a^\dagger a, a] = -a \quad (12)$$

or, more explicitly

$$a^\dagger a a = a a^\dagger a - a = a(a^\dagger a - 1)$$

then

$$a^\dagger a |\phi\rangle = a^\dagger a a |\lambda\rangle = a(a^\dagger a - 1) |\lambda\rangle$$

but $a^\dagger a |\lambda\rangle = \lambda |\lambda\rangle$ so

$$a^\dagger a |\phi\rangle = a(\lambda - 1) |\lambda\rangle = (\lambda - 1) |\phi\rangle \quad (13)$$

Thus, we reach the important conclusion that if $|\lambda\rangle$ is an eigenvector, then so is $a|\lambda\rangle$, but with eigenvalue $\lambda - 1$. That is why a acts as a lowering operator for the spectrum of $a^\dagger a$: it lowers the eigenvalue by one unit

We would therefore be inclined to label $|\phi\rangle$ as $|\lambda-1\rangle$. But $|\phi\rangle = a|\lambda\rangle$ is not normalized, so we better write

$$|\phi\rangle = c_\lambda |\lambda-1\rangle$$

for some c_λ . To figure out this constant we take the absolute value on both sides

$$\langle \lambda-1 | \lambda-1 \rangle |c_\lambda|^2 = \langle \phi | \phi \rangle = \langle \lambda | a^\dagger a | \lambda \rangle = \lambda$$

Thus $|c_\lambda|^2 = \lambda$. The phase of c_λ is arbitrary so we choose c_λ to be real. Then we finally get

$$a|\lambda\rangle = \sqrt{\lambda} |\lambda-1\rangle \quad (14)$$

So here is what we know so far: we know the eigenvalues must be non-negative and we know that if λ is an eigenvalue, then $(\lambda-1)$ will also be one, with eigenvector $a|\lambda\rangle$.

Now let's apply a again:

$$a^2|\lambda\rangle = \sqrt{\lambda} a|\lambda-1\rangle = \sqrt{\lambda(\lambda-1)} |\lambda-2\rangle$$

or, if we apply a k times, we get

$$a^k |\lambda\rangle = \sqrt{\lambda(\lambda-1)\dots(\lambda-k+1)} |\lambda-k\rangle \quad (15)$$

But we cannot keep doing this forever because the eigenvalues cannot be negative. This means that for any given λ there should be some integer m such that

$$a^m |\lambda\rangle \neq 0$$

but $a^{m+1} |\lambda\rangle = 0$

However

$$a^m |\lambda\rangle = \sqrt{\lambda(\lambda-1)\dots(\lambda-m+1)} |\lambda-m\rangle$$

$$a^{m+1} |\lambda\rangle = \sqrt{\lambda(\lambda-1)\dots(\lambda-m)} |\lambda-m-1\rangle$$

Thus we see that the only way for this to happen is to have λ itself be an integer m . If the λ 's were not integers then the hierarchy (15) would never stop and we would get negative eigenvalues.

Thus we conclude that

$$\begin{aligned} a^\dagger a |n\rangle &= n |n\rangle \\ n &= 0, 1, 2, 3, \dots \end{aligned}$$

(16)

the eigenvalues of $a^\dagger a$ are simply the natural numbers. We also know that (14) takes n to $n-1$:

$$a |n\rangle = \sqrt{n} |n-1\rangle$$

(17)

Now let's do the same for a^\dagger . First

$$[a^\dagger a, a^\dagger] = \underbrace{a^\dagger [a, a^\dagger]}_1 + \underbrace{[a^\dagger, a^\dagger] a}_0 = a^\dagger$$

so

$$a^\dagger a a^\dagger = a^\dagger a a^\dagger + a^\dagger = a^\dagger (a^\dagger a + 1)$$

Then

$$a^\dagger a (a^\dagger |m\rangle) = a^\dagger (a^\dagger a + 1) |m\rangle = a^\dagger (m+1) |m\rangle$$

thus

$$a^\dagger |m\rangle = d_m |m+1\rangle$$

for some constant d_m . That is, a^\dagger raises the eigenvector by one unit. The value of d_m is computed as before

$$\langle m+1 | m+1 \rangle |d_m|^2 = \langle m | a a^\dagger |m\rangle = \langle m | (a^\dagger a + 1) |m\rangle = m+1$$

thus

$$a^\dagger |m\rangle = \sqrt{m+1} |m+1\rangle \quad (18)$$

Of all states (16), the one with $n=0$ is special. It is called the vacuum state, and is characterized by the fact that

$$a |0\rangle = 0$$

We say "a annihilates the vacuum", which sounds really cool, like a sci-fi movie.

From the vacuum we can construct all other states by applying at multiple times. For instance

$$a^\dagger |0\rangle = \sqrt{0+1} |1\rangle = |1\rangle$$

$$(a^\dagger)^2 |0\rangle = a^\dagger |1\rangle = \sqrt{2} |2\rangle$$

and so on. Thus

$$|m\rangle = \frac{(a^\dagger)^m}{\sqrt{m!}} |0\rangle \quad (19)$$

And this concludes our algebraic problem.

