

9. Harmonic Oscillator

9.1 Harmonic Oscillator

- 9.1.1 Classical harmonic oscillator and h.o. model
- 9.1.2 Oscillator Hamiltonian: Position and momentum operators
- 9.1.3 Position representation
- 9.1.4 Heisenberg picture
- 9.1.5 Schrödinger picture

9.2 Uncertainty relationships

9.3 Coherent States

- 9.3.1 Expansion in terms of number states
- 9.3.2 Non-Orthogonality
- 9.3.3 Uncertainty relationships
- 9.3.4 X-representation

9.4 Phonons

- 9.4.1 Harmonic oscillator model for a crystal
- 9.4.2 Phonons as normal modes of the lattice vibration
- 9.4.3 Thermal energy density and Specific Heat

9.1 Harmonic Oscillator

We have considered up to this moment only systems with a finite number of energy levels; we are now going to consider a system with an infinite number of energy levels: the quantum harmonic oscillator (h.o.).

The quantum h.o. is a model that describes systems with a characteristic energy spectrum, given by a ladder of evenly spaced energy levels. The energy difference between two consecutive levels is ΔE . The number of levels is infinite, but there must exist a minimum energy, since the energy must always be positive. Given this spectrum, we expect the Hamiltonian will have the form

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

where each level in the ladder is identified by a number n . The name of the model is due to the analogy with characteristics of classical h.o., which we will review first.

9.1.1 Classical harmonic oscillator and h.o. model

A classical h.o. is described by a potential energy $V = \frac{1}{2}kx^2$. If the system has a finite energy E , the motion is bound by two values $\pm x_0$, such that $V(x_0) = E$. The equation of motion is given by $m \frac{d^2x}{dt^2} = -kx$ and the kinetic energy is of course $T = \frac{1}{2}m\dot{x}^2 = \frac{p^2}{2m}$. The energy is constant since it is a conservative system, with no dissipation. Most of the time the particle is in the position x_0 since there the velocity is zero, while at $x = 0$ the velocity is maximum.

The h.o. oscillator in QM is an important model that describes many different physical situations. We will study in depth a particular system described by the h.o., the electromagnetic field. Another system that can be described

by this model is solid-state crystals, where the oscillations of nuclei in the lattice can be described as a systems of coupled oscillators (phonons).

Notice that any potential with a local minimum can be locally described by an h.o.. Provided that the energy is low enough (or x close to x_0), any potential can in fact be expanded in series, giving: $V(x) \approx V(x_0) + b(x - x_0)^2 + \dots$ where $b = \frac{d^2V}{dx^2}|_{x_0}$.

9.1.2 Oscillator Hamiltonian: Position and momentum operators

We can define the operators associated with position and momentum. They are two observables (p, x) with the commutation properties: $[x, p] = i\hbar$. With these two operators, the Hamiltonian of the quantum h.o. is written as:

$$\mathcal{H} = \frac{p^2}{2m} + \frac{kx^2}{2} = \frac{p^2}{2m} + \frac{1}{2}m\omega^2x^2,$$

where we defined a parameter with units of frequency: $\omega = \sqrt{k/m}$.

We use the dimensionless variables,

$$P = \frac{p}{\sqrt{m\omega}}, \quad X = x\sqrt{m\omega}$$

and $\hat{\mathcal{H}} = \mathcal{H}/\omega$, to simplify the expression to $\hat{\mathcal{H}} = \omega(X^2 + P^2)/2$ or $\mathcal{H} = \frac{\omega}{2}(X^2 + P^2)$.

We have said initially that we expect the hamiltonian to have the form $\hat{\mathcal{H}} = (n + \frac{1}{2})|n\rangle\langle n|$, if expressed in an appropriate basis. This simply corresponds to diagonalizing the Hamiltonian (thus the basis $\{|n\rangle\}$ is the energy basis, or the basis formed by the eigenstates of the Hamiltonian). However the diagonalization is not as intuitive as for simple TLS (or n TLS) because we are considering a system with infinite dimensions.

The operator $\hat{\mathcal{H}} = (n + \frac{1}{2})|n\rangle\langle n|$ is our guess for the diagonalized form of the Hamiltonian, which makes explicit the presence of energy levels, labeled by n . Correspondingly, there must be operators that act on the ladder of energy levels. For example, the fundamental operations possible are the raising or lowering of 1 quantum of energy, as well as an operator giving the number of energy quanta: $N|n\rangle = n|n\rangle$. The raising and lowering operators act as the following: $a|n\rangle \propto |n-1\rangle$ and $a^\dagger|n\rangle \propto |n+1\rangle$. They are also called the annihilation and creation operators, as they destroy or create a quantum of energy.

Instead of deriving rigorously these operators, we guess their form in terms of the X and P operators:

$$\begin{aligned} a &= \frac{1}{\sqrt{2\hbar}}(X + iP) = \frac{1}{\sqrt{2\hbar}}(\sqrt{m\omega}x + \frac{i}{\sqrt{m\omega}}p) \\ a^\dagger &= \frac{1}{\sqrt{2\hbar}}(X - iP) = \frac{1}{\sqrt{2\hbar}}(\sqrt{m\omega}x - \frac{i}{\sqrt{m\omega}}p), \end{aligned}$$

and we will check a posteriori that indeed they act as annihilation and creation operators. Notice that a, a^\dagger are not hermitian, but they are one the hermitian conjugate of the other ($a = (a^\dagger)^\dagger$). Also, we define the number operator as $N = a^\dagger a$. The commutation properties are: $[a, a^\dagger] = 1$ and $[N, a] = -a$, $[N, a^\dagger] = a^\dagger$.

