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

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

Here q and p are operators satisfying the canonical commutation relations

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

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

We now introduce the so-called creation and annihilation operators

$$q = \sqrt{\frac{\hbar}{m\omega}}\,\frac{(a^\dagger + a)}{\sqrt{2}} \qquad a = \frac{1}{\sqrt{2}}\left(\sqrt{\frac{m\omega}{\hbar}}\,q + i\frac{p}{\sqrt{m\hbar\omega}}\right) \qquad (3)$$

$$p = i\sqrt{\hbar m\omega}\,\frac{(a^\dagger - a)}{\sqrt{2}} \qquad a^\dagger = \frac{1}{\sqrt{2}}\left(\sqrt{\frac{m\omega}{\hbar}}\,q - i\frac{p}{\sqrt{m\hbar\omega}}\right)$$

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

$$\boxed{[a, a^\dagger] = 1} \tag{4}$$

We now have

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

$$p^2 = \frac{m\hbar\omega}{2}\left(a^\dagger a + aa^\dagger - aa - a^\dagger a^\dagger\right) \tag{5}$$

so

$$\frac{p^2}{2m} = \frac{\hbar\omega}{4}\left(a^\dagger a + aa^\dagger - aa - a^\dagger a^\dagger\right) \tag{6}$$

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

and then (1) becomes

$$H = \frac{\hbar\omega}{2}\left(a^\dagger a + aa^\dagger\right) \tag{7}$$

Finally, using (4) we can write

$$aa^\dagger = 1 + a^\dagger a \tag{8}$$

Hence

$$\boxed{H = \hbar\omega\left(a^\dagger a + 1/2\right)} \tag{9}$$

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 $[\hat{Q}_\psi(\alpha)]$. Everything follows from the algebra.

Let us write

$$a^\dagger a |\lambda\rangle = \lambda |\lambda\rangle \tag{10}$$

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 $|v\rangle = a|\lambda\rangle$ then $\langle\lambda|a^\dagger = \langle v|$ so

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

Hence

$$\lambda \geqslant 0 \tag{11}$$

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

$$[a^\dagger a, a] = a^\dagger \underbrace{[a, a]}_{0} + \underbrace{[a^\dagger, a]}_{-1} a = -a$$

$$\therefore \quad [a^\dagger a, a] = -a \tag{12}$$

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

$$a^\dagger a|\phi\rangle = a(\lambda - 1)|\lambda\rangle = (\lambda - 1)|\phi\rangle \tag{13}$$

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 <u>lowering operator</u> 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

$$a|\lambda\rangle = \sqrt{\lambda}\,|\lambda-1\rangle \tag{14}$$

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

$$a^k|\lambda\rangle = \sqrt{\lambda(\lambda-1)\cdots(\lambda-k+1)}\;|\lambda-k\rangle \tag{15}$$

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

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

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

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

$$\boxed{\begin{aligned} &a^\dagger a |m\rangle = m |m\rangle \\ &m = 0, 1, 2, 3, \ldots \end{aligned}} \qquad (16)$$

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

$$a |m\rangle = \sqrt{m}\ |m-1\rangle \qquad (17)$$

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

$$[a^\dagger a, a^\dagger] = a^\dagger \underbrace{[a, a^\dagger]}_{1} + \underbrace{[a^\dagger, a^\dagger]}_{0} a = a^\dagger$$

so

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

Then

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

Thus

$$a^\dagger |n\rangle = d_n |n+1\rangle$$

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

$$\langle n+1|n+1\rangle\, |d_n|^2 = \langle n| a\, a^\dagger |n\rangle = \langle n|(a^\dagger a + 1)|n\rangle = n+1$$

Thus

$$a^\dagger |n\rangle = \sqrt{n+1}\, |n+1\rangle \qquad (18)$$

Of all states (16), the one with $n=0$ is special. It is called the <u>vacuum state</u>, 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 $a^\dagger$ 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

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

And this concludes our algebraic problem.