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Summary

$$[a, a^\dagger] = 1 \quad [a^\dagger a, a] = -a \quad (20)$$

$$[a^\dagger a, a^\dagger] = a^\dagger$$

$$a^\dagger a |m\rangle = m |m\rangle$$

$$m = 0, 1, 2, \dots$$

(21)

$$a |m\rangle = \sqrt{m} |m-1\rangle$$

$$a^\dagger |m\rangle = \sqrt{m+1} |m+1\rangle$$

(22)

$$a |0\rangle = 0$$

$$|m\rangle = \frac{(a^\dagger)^m}{\sqrt{m!}} |0\rangle$$

(23)

Thermal properties of the QHO

Now that we know all about creation and annihilation operators, let us go back to the QHO and the Hamiltonian (9). Its eigenvectors are $|m\rangle$ and the eigenvalues are

$$E_m = \omega(m + 1/2) \quad (\hbar = 1 \text{ now}) \quad (24)$$

The thermal state is

$$\rho = \frac{e^{-\beta H}}{Z} \quad (25)$$

where

$$\begin{aligned} Z &= \text{tr } e^{-\beta H} = \text{tr } e^{-\beta \omega (a^\dagger a + 1/2)} \\ &= \sum_m \langle m | e^{-\beta \omega (a^\dagger a + 1/2)} | m \rangle \\ &= \sum_m e^{-\beta \omega (m + 1/2)} \\ &= \frac{e^{-\beta \omega / 2}}{1 - e^{-\beta \omega}} \quad \leftarrow \text{we did this before} \end{aligned}$$

Thus

$$\rho = (1 - e^{-\beta \omega}) e^{\beta \omega a^\dagger a} \quad (26)$$

If we want to write it in terms of probabilities, we simply get

$$\begin{aligned} \rho &= \sum_m P_m |m\rangle \langle m| \\ P_m &= (1 - e^{-\beta \omega}) e^{-\beta \omega m} \end{aligned} \quad (27)$$

Now we can compute any expectation value we want at equilibrium

$$\langle A \rangle = \text{tr}(A\rho) = (1 - e^{-\beta\omega}) \text{tr}(A e^{-\beta\omega a^\dagger a})$$

For instance we could compute something like

$$\langle a^\dagger a a a \rangle = (1 - e^{-\beta\omega}) \text{tr}\{a^\dagger a a a e^{-\beta\omega a^\dagger a}\}$$

At first this seems tough. But using only $[a, a^\dagger] = 1$ one may show that

$$a^\dagger a a a = a^\dagger a (a^\dagger a - 1) \tag{28}$$

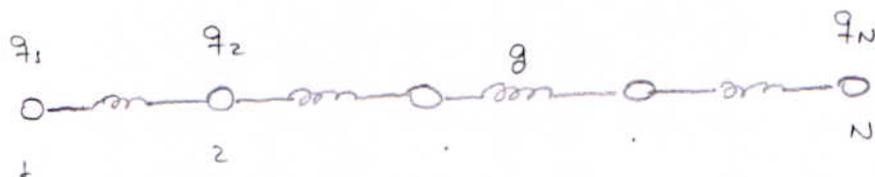
thus

$$\begin{aligned} \langle a^\dagger a a a \rangle &= (1 - e^{-\beta\omega}) \sum_{n=0}^{\infty} \langle n | a^\dagger a (a^\dagger a - 1) e^{-\beta\omega a^\dagger a} | n \rangle \\ &= (1 - e^{-\beta\omega}) \sum_{n=0}^{\infty} n(n-1) e^{-\beta\omega n} \\ &= 2 \bar{n}^2 \qquad \bar{n} = \frac{1}{e^{\beta\omega} - 1} \end{aligned}$$

where, in the last line I simply plugged the sum in Mathematica

One-dimensional harmonic chain

Let us now consider a chain of N harmonic oscillators



We assume each oscillator interacts with its two neighbors and this interaction is harmonic. Thus, we shall take as our Hamiltonian

$$H = \frac{1}{2} \sum_{i=1}^N (p_i^2 + \omega^2 q_i^2) + \frac{g}{2} \sum_{i=1}^N (q_i - q_{i+1})^2 \quad (29)$$

Here I made some tiny assumptions. First I assumed all oscillators have the same mass $m=1$ (I hate masses). Second, I assumed periodic boundary conditions. And third, I added a pinning term $\omega^2 q_i^2$, which ensures that our big molecule doesn't fly off.

Also, in (29) q_i and p_i are operators satisfying

$$[q_i, p_j] = i \delta_{ij} \quad (\hbar=1) \quad (30)$$

that is, the canonical algebra for $i=j$ and nothing for $i \neq j$.