Also we have:

$$\begin{aligned} x &= \sqrt{\frac{\hbar}{2m\omega}}(a^\dagger + a) \\ p &= i\sqrt{\frac{m\omega\hbar}{2}}(a^\dagger - a) \end{aligned}$$

? Question: Prove the commutation relationships of the raising and lowering operators.

$$[a, a^\dagger] = \frac{1}{2\hbar}[X + iP, X - iP] = \frac{1}{2\hbar}([X, -iP] + [iP, X]) = -\frac{i}{\hbar}[X, P] = -\frac{i}{\hbar}[x, p] = 1$$

So we also have $aa^\dagger = [a, a^\dagger] + a^\dagger a = 1 + a^\dagger a = 1 + N$.

$$[N, a] = [a^\dagger a, a] = [a^\dagger, a]a = -a \quad \text{and} \quad [N, a^\dagger] = [a^\dagger a, a^\dagger] = a^\dagger[a, a^\dagger] = a^\dagger$$

□

Notice that from now on we will take as usual $\hbar = 1$.

From the commutation relationships we have:

$$a|n\rangle = [a, N]|n\rangle = an|n\rangle - Na|n\rangle \rightarrow N(a|n\rangle) = (n-1)(a|n\rangle),$$

that is, $a|n\rangle$ is also an eigenvector of the N operator, with eigenvalue $(n-1)$. Thus we confirm that this is the lowering operator: $a|n\rangle = c_n|n-1\rangle$. Similarly, $a^\dagger|n\rangle$ is an eigenvector of N with eigenvalue $n+1$:

$$a^\dagger|n\rangle = [N, a^\dagger]|n\rangle = Na^\dagger|n\rangle - a^\dagger n|n\rangle \rightarrow N(a^\dagger|n\rangle) = (n+1)(a^\dagger|n\rangle).$$

We thus have $a|n\rangle = c_n|n-1\rangle$ and $a^\dagger|n\rangle = d_n|n+1\rangle$. What are the coefficients c_n , d_n ?
Since

$$\langle n|N|n\rangle = \langle n|a^\dagger a|n\rangle = n$$

and

$$\langle n|a^\dagger a|n\rangle = (\langle an|)(a|n\rangle) = \langle n-1|n-1\rangle c_n^2,$$

we must have $c_n = \sqrt{n}$. Analogously, since $aa^\dagger = N+1$, as seen from the commutation relationship:

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

So in the end we have :

$$a|n\rangle = \sqrt{n}|n-1\rangle; \quad a^\dagger|n\rangle = \sqrt{n+1}|n+1\rangle.$$

All the n eigenvalues of N have to be non-negative since $n = \langle n|N|n\rangle = \langle \psi_{n_1}|\psi_{n_1}\rangle \geq 0$ (this follows from the properties of the inner product and the fact that $|\psi_{n_1}\rangle = a|n\rangle$ is just a regular state vector). However, if we apply over and over the a (lowering) operator, we could arrive at negative numbers n : we therefore require that $a|0\rangle = 0$ to truncate this process. The action of the raising operator a^\dagger can then produce any eigenstate, starting from the 0 eigenstate:

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

The matrix representation of these operator in the $|n\rangle$ basis (with infinite-dimensional matrices) is particularly simple, since $\langle n|a|n'\rangle = \delta_{n',n-1}\sqrt{n}$ and $\langle n|a^\dagger|n'\rangle = \delta_{n',n+1}\sqrt{n+1}$:

$$a = \begin{bmatrix} 0 & \sqrt{1} & 0 & \dots \\ 0 & 0 & \sqrt{2} & \dots \\ 0 & 0 & 0 & \dots \end{bmatrix} \quad a^\dagger = \begin{bmatrix} 0 & 0 & 0 & \dots \\ \sqrt{1} & 0 & 0 & \dots \\ 0 & \sqrt{2} & 0 & \dots \end{bmatrix}$$

The Hamiltonian can be written in terms of these operators. We substitute a , a^\dagger at the place of X and P , yielding $\mathcal{H} = \omega(a^\dagger a + \frac{1}{2}) = \omega(N + \frac{1}{2})$ and the minimum energy $\hbar\omega/2$ is called the zero point energy.

9.1.3 Position representation

We have now started from a (physical) description of the h.o. Hamiltonian and made a change of basis in order to arrive at a simple diagonal form of it. Now that we know its eigenkets, we would like to go back to a more intuitive picture of position and momentum. We thus want to express the eigenkets $|n\rangle$ in terms of the position representation (see also section 5.5.1).

The position representation corresponds to expressing a state vector $|\psi\rangle$ in the position basis: $|\psi\rangle = \int dx \langle x|\psi\rangle |x\rangle = \int dx \psi(x) |x\rangle$ (where $|x\rangle$ is the eigenstate of the position operator that is a continuous variable, hence the integral). This defines the wavefunction $\psi(x) = \langle x|\psi\rangle$.