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Summary

$$[a, a^\dagger] = 1 \qquad [a^\dagger a, a] = -a \qquad [a^\dagger a, a^\dagger] = a^\dagger \tag{20}$$

$$a^\dagger a |n\rangle = n |n\rangle \qquad n = 0, 1, 2, \ldots \tag{21}$$

$$a|n\rangle = \sqrt{n}\,|n\rangle$$
$$a^\dagger |n\rangle = \sqrt{n+1}\,|n\rangle \tag{22}$$

$$a|0\rangle = 0 \qquad |n\rangle = \frac{(a^\dagger)^n}{\sqrt{n!}} |0\rangle \tag{23}$$

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 $|n\rangle$ and the eigenvalues are

$$E_n = \omega(n+1/2) \qquad (\hbar = 1 \text{ now}) \tag{24}$$

The thermal state is

$$\rho = \frac{e^{-\beta H}}{Z} \tag{25}$$

where

$$Z = \mathrm{tr}\, e^{-\beta H} = \mathrm{tr}\, e^{-\beta\omega(a^\dagger a + 1/2)}$$

$$= \sum_n \langle n| e^{-\beta\omega(a^\dagger a + 1/2)} |n\rangle$$

$$= \sum_n e^{-\beta\omega(n+1/2)}$$

$$= \frac{e^{-\beta\omega/2}}{1 - e^{-\beta\omega}} \quad \leftarrow \text{We did this before}$$

Thus

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

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

$$\rho = \sum_n p_n |n\rangle\langle n| \tag{27}$$

$$p_n = (1 - e^{-\beta\omega})\, e^{-\beta\omega n}$$

Now we can compute any expectation value we want as

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

For instance we could compute something like

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

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

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

Thus

$$\langle a^\dagger a^\dagger a a \rangle = (1 - e^{-\beta\omega}) \sum_{n=0}^{\infty} \langle n | a^\dagger a \, (a^\dagger a - 1) \, e^{-\beta\omega a^\dagger a} | n \rangle$$

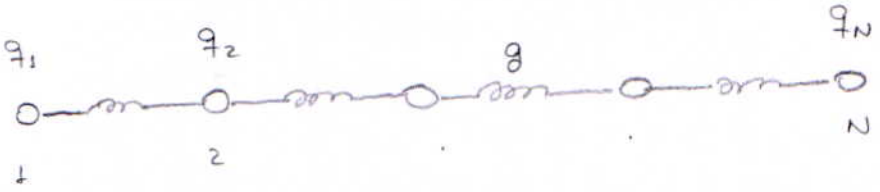
$$= (1 - e^{\beta\omega}) \sum_{n=0}^{\infty} n(n-1) \, e^{-\beta\omega a^\dagger a}$$

$$= 2 \bar{n}^2 \qquad \bar{n} = \frac{1}{e^{\beta\omega} - 1}$$

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 it's two neighbors and this interaction is harmonic. Thus, we shall take as our Hamiltonian

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

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

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

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

To begin let us look at the potential energy only

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

This is a quadratic form in the operators q_i:

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

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

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

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 came from the periodic boundary conditions.

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

$$A = U \Lambda U^T \qquad U U^T = U^T U = 1 \tag{34}$$

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

written in terms of indices we have

$$A_{ij} = \sum_k U_{ik} \lambda_k U_{jk} \tag{35}$$

We now insert this in (32), to find

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

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

We now define a new set of coordinates

$$\boxed{Q_k = \sum_i U_{ik} q_i} \tag{37}$$

The potential energy then becomes

$$V = \frac{1}{2} \sum_k \lambda_k Q_k^2 \tag{38}$$

What we just did is called a <u>normal mode decomposition</u>. 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:

$$P_k = \sum_j U_{jk} p_j \tag{39}$$

It then follows that

$$[Q_k, P_{k'}] = \sum_{ij} U_{ik} U_{jk'} \underbrace{[q_i, p_j]}_{i\delta_{ij}}$$

$$= i \sum_i U_{ik} U_{ik'} \quad \leftarrow \quad (U^T U)_{kk'} = \delta_{kk'}$$