To begin let us look at the potential energy only

$$V = \frac{1}{2} \sum_{i=1}^N \omega^2 q_i^2 + \frac{g}{2} \sum_{i=1}^N (q_i - q_{i+1})^2 \quad (31)$$

This is a quadratic form in the operators q_i :

$$V = \frac{1}{2} \sum_{i,j} A_{ij} q_i q_j \quad (32)$$

where A is an $N \times N$ matrix given by (e.g. for $N=5$)

$$A = \begin{pmatrix} \omega^2 + 2g & -g & 0 & 0 & -g \\ -g & \omega^2 + 2g & -g & 0 & 0 \\ 0 & -g & \omega^2 + 2g & -g & 0 \\ 0 & 0 & -g & \omega^2 + 2g & -g \\ -g & 0 & 0 & -g & \omega^2 + 2g \end{pmatrix} \quad (33)$$

Let me explain: $(q_i - q_{i+1})^2 = q_i^2 + q_{i+1}^2 - 2q_i q_{i+1}$, so when we sum over i , each q_i end up appearing twice. That's why we have $2g$ in the diagonal. The $-g$ in the off-diagonal bands are from $-2q_i q_{i+1}$, which I split in half to make A symmetric. We also have the lonely $-g$'s in the upper-right corner and lower-left corner. They come from the periodic boundary conditions.

The matrix A is symmetric ($A^T = A$) and thus may be diagonalized by an orthogonal transformation

$$A = U \Lambda U^T \quad U U^T = U^T U = I \quad (34)$$

$$\Lambda = \text{diag}(\lambda_1, \lambda_2, \dots)$$

written in terms of indices we have

$$A_{ij} = \sum_k U_{ik} \lambda_k U_{jk} \quad (35)$$

We now insert this in (32), to find

$$V = \frac{1}{2} \sum_{i,j} \sum_k U_{ik} \lambda_k U_{jk} q_i q_j$$

$$= \frac{1}{2} \sum_k \lambda_k \left[\sum_i U_{ik} q_i \right] \left[\sum_j U_{jk} q_j \right] \quad (36)$$

We now define a new set of coordinates

$$Q_k = \sum_i U_{ik} q_i \quad (37)$$

The potential energy then becomes

$$V = \frac{1}{2} \sum_k \lambda_k Q_k^2 \quad (38)$$

what we just did is called a normal mode decomposition.
 The Q_k are the normal modes. They represent a new choice of coordinates where the potential energy is "diagonal", in the sense that it represents a set of independent harmonic oscillators.

We now do the same transformation for the momenta:

$$P_k = \sum_j U_{jk} P_j \quad (39)$$

It then follows that

$$\begin{aligned} [Q_k, P_{k'}] &= \sum_{ij} U_{ik} U_{j k'} [Q_i, P_j] \\ &= i \sum_i U_{ik} U_{i k'} \quad \leftarrow (U^T U)_{kk'} = \delta_{kk'} \\ &= i \delta_{kk'} \end{aligned}$$

Thus

$$[Q_k, P_{k'}] = i \delta_{kk'} \quad (40)$$

Hence, we see that the new set of normal mode coordinates (Q_k, P_k) also satisfies the canonical algebra. This is always true for a transformation of the form (37), (39), for any orthogonal matrix U .

One may also check that

$$\begin{aligned} \sum_k P_k^2 &= \sum_{i,j,k} U_{ik} U_{jk} P_i P_j \\ &= \sum_{ij} \left[\underbrace{\sum_k U_{ik} U_{jk}}_{\delta_{ij}} \right] P_i P_j \end{aligned}$$

$$\therefore \sum_k P_k^2 = \sum_i P_i^2 \quad (41)$$

Thus the Hamiltonian is now transformed as

$$\begin{aligned} H &= \frac{1}{2} \sum_i P_i^2 + \frac{1}{2} \sum_{ij} A_{ij} Q_i Q_j \\ &= \frac{1}{2} \sum_k (P_k^2 + \lambda_k Q_k^2) \end{aligned} \quad (42)$$

This is the general procedure of the normal mode decomposition. We start with a system of n interacting oscillators and we move to a new representation where we have n independent oscillators with frequencies

$$\Omega_k = \sqrt{\lambda_k} \quad (43)$$

Incidentally, note how this implies that the eigenvalues λ_k of the matrix A should be non-negative. That is, A should be positive semi-definite. This is a condition on mechanical stability.

Ok. So far we discussed a general procedure for an arbitrary A , this is cool because it can be used to study arbitrary harmonic networks.

Now let's specialize to the A in Eq (33). In this case it turns out that it's more convenient to use a unitary transformation ($UU^T = I$) instead of an orthogonal one. I want to discuss in some detail how to do this, as I think is a rather important mathematical procedure.

We want to find the eigenvalues and eigenvectors of A . So something like

$$A \vec{v}_k = \lambda_k \vec{v}_k \quad (44)$$

then from all \vec{v}_j we construct U by stacking them in columns

$$U = \left(\begin{array}{c|c|c} | & | & \\ \vec{v}_1 & \vec{v}_2 & \dots & \vec{v}_N \\ | & | & & | \end{array} \right) \quad (45)$$

So let us write one such eigenvector as

$$\vec{v}_j = \begin{pmatrix} b_{j1} \\ b_{j2} \\ \vdots \\ b_{jN} \end{pmatrix}$$