The wave function description in the x representation of the quantum h.o. can be found by starting with the ground state wavefunction. Since $a|0\rangle = 0$ we have $\frac{1}{\sqrt{2}}(X + iP)|0\rangle = \frac{1}{\sqrt{2}}(\sqrt{m\omega}x + \frac{ip}{\sqrt{m\omega}})|0\rangle = 0$. In the x representation, given $\psi_0(x) = \langle x|0\rangle$

$$\frac{1}{\sqrt{2}} \langle x|(\sqrt{m\omega}x + \frac{ip}{\sqrt{m\omega}})|0\rangle = 0 \quad \rightarrow \quad (m\omega x + \frac{d}{dx})\psi_0(x) = 0 \quad \rightarrow \quad \psi_0(x) \propto e^{-m\omega x^2/2}$$

The other eigenstates are built using Hermite Polynomials $H_n(x)$, using the formula³¹ $|n\rangle = \frac{(a^\dagger)^n}{\sqrt{n!}} |0\rangle$ to derive differential equations:

$$\psi_n(x) = \langle x|n\rangle = \frac{1}{\sqrt{n!2^n}} \left[\sqrt{m\omega}x - \frac{1}{\sqrt{m\omega}} \frac{d}{dx} \right]^n \psi_0(x)$$

with solutions $\psi_n(x) = \langle x|n\rangle = \frac{1}{\sqrt{2^n n!}} H_n(x) \psi_0(x)$.

The $n = 2$ and $n = 3$ wavefunctions are plotted in the following figure, while the second figure displays the probability distribution function. Notice the different parity for even and odd number and the number of zeros of these functions.

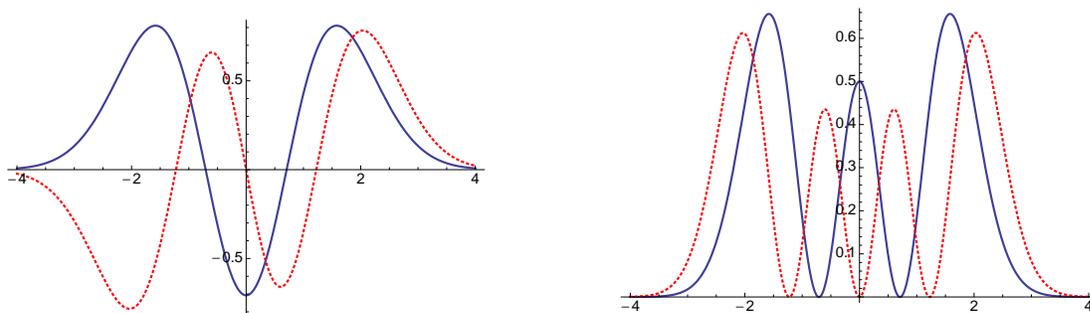


Fig. 12: Left: Harmonic oscillator wavefunction. Right: corresponding probability distribution function for $n = 2$ (blue) and $n = 3$ (Red, dotted).

Classically, the probability that the oscillating particle is at a given value of x is simply the fraction of time that it spends there, which is inversely proportional to its velocity $v(x) = x_0\omega \sqrt{1 - \frac{x^2}{x_0^2}}$ at that position. For large n , the probability distribution becomes close to the classical one:

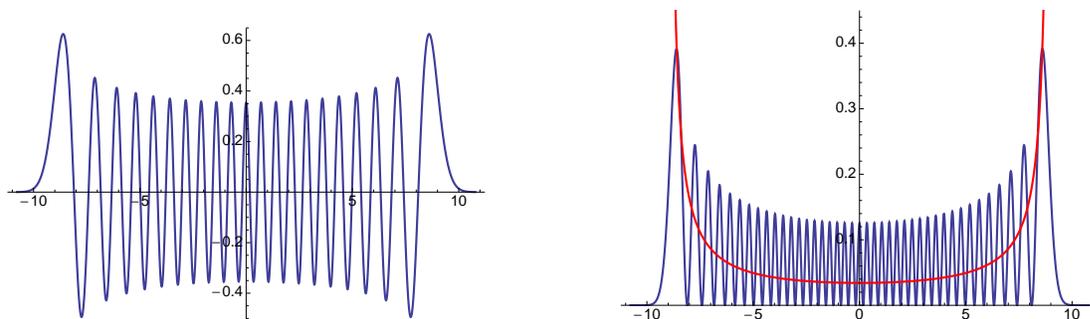


Fig. 13: Left: Harmonic oscillator wavefunction. Right: corresponding probability distribution function for $n = 40$. In Red, the classical probability.

³¹ For more details on Hermite Polynomials and their generator function, look on Cohen-Tannoudji. Online information from: Eric W. Weisstein. [Hermite Polynomial](#). From MathWorld—A Wolfram Web Resource.