$$= i \delta_{kk'}$$

Thus

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

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

$$\sum_u P_u^2 = \sum_{i,j,u} U_{iu} U_{ju} P_i P_j$$

$$= \sum_{ij} \underbrace{\left[\sum_u U_{iu} U_{ju} \right]}_{\delta_{ij}} P_i P_j \quad .$$

$$\therefore \quad \sum_u P_u^2 = \sum_i P_i^2 \tag{41}$$

Thus the Hamiltonian is now transformed as

$$H = \frac{1}{2} \sum_i P_i^2 + \frac{1}{2} \sum_{ij} A_{ij} q_i q_j$$

$$= \frac{1}{2} \sum_u \left(P_u^2 + \lambda_u Q_u^2 \right) \tag{42}$$

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

$$\Omega_u = \sqrt{\lambda_u} \tag{43}$$

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

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 ($UU^\dagger = 1$) instead of an orthogonal one. I want to discuss in some detail how to do this, as I think it a rather important mathematical procedure.

We want to find the eigenvalues and eigenvectors of A.

So some things like

$$A\,\vec{v}_k = \lambda_k \vec{v}_k \tag{44}$$

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

$$U = \begin{pmatrix} | & | & & | \\ \vec{v}_1 & \vec{v}_2 & \cdots & \vec{v}_N \\ | & | & & | \end{pmatrix} \tag{45}$$

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

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

We can see the pattern:

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

I like this because it shows how a eigenvalue/eigenvector equation can also be interpreted as a <u>recurrence relation</u> 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

$$b_j = c\, e^{ikx_j} \tag{48}$$

where k is a number to be determined and $x_j = j$ (it 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

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

Cancelling out $c\,e^{ikx_j}$ we get

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

or

$$\boxed{\lambda_k = \omega^2 + 2g\,(1-\cos k)} \qquad (49)$$

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

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

This means

$$k = \frac{2\pi \ell}{N}, \qquad \ell = 0, \pm 1, \pm 2, \cdots \tag{51}$$

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

$$\vec{v}_k = C \begin{pmatrix} e^{ikx_1} \\ e^{ikx_2} \\ \vdots \\ e^{ikx_N} \end{pmatrix} \tag{52}$$

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

$$k \in [-\pi, \pi] \tag{53}$$

which in solid state physics is called the first Brillouin zone

Thus, we usually choose

$$-\frac{N}{2} < \ell \leq \frac{N}{2} \tag{54}$$

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

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

Using the result for a truncated geometric series

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

we get

$$\vec{v}_k^{\,\dagger}\,v_{k'} = |c|^2 \, e^{i(k-k')} \left(\frac{1-e^{iN(k-k')}}{1-e^{i(k-k')}}\right)$$

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

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

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

$$\|v_k\|^2 = |c|^2 N$$

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

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

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

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

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

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

$$A\vec{v}_k = \lambda_k \vec{v}_k \tag{58}$$

where

$$v_k = \frac{1}{\sqrt{N}} \begin{pmatrix} e^{ikx_1} \\ e^{ikx_2} \\ \vdots \\ e^{ikx_N} \end{pmatrix} \tag{59}$$

and

$$\lambda_k = \omega^2 + 2g(1-\cos k) \tag{60}$$

$$k = \frac{2\pi \ell}{N}, \qquad \ell = 0, \pm 1, \pm 2, \ldots, \pm \frac{N}{2} \tag{61}$$

Or, in terms of a matrix transformation

$$A = U \Lambda U^{\dagger} \tag{62}$$

where

$$\Lambda_{kk} = \lambda_k \tag{63}$$

$$U_{ik} = \frac{1}{\sqrt{N}} e^{ikx_i} \tag{64}$$

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.