For now I will drop the index j

we now multiply A and \vec{v} . For instance in the $N=5$ problem of (33) we get

$$A \begin{pmatrix} b_1 \\ b_2 \\ b_3 \\ b_4 \\ b_5 \end{pmatrix} = \begin{pmatrix} (\omega^2 + 2g) b_1 - g b_2 - g b_5 \\ (\omega^2 + 2g) b_2 - g b_1 - g b_3 \\ (\omega^2 + 2g) b_3 - g b_2 - g b_4 \\ (\omega^2 + 2g) b_4 - g b_3 - g b_5 \\ (\omega^2 + 2g) b_5 - g b_4 - g b_1 \end{pmatrix} = \lambda \begin{pmatrix} b_1 \\ b_2 \\ b_3 \\ b_4 \\ b_5 \end{pmatrix} \quad (46)$$

We can see the pattern:

$$(\omega^2 + 2g) b_i - g b_{i-1} - g b_{i+1} = \lambda b_i \quad (47)$$

I like this because it shows how a eigenvalue/eigenvector equation can also be interpreted as a recurrence relation what we need to do now is find the λ 's and the b_j 's which satisfy this recurrence relation. Moreover, this relation is also subject to the boundary conditions specified in the first and last lines of (46): namely $b_0 = b_N$ and $b_{N+1} = b_1$. With this, Eq (47) will be true for all j .

we now try the ansatz

$$b_j = c e^{i k x_j} \quad (48)$$

where k is a number to be determined and $x_j = j$ (is just so we don't confuse with the i in front). The k 's therefore are introduced to play the role of the quantum number labeling the eigenvectors and eigenvalues, as in (44)

Substituting (48) in (47) we get

$$c \left[(\omega^2 + 2g) e^{ikx_j} - g e^{ikx_j} e^{-ik} - g e^{ikx_j} e^{ik} \right] = \lambda A e^{ikx_j}$$

Canceling out $c e^{ikx_j}$ we get

$$\lambda = (\omega^2 + 2g) - g(e^{-ik} + e^{ik})$$

or

$$\lambda_k = \omega^2 + 2g(1 - \cos k) \quad (49)$$

Thus we conclude that (48) is indeed a valid solution, provided the eigenvalues λ follow (49).

Next we impose the boundary conditions

$$b_{N+1} = c e^{ikx_{N+1}} = c e^{ikN} e^{ik} =$$

But this should be equal to

$$b_1 = c e^{ik}$$

Thus we conclude that

$$e^{ikN} = 1 \quad (50)$$

This means

$$k = \frac{2\pi l}{N}, \quad l = 0, \pm 1, \pm 2, \dots \quad (51)$$

The boundary conditions therefore establish the quantum numbers labeling the eigenvalues and eigenvectors. That is, the eigenvector $\vec{\psi}_k$ in (44) is now written as

$$\vec{\psi}_k = c \begin{pmatrix} e^{ikx_1} \\ e^{ikx_2} \\ \vdots \\ e^{ikx_N} \end{pmatrix} \quad (52)$$

and each of the allowed values of k represent a different eigenvector.

But our matrix is $N \times N$, so we only need N distinct eigenvectors. It turns out that if we change k by 2π , nothing happens

$$e^{i(k+2\pi)x_j} = e^{ikx_j} \underbrace{e^{i2\pi x_j}}_1$$

Thus in (51) we only need to choose k in an interval of length 2π . The standard choice is

$$k \in [-\pi, \pi] \quad (53)$$

which in solid state physics is called the first Brillouin zone. Thus, we usually choose

$$-\frac{N}{2} < l \leq \frac{N}{2} \quad (54)$$

The last piece of info we need is the normalization constant c of the eigenvectors. We have

$$\vec{v}_k^\dagger \vec{v}_{k'} = |c|^2 \sum_j e^{i(k-k')x_j} \quad (55)$$

Using the result for a truncated geometric series

$$\sum_{j=1}^N y^j = \frac{y(1-y^N)}{1-y}$$

we get

$$\vec{v}_k^\dagger \vec{v}_{k'} = |c|^2 e^{i(k-k')x_j} \frac{(1 - e^{iN(k-k')x_j})}{1 - e^{i(k-k')x_j}}$$

But $k = 2\pi l/N$ so

$$e^{iN(k-k')x_j} = e^{i2\pi(l-l')} = 1$$

Hence $\vec{v}_k^\dagger \vec{v}_{k'} = 0$. The only exception is when $k = k'$, where (55) gives instead

$$\|\vec{v}_k\|^2 = |c|^2 N$$

Thus we choose $c = 1/\sqrt{N}$ to make these guys normalized.