9.1.4 Heisenberg picture

We want now to study the time-evolution of the h.o. We first start with analyzing the evolution of the operators in the Heisenberg picture. We have

$$\frac{da}{dt} = i[\mathcal{H}, a] = i[\omega(a^\dagger a + \frac{1}{2}), a] = -i\omega a \quad \rightarrow \quad a(t) = a(0)e^{-i\omega t}$$

Similarly:

$$\frac{da^\dagger}{dt} = i[\mathcal{H}, a^\dagger] = i[\omega(a^\dagger a + \frac{1}{2}), a^\dagger] = i\omega a^\dagger \quad \rightarrow \quad a^\dagger(t) = a^\dagger(0)e^{i\omega t}$$

Notice that we could have found this last relationship just by taking the hermitian conjugate of the first one. Using these results, we can also find the time evolution of the position and momentum operators:

$$x(t) = x(0) \cos(\omega t) + \frac{p(0)}{m\omega} \sin(\omega t)$$

$$p(t) = p(0) \cos(\omega t) - m\omega x(0) \sin(\omega t)$$

and the corresponding expectation values, e.g.

$$\langle x(t) \rangle = \langle x(0) \rangle \cos(\omega t) + \frac{\langle p(0) \rangle}{m\omega} \sin(\omega t)$$

9.1.5 Schrödinger picture

An initial state can be expressed in terms of the number eigenvectors: $|\psi\rangle = \sum_n c_n |n\rangle$. Then its evolution is simply: $|\psi(t)\rangle = \sum_n c_n e^{-in\omega t} |n\rangle$. From this expression, one can calculate e.g.

$$\langle x(t) \rangle = \sum_{n,m} c_n c_m^* \langle m | x | n \rangle e^{-i\omega t(n-m)}.$$

Since x only connects states that differ by $n - m = \pm 1$, it's easy to see that the double sum simplifies and we retrieve the expression above, found in the Heisenberg picture.

9.2 Uncertainty relationships

The operators x and p for a quantum h.o. do not commute, so they do not share any eigenstate, nor they share eigenstates with the Hamiltonian. In particular the diagonal elements of x and p in the $|n\rangle$ -basis representation are both zero, therefore the expectation values are also zero. In a series of measurements, it is possible to get a range of values; we associate this dispersion of values with the root mean square value of the eigenvalues:

$$\Delta x = \sqrt{\langle x^2 \rangle - \langle x \rangle^2} \tag{3}$$

$$\Delta p = \sqrt{\langle p^2 \rangle - \langle p \rangle^2} \tag{4}$$

Given the expression for x and p in terms of a and a^\dagger we can calculate $\langle x^2 \rangle$:

$$\langle x^2 \rangle = \frac{\hbar}{2m\omega} \langle n | aa + a^\dagger a^\dagger + a^\dagger a + aa^\dagger | n \rangle \tag{5}$$

$$= \frac{\hbar}{2m\omega} \langle n | a^\dagger a + aa^\dagger | n \rangle = \frac{\hbar}{2m\omega} (2n + 1) \tag{6}$$

and in the same way, we can calculate $\langle p^2 \rangle$: $\langle p^2 \rangle = \frac{m\hbar\omega}{2} (2n + 1)$. Since the expectation values are zero ($\langle x \rangle = \langle p \rangle = 0$), the deviations are just: $\Delta x = \sqrt{\langle x^2 \rangle}$ and $\Delta p = \sqrt{\langle p^2 \rangle}$ and the uncertainty relation can be expressed by:

$$\Delta p \Delta x = \frac{\hbar}{2} (2n + 1) \tag{7}$$

We see that in general $\Delta p \Delta x \geq \frac{\hbar}{2}$, with equality for $n = 0$: the ground state of the harmonic oscillator is a state of minimum uncertainty. More generally, for any potential $V(x)$, the ground state of a local minimum is always a state of minimum uncertainty (since the potential can be always approximated by an harmonic potential).

We expect that higher energy states do not saturate the uncertainty bound. Classically, when a system has some finite energy, the particle is moving around so $\Delta x = \sqrt{2}x_0$. At the minimum energy (that classically is 0), the particle is at rest, localized ($\Delta x = 0$). For the quantum h.o., even the minimum energy state is not localized, but rather it is a gaussian packet (as described by $\psi_0(x)$) thus the state does have some uncertainty in its position. Still, as expected from the classical intuition, this uncertainty is the minimum possible.

From the expectation values $\langle x^2 \rangle$ and $\langle p^2 \rangle$ we can calculate the average kinetic and potential energy. We find that the average potential and kinetic energy are the same, $\langle T \rangle = \langle V \rangle = \frac{\hbar\omega}{4} = \langle E \rangle / 2$, as for classical conservative systems (virial theorem).

9.3 Coherent States

We now want to look at some connexion of the quantum h.o. with the classical one. We have seen that in the limit of vanishing energy, the classical and quantum oscillators are very different, since the minimum energy for the quantum h.o. is non-zero, while the classical h.o. is totally localized. On the opposite side, we saw that at high energy (high n) the energy difference between two levels vanishes, $\frac{\Delta E}{E} = \frac{\hbar\omega}{(n+1/2)\hbar\omega} \approx 0$; thus the energy becomes continuous, as it would be in the classical case. Still, to find a quantum-to-classical correspondence it is not enough to choose a stationary eigenstate of the Hamiltonian with a high energy (high n): this state would still have zero expectation value for the momentum and position. In contrast, the position evolution in classical mechanics is $x_{cl} = x_0 \cos \omega t$: ideally we would like to find a state $|\psi_{cl}\rangle$ such that $\langle x(t) \rangle = \langle \psi_{cl}(t) | x | \psi_{cl}(t) \rangle = x_{cl}$, as usually stated by Ehrenfest theorem. *Coherent states* achieve this result. For this reasons, these states are also called quasi-classical.