Phonons

We are now ready to go back to the physical problem of our 3D 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

$$V = \frac{1}{2} \sum_{ij} A_{ij} q_i q_j$$

$$= \frac{1}{2} \sum_{ij} \sum_{k} U_{ik} \lambda_k U^{*}_{jk} q_i q_j$$

$$= \frac{1}{2} \sum_{k} \lambda_k \left[\sum_{i} U_{ik} q_i \right] \left[\sum_{j} U^{*}_{jk} q_j \right] \qquad (65)$$

We now define

$$\boxed{Q_k = \sum_{i} U_{ik} q_i = \frac{1}{\sqrt{N}} \sum_{i} e^{ikx_i} q_i} \qquad (66)$$

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

$$Q_k^{\dagger} = Q_{-k} \qquad (67)$$

Hence, Eq (65) becomes

$$V = \frac{1}{2} \sum_{k} \lambda_k Q_k Q_{-k} \qquad (68)$$

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

$$\boxed{\mathcal{P}_k = \sum_i U^*_{ik}\, p_i = \frac{1}{\sqrt{N}} \sum_i e^{-ikx_i}\, p_i} \tag{69}$$

we then get

$$[\Theta_k, \mathcal{P}_{k'}] = \frac{1}{N} \sum_{ij} e^{i(kx_i - k'x_j)} \underbrace{[q_i, p_j]}_{i\delta_{ij}}$$

$$= i \underbrace{\frac{1}{N} \sum_i e^{i(k-k')x_i}}_{\delta_{kk'} \text{ by Eq (56)}}$$

thus

$$\boxed{[\Theta_k, \mathcal{P}_{k'}] = i\,\delta_{kk'}} \tag{70}$$

so Θ_k and $\mathcal{P}_k$ continue to be canonically conjugated variables.

I will leave for you as an exercise to check that

$$\sum_i p_i^2 = \sum_k \mathcal{P}_k \mathcal{P}_{-k} \tag{71}$$

where, as with Θ_k, $\mathcal{P}_{-k} = \mathcal{P}_k^\dagger$

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

$$H = \frac{1}{2} \sum_k \left(\Pi_k \Pi_{-k} + \Omega_k^2 Q_k Q_{-k} \right) \tag{72}$$

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

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

Hence, despite the weird appearance of the non Hermitian operators Q_k and Π_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

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

$$\text{or}$$

$$a_k^\dagger = \sqrt{\frac{\Omega_k}{2}} \left(Q_{-k} - i \frac{\Pi_k}{\Omega_k} \right) \qquad \Pi_k = i \sqrt{\frac{\Omega_k}{2}} (a_k^\dagger - a_{-k}) \tag{74}$$

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

One may then check that

$$[a_u, a_u^\dagger] = \frac{\Omega_u}{2}\left[Q_u + \frac{i P_{-u}}{\Omega_u},\ Q_{-u} - \frac{i P_u}{\Omega_u}\right]$$

$$= \frac{\Omega_u}{2}\left(-\frac{i}{\Omega_u}\right)\underbrace{[Q_u, P_u]}_{i} + \frac{\Omega_u}{2}\frac{i}{\Omega_u}\underbrace{[P_{-u}, Q_{-u}]}_{-i}$$

$$= \frac{1}{2} + \frac{1}{2} = 1$$

Thus

$$\boxed{[a_u, a_{u'}^\dagger] = \delta_{uu'}} \tag{75}$$

these operators therefore represent an <u>independent set of creation and annihilation operators</u>

we also have

$$Q_u Q_{-u} = \frac{1}{2\Omega_u}(a_u + a_{-u}^\dagger)(a_{-u} + a_u^\dagger) \tag{76}$$

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

$$P_u P_{-u} = -\frac{\Omega_u}{2}(a_u^\dagger - a_{-u})(a_{-u}^\dagger - a_u) \tag{77}$$

$$= -\frac{\Omega_u}{2}(a_u^\dagger a_{-u}^\dagger + a_{-u} a_u - a_u^\dagger a_u - a_{-u} a_{-u}^\dagger)$$