It is convenient to write down these results in a big box

$$\frac{1}{N} \sum_j e^{i(k-k')x_j} = \delta_{kk'} \quad (56)$$

The same is also true for a sum over k , for the same reason

$$\frac{1}{N} \sum_k e^{ik(x_i - x_j)} = \delta_{ij} \quad (57)$$

Let's summarize what we have accomplished. We started with a tridiagonal cyclic matrix

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

and we showed that it can be diagonalized by a Fourier transform

$$A \vec{u} = \lambda_u \vec{u} \quad (58)$$

where

$$\vec{u} = \frac{1}{\sqrt{N}} \begin{pmatrix} e^{ikx_1} \\ e^{ikx_2} \\ \vdots \\ e^{ikx_N} \end{pmatrix} \quad (59)$$

and

$$\lambda_u = \omega^2 2g (1 - \cos k) \quad (60)$$

$$k = \frac{2\pi l}{N}, \quad l = 0, \pm 1, \pm 2, \dots, \pm \frac{N}{2} \quad (61)$$

or, in terms of a matrix transformation

$$A = U \Lambda U^\dagger \quad (62)$$

where

$$\Lambda_{kk} = \lambda_k \quad (63)$$

$$U_{ik} = \frac{1}{\sqrt{N}} e^{ikx_i} \quad (64)$$

I know what we just did sounded like a lot of effort. But it was worth it in my opinion. What we just did will appear several other times in this course, and I wanted you to see in detail where it comes from.

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We are now ready to go back to the physical problem of our 1D harmonic chain, Eq (29). The matrix A we just diagonalize is the matrix appearing in the potential energy (32). So inserting $A = U\Lambda U^\dagger$ we get

$$\begin{aligned} V &= \frac{1}{2} \sum_{ij} A_{ij} q_i q_j \\ &= \frac{1}{2} \sum_{ij} \sum_{\mu} U_{i\mu} \lambda_{\mu} U_{j\mu}^* q_i q_j \\ &= \frac{1}{2} \sum_{\mu} \lambda_{\mu} \left[\sum_i U_{i\mu} q_i \right] \left[\sum_j U_{j\mu}^* q_j \right] \end{aligned} \quad (65)$$

We now define

$$Q_{\mu} = \sum_i U_{i\mu} q_i = \frac{1}{\sqrt{N}} \sum_i e^{ik\mu i} q_i \quad (66)$$

Notice, however, that unlike (37), since we now chose a matrix U which is complex, Q_{μ} is no longer Hermitian. Instead

$$Q_{\mu}^{\dagger} = Q_{-\mu} \quad (67)$$

Hence, Eq (65) becomes

$$V = \frac{1}{2} \sum_{\mu} \lambda_{\mu} Q_{\mu} Q_{-\mu} \quad (68)$$

We also transform the momenta in a similar way. But now it is convenient to write

$$\boxed{P_u = \sum_i U_{iu}^* P_i = \frac{1}{\sqrt{N}} \sum_i e^{-i k u x_i} P_i} \quad (69)$$

We then get

$$\begin{aligned} [Q_u, P_{u'}] &= \frac{1}{N} \sum_{ij} e^{i(kx_i - k'x_j)} \underbrace{[q_i, p_j]}_{i \delta_{ij}} \\ &= i \frac{1}{N} \sum_i e^{i(k-k')x_i} \\ &\quad \underbrace{\hspace{10em}}_{\delta_{uu'} \text{ by Eq (56)}} \end{aligned}$$

thus

$$\boxed{[Q_u, P_{u'}] = i \delta_{uu'}} \quad (70)$$

so Q_u and P_u continue to be canonically conjugated variables.

I will leave for you as an exercise to check that

$$\sum_i p_i^2 = \sum_u P_u P_{-u} \quad (71)$$

where, as with Q_u , $P_{-u} = P_u^\dagger$

From all this mess, we finally emerge victorious! The Hamiltonian of the 1D chain, Eq (29), is finally put in diagonal form as

$$H = \frac{1}{2} \sum_k (P_k P_{-k} + \Omega_k^2 Q_k Q_{-k}) \quad (72)$$

where $\Omega_k^2 = \lambda_k$ or, more explicitly

$$\Omega_k = \sqrt{\omega^2 + 2g(1 - \cos k)} \quad (73)$$

Hence, despite the weird appearance of the non Hermitian operators Q_k and P_k , we still get that our 1D harmonic chain can still be decomposed into normal modes k which oscillate independently with frequency Ω_k .

The final touch is to define creation and annihilation operators according to

$$\begin{aligned} a_k &= \sqrt{\frac{\Omega_k}{2}} \left(Q_k + i \frac{P_{-k}}{\Omega_k} \right) & Q_k &= \frac{1}{\sqrt{2\Omega_k}} (a_k + a_{-k}^\dagger) \\ a_k^\dagger &= \sqrt{\frac{\Omega_k}{2}} \left(Q_{-k} - i \frac{P_k}{\Omega_k} \right) & P_k &= i \sqrt{\frac{\Omega_k}{2}} (a_k^\dagger - a_{-k}) \end{aligned} \quad (74)$$

where I exploited the fact that $\Omega_k = \Omega_{-k}$.