The coherent state was defined by Roy J. Glauber³². He was looking for a superposition of eigenstates that looked as classical as possible, without invoking any decoherence or the action of an external environment. The coherent states are pure quantum states, however when we look at expectation values with respect to these states, the limit of high energy we recover the classical results. For example, although the operator x and p do not commute and give rise to the known uncertainty relationships, when we consider the high energy limit of their expectation values the uncertainties become a vanishing contribution.

Glauber idea was to introduce a complex classical variable $\alpha = \frac{1}{\sqrt{2}}(X + iP)$ (where X and P are the dimensionless variables defined previously). The classical equations of motion for x and p define the evolution of the variable α :

$$\frac{dx}{dt} = \frac{p(t)}{m}, \quad \frac{dp}{dt} = -m\omega^2 x \quad \rightarrow \quad \frac{d\alpha}{dt} = -i\omega\alpha(t)$$

The evolution of α is therefore just a rotation in its phase space: $\alpha(t) = \alpha(0)e^{-i\omega t}$. This is usual for a conservative system (in classical mechanics) or closed systems in QM. The initial conditions thus specify the overall evolution, $\alpha_0 = \alpha(0)$ contains all the important information.

Since $X = \sqrt{2}Re(\alpha)$ and $P = \sqrt{2}Im(\alpha)$, the expectation values for X and P oscillate, as usual in the classical case (again, here X and P are just normalized, classical variable).

$$\begin{aligned} \langle X \rangle &= \frac{1}{\sqrt{2}}(\alpha_0 e^{-i\omega t} + \alpha_0^* e^{i\omega t}) \\ \langle P \rangle &= \frac{-i}{\sqrt{2}}(\alpha_0 e^{-i\omega t} - \alpha_0^* e^{i\omega t}) \end{aligned}$$

The classical energy, given by $\omega/2(X^2 + P^2) = \omega\alpha_0^2$, is constant at all time.

Now consider the QM problem, where the variables are replaced by the corresponding operators:

$$X = (a + a^\dagger)/\sqrt{2}, \quad P = -i(a - a^\dagger)/\sqrt{2}, \quad \mathcal{H} = \omega(a^\dagger a + \frac{1}{2}),$$

and consider the evolution of the operator a in the Heisenberg picture. Its expectation value is given by

$$\frac{d\langle a \rangle}{dt} = -i\langle [a, \mathcal{H}] \rangle = -i\langle [a, \omega a^\dagger a] \rangle = -i\omega\langle a \rangle$$

³² Roy J. Glauber, *Coherent and Incoherent States of the Radiation Field*, *Phys. Rev.* **131** 2766–2788 (1963).

Therefore the expectation value evolution is the same as for the α variable:

$$\langle a(t) \rangle = \langle a(0) \rangle = e^{-i\omega t}, \quad \langle a(t)^\dagger \rangle = \langle a(0)^\dagger \rangle e^{i\omega t}$$

Inspired by this result, we consider a state that is an eigenstate of the annihilation operator a : $a|\alpha\rangle = \alpha|\alpha\rangle$. With respect to this state we have $\langle X \rangle = \langle \alpha | (a + ia^\dagger) | \alpha \rangle / \sqrt{2} = (\alpha + \alpha^*) / \sqrt{2} = \text{Re}(\alpha) / \sqrt{2} \neq 0$. The evolution of $\langle X \rangle$ will then have the same oscillatory character as for its classical counterpart. This eigenstate of the annihilation operator has the desired property and we thus identify it with a coherent state.

The expectation values of position and momentum with respect to a coherent state give rise to the classical result. However, when considering the expectation value of the energy, there are still two contributions: the first one contributes to the classical energy ($\omega a^\dagger a \rightarrow E = \omega |\alpha_0|^2$), while the second term is a purely QM contribution (zero point energy). The classical limit is reached at higher energy where the first contribution is much larger than the zero-point energy $\hbar\omega/2$.

9.3.1 Expansion in terms of number states

The coherent state can of course be expressed in terms of number eigenstates: $|\alpha\rangle = \sum_n c_n |n\rangle$. We want to derive the coefficients c_n . From

$$a|\alpha\rangle = \alpha|\alpha\rangle \rightarrow \sum_{n=0}^{\infty} c_n a|n\rangle = \sum_{n=1}^{\infty} c_n \sqrt{n} |n-1\rangle = \sum_{n=0}^{\infty} c_{n+1} \sqrt{n+1} |n\rangle$$

we obtain

$$\sum_{n=0}^{\infty} (\alpha c_n - c_{n+1} \sqrt{n+1}) |n\rangle = 0 \rightarrow \alpha c_n = c_{n+1} \sqrt{n+1}$$

We thus have a series of equations,

$$\begin{cases} c_1 = \alpha c_0 \\ c_2 = \frac{\alpha}{\sqrt{2}} c_1 = \frac{\alpha^2}{\sqrt{2}} c_0 \\ c_3 = \frac{\alpha}{\sqrt{3}} c_2 = \frac{\alpha^3}{\sqrt{6}} c_0 \end{cases}$$