Thus the Hamiltonian (72) becomes

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

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

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

$$\boxed{H = \sum_u \Omega_u \left(a_u^\dagger a_u + 1/2 \right)} \qquad (78)$$

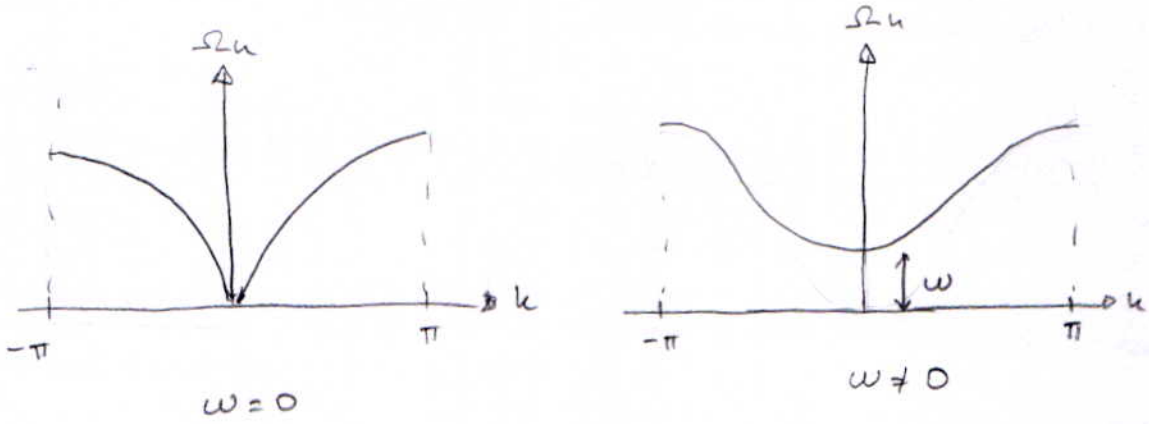
We therefore conclude that the 1D can be represented as an independent set of harmonic oscillators, labeled by k and with frequencies

$$\Omega_u = \sqrt{\omega^2 + 2g(1 - \cos k)} \qquad (79)$$

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 (Ω_u, f_u) are delocalized, as can be seen in (66): they are plane wave decompositions of the actual displacements q_i.

Now let's plot Ω_k 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 Ω_k in the vicinity of $k=0$. Expanding the cosine in a Taylor series we get

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

Hence (79) becomes

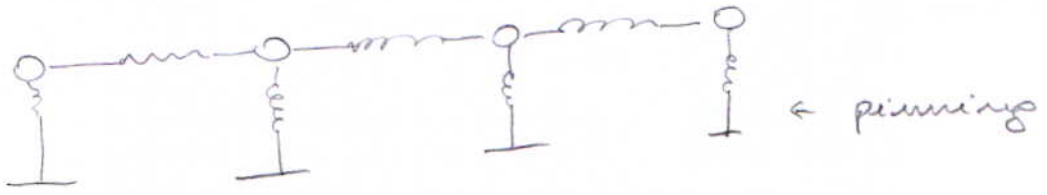
$$\boxed{\Omega_k \simeq \sqrt{\omega^2 + g k^2}} \tag{80}$$

Holy shit! This is the relativistic dispersion relation!

$$\boxed{E = \sqrt{m^2 c^4 + p^2 c^2}} \tag{81}$$

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

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

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

$$|\vec{N}\rangle = \bigotimes_{k=1}^{N} |N_k\rangle \tag{82}$$

which is a short-hand notation for

$$|\vec{N}\rangle = |N_{k_1}\rangle \otimes |N_{k_2}\rangle \otimes |N_{k_3}\rangle \otimes \cdots$$

where $k_1, k_2, \cdots$ 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 $0, 1, 2, 3, \ldots$ phonons on that k.

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

$$a_k |0\rangle = 0 \qquad \forall\, k \tag{83}$$

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

$$|1_k\rangle = a_k^\dagger |0\rangle \tag{84}$$

Then states with 2 phonons

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

and so on.

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

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

$$H|1_k\rangle = \sum_{k'} \Omega_{k'} \left(a^\dagger_{k'} a_{k'} + 1/2\right)|1_k\rangle$$

$$= \sum_{k'} \Omega_{k'} a^\dagger_{k'} a_{k'}|1_k\rangle + \frac{\Omega_{k'}}{2}|1_k\rangle$$

But $a^\dagger_{k'} a_{k'}$ 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

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

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

$$E(1_k) = \Omega_k + E_{gs}$$

Similarly, the energy of two phonons would be

$$E(1_k, 1_{k'}) = \Omega_k + \Omega_{k'} + E_{gs}$$