One may then check that

$$\begin{aligned} [a_u, a_u^\dagger] &= \frac{\Omega_u}{2} \left[Q_u + \frac{i P_u}{\Omega_u}, Q_u - \frac{i P_u}{\Omega_u} \right] \\ &= \frac{\Omega_u}{2} \left(\frac{-i}{\Omega_u} \right) \underbrace{[Q_u, P_u]}_i + \frac{\Omega_u}{2} \frac{i}{\Omega_u} \underbrace{[P_u, Q_u]}_{-i} \\ &= \frac{1}{2} + \frac{1}{2} = 1 \end{aligned}$$

thus

$$\boxed{[a_u, a_u^\dagger] = \delta_{uu'}} \quad (75)$$

these operators therefore represent an independent set of creation and annihilation operators

we also have

$$\begin{aligned} Q_u Q_{-u} &= \frac{1}{2\Omega_u} (a_u + a_{-u}^\dagger)(a_{-u} + a_u^\dagger) \\ &= \frac{1}{2\Omega_u} (a_u a_{-u} + a_{-u}^\dagger a_u^\dagger + a_u a_u^\dagger + a_{-u}^\dagger a_{-u}) \end{aligned} \quad (76)$$

$$\begin{aligned} P_u P_{-u} &= -\frac{\Omega_u}{2} (a_u^\dagger - a_{-u})(a_{-u}^\dagger - a_u) \\ &= -\frac{\Omega_u}{2} (a_u^\dagger a_{-u}^\dagger + a_{-u} a_u - a_u^\dagger a_u - a_{-u} a_{-u}^\dagger) \end{aligned} \quad (77)$$

Thus the Hamiltonian (72) becomes

$$H = \frac{1}{2} \sum_u \left\{ \Omega_u (a_u a_u^\dagger + a_{-u}^\dagger a_{-u} + a_u^\dagger a_u + a_{-u} a_{-u}^\dagger) \right\}$$

$$= \frac{1}{2} \sum_u \left[\Omega_u (a_u^\dagger a_u + 1/2) + \Omega_u (a_{-u}^\dagger a_{-u} + 1/2) \right]$$

To finish, we note that we are summing over both positive and negative k , so we can change $k \rightarrow -k$ in the last term only. This then makes it identical to the first term. As a result we get

$$H = \sum_u \Omega_u (a_u^\dagger a_u + 1/2) \quad (78)$$

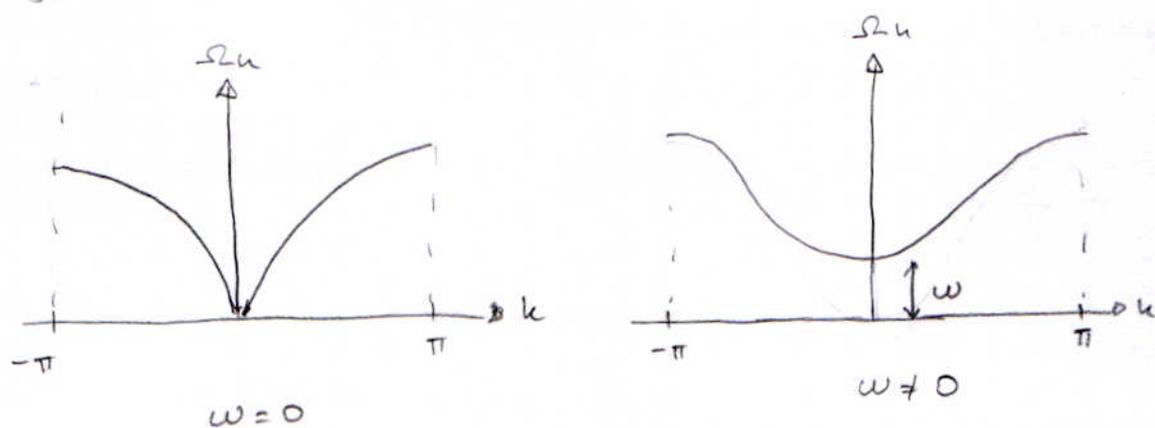
We therefore conclude that the 1D can be represented as an independent set of harmonic oscillators, labeled by k and with frequencies

$$\Omega_u = \sqrt{\omega_D^2 \epsilon g (1 - \cos k)} \quad (79)$$

Now let's talk about the interpretation of these results. The first thing I want to point out is the interpretation of this quantum number k as a kind of momentum. First, anything that appears as e^{ikx_j} is associated with plane waves and the k of a plane wave is a kind of momentum. This happens here as well. The normal modes (a_u, a_u^\dagger) are delocalized, as can be seen in (66): they are plane wave decompositions of the local displacements q_i .

Now let's plot Ωu as a function of k . Recall that $k \in [-\pi, \pi]$.

we then get



This is called a dispersion relation, or energy-momentum relation (if Ω is a frequency, $\hbar\Omega$ is energy, so energy and frequency is the same thing).

Suppose now that we are interested in Ωu in the vicinity of $k=0$. Expanding the cosine in a Taylor series we get

$$1 - \cos k \approx \frac{k^2}{2}$$

Hence (79) becomes

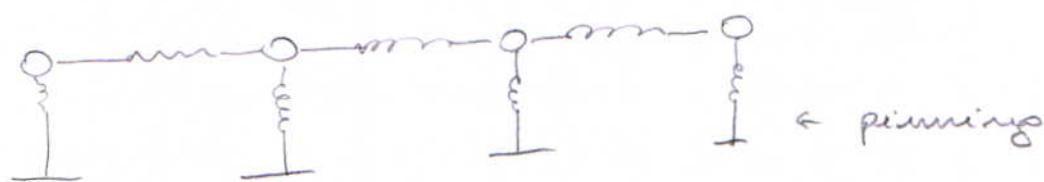
$$\Omega u \approx \sqrt{\omega^2 + gk^2} \quad (80)$$

Holy shit! This is the relativistic dispersion relation!

$$E = \sqrt{m^2 c^4 + p^2 c^2} \quad (81)$$

I think this is really really cool: the pinning frequency ω is the "mass" and g is the "speed" (with k being the momentum p).