So in general $c_n = \frac{\alpha^n}{\sqrt{n!}} c_0$. We finally obtain c_0 from the normalization condition $\langle \alpha | \alpha \rangle = 1$:

$$|c_0|^2 = \left(\sum_{m,n} \frac{\alpha^n (\alpha^*)^m}{\sqrt{n!m!}} \langle m | n \rangle \right)^{-1} = \left(\sum_n \frac{|\alpha|^{2n}}{n!} \right)^{-1} = e^{-|\alpha|^2}$$

The coherent state can thus be expressed in terms of the number states as

$$|\alpha\rangle = e^{-\frac{1}{2}|\alpha|^2} \sum_{n=0}^{\infty} \frac{\alpha^n}{\sqrt{n!}} |n\rangle$$

This also gives the probability for obtaining a particular energy level n when the system is in a quantum coherent state:

$$P_\alpha(n) = |\langle n | \alpha \rangle|^2 = e^{-\langle n \rangle} \frac{\langle n \rangle^n}{n!}$$

where we have used that the average number of photons is $\langle n \rangle = \langle \alpha | a^\dagger a | \alpha \rangle = |\alpha|^2$. Notice also that $\Delta n^2 = |\alpha|^2$. We thus see that the coherent states have a Poissonian distribution.

9.3.2 Non-Orthogonality

The coherent states $|\alpha\rangle$ do not form a proper basis, since they are eigenvectors of a non-hermitian operator. In particular they are not orthogonal (even if they are normalized by the choice of c_0):

$$\langle\alpha|\beta\rangle = \sum_{n,m} e^{-(|\alpha|^2+|\beta|^2)/2} (\alpha^*)^n \beta^m / \sqrt{n!m!} \langle n|m\rangle = e^{-(|\alpha|^2+|\beta|^2)/2} \sum_n (\alpha^*\beta)^n / n! = e^{-(|\alpha|^2+|\beta|^2-2\alpha^*\beta)/2}$$

Although not orthogonal, their superposition goes to zero as $|\alpha - \beta| \rightarrow 0$, since

$$|\langle\alpha|\beta\rangle|^2 = e^{-(|\alpha|^2+|\beta|^2-2\alpha^*\beta)/2} e^{-(|\alpha|^2+|\beta|^2-2\alpha\beta^*)/2} = e^{-|\alpha-\beta|^2}$$

Also, the set of coherent states is complete:

$$\int |\alpha\rangle \langle\alpha| d\alpha/\pi = \mathbb{1}$$

Because of this closure relation, any state can be written in terms of coherent state superposition, thus the coherent states form an overcomplete basis.

9.3.3 Uncertainty relationships

We have already seen that

$$\langle X \rangle = \sqrt{2} \operatorname{Re}[\alpha] = \frac{1}{\sqrt{2}}(\alpha + \alpha^*), \quad \langle P \rangle = -i\sqrt{2} \operatorname{Im}[\alpha] = \frac{i}{\sqrt{2}}(\alpha^* - \alpha)$$

Now consider the variance. We have:

$$\langle X^2 \rangle = \frac{1}{2} \langle \alpha | a^2 + (a^\dagger)^2 + aa^\dagger + a^\dagger a | \alpha \rangle = \frac{1}{2}(\alpha^2 + (\alpha^*)^2 + 2\alpha^*\alpha + 1)$$

and

$$\langle P^2 \rangle = \frac{1}{2} \langle \alpha | a^2 + (a^\dagger)^2 - aa^\dagger - a^\dagger a | \alpha \rangle = -\frac{1}{2}(\alpha^2 + (\alpha^*)^2 - 2\alpha^*\alpha - 1) = \frac{1}{2}[1 - (\alpha - \alpha^*)^2]$$

and for example:

$$\Delta X^2 = \frac{1}{2}[(\alpha^2 + (\alpha^*)^2 + 2\alpha^*\alpha + 1) - (\alpha + \alpha^*)^2] = \frac{1}{2}$$

We then have $\Delta X^2 = \frac{1}{2}$ and $\Delta P^2 = \frac{1}{2}$ so that the uncertainty relationship is saturated:

$$\Delta X \Delta P = \frac{1}{2}$$

The coherent state is thus a minimum uncertainty state (as the number states were).

? Question: What are the uncertainty relationship in terms of the variables x and p ?

$$\langle x \rangle = \sqrt{\frac{\hbar}{2m\omega}}(\alpha + \alpha^*), \quad \langle p \rangle = i\sqrt{\frac{\hbar m\omega}{2}}(\alpha - \alpha^*)$$

and

$$\begin{aligned} \langle x^2 \rangle &= \frac{\hbar}{2m\omega}(\alpha^2 + (\alpha^*)^2 + 2\alpha^*\alpha + 1) \\ \langle p^2 \rangle &= \frac{\hbar m\omega}{2}(\alpha^2 + (\alpha^*)^2 - 2\alpha^*\alpha - 1) \end{aligned}$$

We thus have the uncertainties for x and p and their uncertainty relationship

$$\Delta x^2 = \frac{\hbar}{2m\omega}, \quad \Delta p^2 = \frac{\hbar m\omega}{2} \rightarrow \Delta x \Delta p = \frac{\hbar}{2}$$

