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

$$H = \frac{p^2}{2m} + \frac{1}{2} m \omega^2 q^2 \tag{1}$$

Here q and p are operators satisfying the canonical commutation relations

$$[q, p] = i\hbar \tag{2}$$

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

We now introduce the so-called creation and annihilation operators

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

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

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

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

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

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 [Eq (4)]. 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

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

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

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

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

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

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

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

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

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

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

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

However

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

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

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

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

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

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

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 $a^\dagger$ 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

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

And this concludes our algebraic problem.

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<u>Summary</u>

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

$$a^\dagger a |n\rangle = n |n\rangle \qquad n = 0, 1, 2, \ldots \qquad (21)$$

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

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

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

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

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

$$\begin{aligned} \rho &= \sum_n q_n |n\rangle\langle n| \\ q_n &= (1-e^{-\beta\omega})\, e^{-\beta\omega n} \end{aligned} \tag{27}$$

Now we can compute any expectation value we want as

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

For instance we could compute something like

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

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