But mass of what? Well, that's the point. We can interpret the operator a_k^\dagger in (78) as the operator that creates a "particle" (which we call a quasi-particle) that has momentum k and dispersion relation Ω_k . These quasi-particles are the phonons. They represent quantum excitations of the vibrational modes of the chain. And these excitations move as massive particles, where the mass is related to the pinning ω



and they move with a speed of sound g .

Fock space

Let's now talk about the eigenstates of our Hamiltonian

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

Each set of $a_k^\dagger a_k$ acts like an independent harmonic oscillator so that the natural basis is

$$|\vec{M}\rangle = \bigotimes_{k=1}^N |M_k\rangle \quad (82)$$

which is a short-hand notation for

$$|\vec{M}\rangle = |M_{k_1}\rangle \otimes |M_{k_2}\rangle \otimes |M_{k_3}\rangle \otimes \dots$$

where k_1, k_2, \dots are all the allowed values of k . Thus, for a chain of N sites we have N allowed values of k and, for each value, we can have $0, 1, 2, 3, \dots$ phonons at that k .

Thus, we start with the vacuum $|0\rangle$, which is defined such that

$$a_k |0\rangle = 0 \quad \forall k \quad (83)$$

then we have states with one phonon in a given mode k

$$|1_k\rangle = a_k^\dagger |0\rangle \quad (84)$$

then states with 2 phonons

$$|1_k, 1_{k'}\rangle = a_k^\dagger a_{k'}^\dagger |0\rangle \quad (85)$$

and so on.

This type of Hilbert space where we put the number of quasi-particles in each mode k , is called Fock space (don't confuse the "o" with an "u"!).

All states in Fock space are eigenstates of the Hamiltonian. For instance

$$\begin{aligned} H |1u\rangle &= \sum_{k'} \Omega_{k'} (a_{k'}^\dagger a_{k'} + 1/2) |1u\rangle \\ &= \sum_{k'} \Omega_{k'} a_{k'}^\dagger a_{k'} |1u\rangle + \frac{\Omega_{k'}}{2} |1u\rangle \end{aligned}$$

But $a_{k'}^\dagger a_{k'}$ is a number operator: it counts the number of quanta in mode k' . Thus it will give zero for all k' which are not k , and will give 1 for $k' = k$. Thus

$$H |1u\rangle = \Omega_u |1u\rangle + \left(\sum_{k'} \frac{\Omega_{k'}}{2} \right) |1u\rangle$$

The last term is just the vacuum / ground state energy

$$E_{gs} = \sum_{k'} \frac{\Omega_{k'}}{2}$$

Thus we see that the energy of a state with one phonon in mode k is

$$E(1u) = \Omega_u + E_{gs}$$

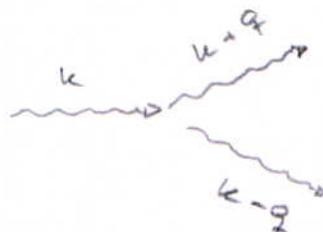
Similarly, the energy of two phonons would be

$$E(1u, 1u') = \Omega_u + \Omega_{u'} + E_{gs}$$

In our Hamiltonian the phonons do not interact, so if we add more and more phonons the energy simply stacks up.

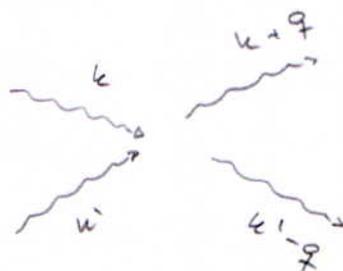
In anharmonic chains the additional anharmonic potential will lead to phonon-phonon interactions. For instance, this could mean terms like

$$a_{u+q}^\dagger a_{u-q}^\dagger a_u$$



or

$$a_{u+q}^\dagger a_{u-q}^\dagger a_u^\dagger a_u$$



Each a_u means annihilating a phonon and each a_u^\dagger means creating one. Thus we see that phonon-phonon interactions may be thought of as scattering events, where phonons are annihilated and then created.

Thermal properties

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

$$H = \frac{1}{2} \sum_{i=1}^N (p_i^2 + \omega^2 q_i^2) + \frac{g}{2} \sum_{i=1}^N (q_i - q_{i+1})^2 \quad (86)$$

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 $\bar{e}^{\beta H}$?