□

9.3.4 X-representation

We now want to obtain an expression for the wavefunction representing a coherent state, that is, we want to find the x-representation of the coherent state: $\langle x | \alpha \rangle$. For this, we start from the equation

$$\langle x | a | \alpha \rangle = \alpha \langle x | \alpha \rangle$$

as well as the explicit form of a in terms of x and p , $a = \frac{\sqrt{m\omega}}{\sqrt{2\hbar}}x + \frac{i}{\sqrt{2m\omega\hbar}}p$

$$\langle x | a | \alpha \rangle = \langle x | \left(\sqrt{\frac{m\omega}{2\hbar}}x + i\sqrt{\frac{1}{2\hbar m\omega}}p \right) | \alpha \rangle$$

Now we define the wavefunction in the x-representation $\langle x | \alpha \rangle = \psi_\alpha(x)$ and we remember that

$$\langle x | p | \psi \rangle = -i\hbar\partial_x\psi(x)$$

and $\langle x | p | x' \rangle = -i\hbar\partial_x\delta(x - x')$ to obtain:

$$\langle x | \left(\sqrt{\frac{m\omega}{2\hbar}}x + i\sqrt{\frac{1}{2\hbar m\omega}}p \right) | \alpha \rangle = \left(\sqrt{\frac{m\omega}{2\hbar}}x + \sqrt{\frac{\hbar}{2m\omega}}\frac{\partial}{\partial x} \right) \langle x | \alpha \rangle$$

Equating with the expression obtained before yields the differential equation:

$$\frac{\partial}{\partial x}\psi_\alpha(x) = \left(\sqrt{\frac{2m\omega}{\hbar}}\alpha - \frac{m\omega}{\hbar}x \right) \psi_\alpha(x)$$

with solution

$$\psi_\alpha(x) = Ae^{\sqrt{\frac{2m\omega}{\hbar}}\alpha x} e^{-\frac{m\omega}{2\hbar}x^2}$$

The constant A can be as usual obtained from the normalization condition:

$$\int_{-\infty}^{\infty} |\psi_\alpha(x)|^2 dx = 1 \rightarrow A = \left(\frac{m\omega}{2\pi\hbar} \right)^{1/4} e^{-\frac{\alpha^2}{2}}$$

The wavefunction representation is thus a Gaussian wavepacket:

$$\psi_\alpha(x) = \left(\frac{m\omega}{2\pi\hbar} \right)^{1/4} e^{-\frac{\alpha^2}{2}} e^{\sqrt{\frac{2m\omega}{\hbar}}\alpha x} e^{-\frac{m\omega}{2\hbar}x^2}$$

(not just a simple Gaussian, since α can be complex).

9.4 Phonons

We have introduced the harmonic oscillator as an interesting model because of the energy level structure it gives rise to. A second reason for its utility is that it can model many different systems around their equilibrium point. Here we show how it can be used to describe vibrations in a crystal lattice and how the quantum-mechanical description can be used to derive some of the lattice properties, such as its specific heat.

9.4.1 Harmonic oscillator model for a crystal

We consider a crystal formed by ions of mass M in a lattice (for simplicity we will consider a monoatomic, one-dimensional lattice).

The ion equilibrium positions are $R_n = nd$, with d the lattice constant, but the actual position of the ions is $r_n = R_n + x_n$, where x_n is the displacement from the equilibrium.

The interaction potential among the ions is

$$U = \frac{1}{2} \sum_{n,m} \mathcal{U}(r_n - r_m) = \frac{1}{2} \sum_{n,m} \mathcal{U}(R_n - R_m + x_n - x_m)$$

Assuming the displacement x_n is small, we can expand the potential as:

$$U = \frac{1}{2} \sum_{n,m} \mathcal{U}(R_n - R_m) + \frac{1}{2} \sum_{n,m} (x_n - x_m) \partial \mathcal{U}(R_n - R_m) + \frac{1}{4} \sum_{n,m} (x_n - x_m)^2 \partial^2 \mathcal{U}(R_n - R_m)$$

The first term $U_{eq} = \frac{1}{2} \sum_{n,m} \mathcal{U}(R_n - R_m)$ is the interaction potential at equilibrium, which is not of interest here. Consider the linear term:

$$\frac{1}{2} \sum_{n,m} (x_n - x_m) \partial \mathcal{U}(R_n - R_m) = \frac{1}{2} \sum_n x_n \sum_m [\partial \mathcal{U}(R_n - R_m) - \partial \mathcal{U}(R_m - R_n)] = \sum_n x_n \sum_m \partial \mathcal{U}(R_n - R_m)$$

The term $\sum_m \partial \mathcal{U}(R_n - R_m) = F_n$ is the total force exerted on the atom n by all the other atoms. When all the atoms are at equilibrium, this force must be zero, since there can be no net force at equilibrium. We are then left with only the second order term:

$$U = \frac{1}{2} \sum_{n,m} (x_n - x_m)^2 \partial_x^2 \mathcal{U}$$

If we assume that only neighboring ions interact, to second order, we retrieve an harmonic potential:

$$U = \frac{1}{2} K \sum_n (x_n - x_{n+1})^2$$

Then, the Hamiltonian can be written as:

$$\mathcal{H} = \sum_n \frac{p_n^2}{2M} + \frac{1}{2} K \sum_n (x_n - x_{n+1})^2$$

while the equation of motion for each oscillator is:

$$M \ddot{x}_n = - \frac{\partial U}{\partial x_n} = -K [2x_n - x_{n-1} - x_{n+1}]$$

