0.1 Repetition of the harmonic oscillator

The Hamiltonian for the harmonic oscillator $H = k^2/2m + m\omega^2 x^2/2$ can be written as

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

with $p = k/\sqrt{m\hbar\omega}$, and $q = \sqrt{m\omega/\hbar}x$. The commutation relation between p and q is:

$$[p, q] = pq - qp = -i$$

If we define operators

$$b = (q + ip)/\sqrt{2}$$

$$b^\dagger = (q - ip)/\sqrt{(2)}$$

then the hamiltonian reads

$$H = \hbar\omega\left(b^\dagger b + \frac{1}{2}\right),$$

and the commutator

$$[b, b^\dagger] = 1.$$

We also may compute the commutator of these operator with the hamiltonian to give

$$[H, b^\dagger] = \hbar\omega\left\{\left(b^\dagger b b^\dagger + \frac{1}{2}b^\dagger\right) - \left(b^\dagger b^\dagger b + \frac{1}{2}b^\dagger\right)\right\} = \hbar\omega b^\dagger[b, b^\dagger] = \hbar\omega b^\dagger,$$

and

$$[H, b] = -\hbar\omega b$$

Then

$$[H, b^\dagger]\,|\phi_E\rangle = Hb^\dagger\,|\phi_E\rangle - b^\dagger H\,|\phi_E\rangle = \hbar\omega b^\dagger\,|\phi_E\rangle$$

$$Hb^\dagger\,|\phi_E\rangle = (E + \hbar\omega)b^\dagger\,|\phi_E\rangle\,,$$

and

$$Hb\,|\phi_E\rangle = (E - \hbar\omega)b\,|\phi_E\rangle$$

This way we find new states like $b\,|\phi_E\rangle$ with energy $(E - \hbar\omega)$. Since the hamiltonian is positive definite, there must be an end to finding lower energy states such that for this lowest energy state $|\phi_0\rangle$ we have $b\,|\phi_0\rangle = 0$. In order to find this energy we first look in detail what b and $b^\dagger$ actually do, starting with a proper normalization. Since we know that $b^\dagger\,|\phi_E\rangle = A_E\,|\phi_{E+\hbar\omega}\rangle$ (see above), we can find the normalization constant:

$$|A_E|^2 = \langle\phi_E|\,bb^\dagger\,|\phi_E\rangle = \langle\phi_E|\,\frac{H}{\hbar\omega} + \frac{1}{2}\,|\phi_E\rangle = \frac{E + \hbar\omega/2}{\hbar\omega}$$

So, now we have

$$b^\dagger |\phi_E\rangle = \sqrt{\frac{E + \hbar\omega/2}{\hbar\omega}} |\phi_{E+\hbar\omega}\rangle$$

$$b |\phi_E\rangle = \sqrt{\frac{E - \hbar\omega/2}{\hbar\omega}} |\phi_{E-\hbar\omega}\rangle$$

The lowest state is obviously found for $E = \hbar\omega/2$ so that $b\left|\phi_{\hbar\omega/2}\right\rangle = 0$ Now we can label the states by a number $n > 0$ representing the energy $(n + 1/2)\hbar\omega$, and since

$$\langle\phi_E| b^\dagger b |\phi_E\rangle = \langle\phi_E| bb^\dagger - 1 |\phi_E\rangle = n$$

the eigenstates of $b^\dagger b$ as $|n\rangle$. That is we can rewrite the problem as

$$b^\dagger |n\rangle = \sqrt{n+1} |n+1\rangle$$

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

$$H |n\rangle = \hbar\omega \left(\tilde{n} + \frac{1}{2}\right) |n\rangle$$

from which we can easily evaluate the probability of any physical observable. As an example let us look at the mean square amplitude in the ground state. We have $q = (b + b^\dagger)/\sqrt{2}$ or $x = (b + b^\dagger)/\sqrt{2m\omega/\hbar}$ so that $|x^2| \propto (b + b^\dagger)^2 = (bb + b^\dagger b^\dagger + bb^\dagger + b^\dagger b)$. The squared amplitude is then

$$\left|x^2\right| = \hbar \frac{\langle 0| bb^\dagger |0\rangle}{2m\omega} = \frac{\hbar}{2m\omega}.$$

It is equally easy to verify that $|x| = 0$ as expected. If we use the wavefunctions $|n\rangle$ as a basis, we now see that the Hamilton matrix is nicely diagonalized to:

$$\hbar\omega \begin{pmatrix} 1/2 & 0 & \dots \\ 0 & 3/2 & \\ \vdots & & \ddots \end{pmatrix}$$

This restatement of the problem in terms of raising (creation) and lowering (annihilation) operators, and the occupation operator $\tilde{n}$ has proven to be usefull in solving the harmonic oscillator model, even though we can also solve the problem more directly. For many body problems, the second quantization language of introduced here turns out to be indispensible. We can not treat the momentum and position operators of, say, 10^{23} particles in a similar way we can directly solve the harmonic oscillator problem.

0.2 Intuitive extension to lattice vibrations

The lattice modes are labeled by their branch index, s, and k-vectors $\omega_{s,k}$. Each of these states can be considered as a harmonic oscillator like state. In analogy to the harmonic oscillator one can therefore write for the Hamilton operator for state k (we will restrict ourselves to one branch).

$$H_k = \hbar\omega_k \left(b_k^\dagger b_k + \frac{1}{2} \right) \tag{1}$$

To calculate an expectation value one needs to then sum matrix elements over all k-states. For example if we would like to calculate the amplitude of the fluctuations, $\langle x^2 \rangle$, we first need to express x in terms of our operators and then calculate the expectation value for a given k state:

$$x_k = \frac{1}{2}\sqrt{2}\sqrt{\frac{\hbar}{m\omega_k}} \left(b + b^\dagger \right) \tag{2}$$

$$\langle n_k | \left[\frac{1}{2}\sqrt{2}\sqrt{\frac{\hbar}{m\omega_k}} \left(b + b^\dagger \right) \right]^2 | n_k \rangle \tag{3}$$

In the ground state this gives:

$$\langle 0 | \, x_k^2 \, | 0 \rangle = \frac{\hbar}{2m\omega_k} \tag{4}$$

Now we can make the sum over the k-states, which with the help of the density of states in k-space can be converted into an integral:

$$\left\langle x^2 \right\rangle = \sum_{k \in BZ} \frac{\hbar}{2m\omega_k} = \int_{-\pi}^{\pi} \frac{\hbar}{2m\omega_k} D(k) dk \tag{5}$$

In d dimensions (one atom per cell, unit cell length = 1) this gives with $\omega_k = \omega_0 |\sin(k/2)|$ and $D(k) = A_d k^{d-1}$:

$$\left\langle x^2 \right\rangle = A_d \int_{-\pi}^{\pi} \frac{\hbar}{2m\omega_k} k^d dk \tag{6}$$

For 2 and 3 dimensions the integral is finite. In 1 dimension the integral diverges as

$$\lim_{\delta \to 0} 4 \ln \left(\cot \frac{\delta}{4} \right) \tag{7}$$