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

$$H = \sum_k \Omega_k (a_k^\dagger a_k + 1/2) \quad (87)$$

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

$$Z = \text{tr} \bar{e}^{-\beta H} = \text{tr} \bar{e}^{-\beta \sum_k \Omega_k (a_k^\dagger a_k + 1/2)}$$

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

$$\begin{aligned} Z &= \text{tr} \left[\prod_k \bar{e}^{-\beta \Omega_k (a_k^\dagger a_k + 1/2)} \right] \\ &= \prod_k \text{tr}_k \left(\bar{e}^{-\beta \Omega_k (a_k^\dagger a_k + 1/2)} \right) \end{aligned}$$

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

Thus

is Hsuypng constant

$$Z = \prod_k \frac{e^{-\beta \Omega_k / 2}}{(1 - e^{-\beta \Omega_k})} = \prod_k Z_k \quad (88)$$

Similarly, the Gibbs state becomes simply

$$\rho = \prod_k \rho_k = \prod_k (1 - e^{-\beta \Omega_k}) e^{-\beta \Omega_k a_k^\dagger a_k} \quad (89)$$

For instance, we know that for one harmonic oscillator

$$\Omega (\langle a^\dagger a \rangle + 1/2) = \Omega (\bar{n} + 1/2) = \frac{\Omega}{2} \coth\left(\frac{\Omega}{2T}\right) \quad (90)$$

where

$$\bar{n} = \frac{1}{e^{\beta \Omega} - 1} \quad (91)$$

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

$$U = \langle H \rangle = \sum_k \Omega_k (\bar{n}_k + 1/2) = \sum_k \frac{\Omega_k}{2} \coth\left(\frac{\Omega_k}{2T}\right) \quad (92)$$

A similar reasoning holds for all other thermodynamic quantities

But now suppose we want to compute something more specific. For instance, I want to know $\langle q_i \rangle$ for some i . This is the average of the displacement of the i -th oscillator. Of course, we can anticipate that $\langle q_i \rangle = 0$ since the oscillator is equally likely to be displaced to the left or to the right. But let's see if we can see where this comes from.

Our Gibbs state is written in terms of a_n and a_n^\dagger , so the first step is to express q_i in terms of these guys. Now, from (66) we have

$$Q_n = \frac{1}{\sqrt{N}} \sum_i e^{ikx_i} q_i$$

Now multiply by $\frac{e^{-ikx_j}}{\sqrt{N}}$ and sum over k :

$$\begin{aligned} \frac{1}{\sqrt{N}} \sum_n Q_n e^{-ikx_j} &= \frac{1}{N} \sum_{ik} e^{ik(x_i - x_j)} q_i \quad \leftarrow \text{use (57)} \\ &= \sum_j \delta_{ij} q_i = q_j \end{aligned}$$

thus

$$q_i = \frac{1}{\sqrt{N}} \sum_n e^{-ikx_i} Q_n \quad (93)$$

Next we also use (74) to get

$$q_i = \frac{1}{\sqrt{N}} \sum_n e^{-ikx_i} \frac{1}{\sqrt{2\Omega_n}} (a_n + a_n^\dagger)$$

It is convenient to exchange $k \leftrightarrow -k$ in the last term, finally leading us to

$$q_i = \frac{1}{\sqrt{N}} \sum_k \frac{1}{\sqrt{2\Omega_k}} (a_k e^{-ikx_i} + a_k^\dagger e^{ikx_i}) \quad (94)$$

Using this we can now compute

$$\langle q_i \rangle = \frac{1}{\sqrt{N}} \sum_k \frac{1}{\sqrt{2\Omega_k}} \{ \langle a_k \rangle e^{-ikx_i} + \langle a_k^\dagger \rangle e^{ikx_i} \} \quad (95)$$

It is important that you gain some intuition as to how to compute these kinds of expectation values.

If we have 1 oscillator, $\rho = e^{-\beta \Omega a^\dagger a} / Z$, then

$$\begin{aligned} \langle a \rangle &= \text{tr}(a e^{-\beta \Omega a^\dagger a} / Z) \\ &= \frac{1}{Z} \sum_n \langle n | a e^{-\beta \Omega a^\dagger a} | n \rangle \\ &= \frac{1}{Z} \sum_n \underbrace{\langle n | a | n \rangle}_0 e^{-\beta \Omega n} \\ &= 0 \end{aligned}$$

If we have 2 oscillators, $\rho = \frac{e^{-\beta\Omega_1 a_1^\dagger a_1}}{Z_1} \otimes \frac{e^{-\beta\Omega_2 a_2^\dagger a_2}}{Z_2}$ and

$$\begin{aligned} \langle a_1 \rangle &= \text{tr} \left\{ a_1 \frac{e^{-\beta\Omega_1 a_1^\dagger a_1}}{Z_1} \frac{e^{-\beta\Omega_2 a_2^\dagger a_2}}{Z_2} \right\} \\ &= \underbrace{\text{tr} \left\{ a_1 \frac{e^{-\beta\Omega_1 a_1^\dagger a_1}}{Z_1} \right\}}_0 \underbrace{\text{tr} \left\{ \frac{e^{-\beta\Omega_2 a_2^\dagger a_2}}{Z_2} \right\}}_1 \end{aligned}$$

thus, the average goes as if a_2 was not even there. Going back to (95), we then conclude that

$$\langle q_2 \rangle = 0$$

(96)