9.4.2 Phonons as normal modes of the lattice vibration

The classical oscillator model is solved by guessing a solution in terms of waves (normal modes of the oscillation):

$$x_k(t) \propto e^{-ikR_n} e^{-i\omega_k t}$$

This solution is motivated by the translation symmetry of the lattice. We can check that the solution we guessed is the correct one, by inserting it in the equation of motion

$$M\ddot{x}_n = -\frac{\partial U}{\partial x_n} \rightarrow -M\omega_k^2 x_n = -K[2x_n - x_{n-1} - x_{n+1}] = -Kx_n[2 - e^{ikd} - e^{-ikd}]$$

Thus if we set $\omega_k^2 = \frac{K}{M}2[1 - \cos(kd)]$ the equation is verified. The relationship:

$$\omega(k) = 2\omega_0 \left| \sin\left(\frac{kd}{2}\right) \right|,$$

with $\omega_0 = \sqrt{K/M}$, is called the **dispersion** relation, which describes the frequency (energy) of the wave as a function of the wavelength.

This solution describes waves propagating in the chain with *phase* velocity $c = \omega/k$ and *group* velocity $v_g = \frac{\partial \omega}{\partial k}$ (the speed of sound in the given material). At small k the two velocities are equal, but for large k (small spacing between ions) we have $v_g \rightarrow 0$.

We can now turn to the corresponding quantum-mechanical model, by replacing the position and momentum coordinates in the Hamiltonian by the corresponding operators:

$$\mathcal{H} = \sum_n \frac{p_n^2}{2M} + \frac{1}{2}K \sum_n (x_n - x_{n+1})^2$$

Inspired by the classical solution, we also look for solutions (i.e. eigenvectors that diagonalize the Hamiltonian) in terms of waves. Then in this basis, x_n and p_n will be expressed as linear combinations of waves with different wavevectors, e.g.:

$$x_n = \frac{1}{\sqrt{N}} \sum_k X_k e^{ikR_n}$$

We then rewrite the operator X_k (and P_k) in terms of the creation and annihilation operators a_k, a_k^\dagger :

$$x_n = \frac{1}{\sqrt{NM}} \sum_k \frac{1}{\sqrt{2\omega_k}} \left(a_k e^{ikR_n} + a_k^\dagger e^{-ikR_n} \right)$$

and

$$p_n = -i\sqrt{\frac{M}{N}} \sum_k \sqrt{\frac{\omega_k}{2}} \left(a_k e^{-ikR_n} - a_k^\dagger e^{ikR_n} \right)$$

Similar to the solution for the simple h.o. we want to verify that the operators a_k, a_k^\dagger diagonalize the Hamiltonian. We thus first calculate the kinetic energy, $T = \sum_n \frac{p_n^2}{2M}$.

$$p_n^2 = -\frac{M}{N} \sum_{k,h} \sqrt{\frac{\omega_k \omega_h}{4}} \left[a_k^\dagger a_h^\dagger e^{-i(k+h)R_n} - a_k^\dagger a_h e^{-i(k-h)R_n} + a_k a_h e^{i(k+h)R_n} - a_k a_h^\dagger e^{i(k-h)R_n} \right]$$

We then take the sum over n , remember that $R_n = nd$ where n is an integer and d the distance between two ions, and invert the order of the sums:

$$T = -\frac{1}{4N} \sum_{k,h} \sqrt{\omega_k \omega_h} \left[a_k^\dagger a_h^\dagger \sum_n e^{-i(k+h)R_n} - a_k^\dagger a_h \sum_n e^{-i(k-h)R_n} + \dots \right]$$

The sums $\sum_n e^{-i(k+h)R_n} = \sum_n e^{-i(k+h)nd}$ are zero unless the exponent argument $h + k$ is zero:

$$T = -\frac{1}{4N} \sum_{k,h} \sqrt{\omega_k \omega_h} \left[a_k^\dagger a_h^\dagger \delta_{k,-h} - a_k^\dagger a_h \delta_{k,h} + \dots \right]$$

We thus obtain:

$$T = -\frac{1}{4} \sum_k \omega_k \left[a_k^\dagger a_{-k}^\dagger - a_k^\dagger a_k + a_k a_{-k} - a_k a_k^\dagger \right]$$

We then calculate the potential energy. First we calculate $x_n - x_{n+1}$:

$$\begin{aligned} x_n - x_{n+1} &= \frac{1}{\sqrt{NM}} \sum_k \frac{1}{\sqrt{2\omega_k}} \left(a_k e^{ikR_n} + a_k^\dagger e^{-ikR_n} - a_k e^{ikR_{n+1}} - a_k^\dagger e^{-ikR_{n+1}} \right) \\ &= \frac{1}{\sqrt{NM}} \sum_k \frac{1}{\sqrt{2\omega_k}} \left(a_k e^{ikR_n} (1 - e^{ikd}) + a_k^\dagger e^{-ikR_n} (1 - e^{-ikd}) \right) \\ &= \frac{1}{\sqrt{NM}} \sum_k \frac{-2i}{\sqrt{2\omega_k}} \sin\left(\frac{kd}{2}\right) \left(a_k e^{ik(R_n+d/2)} + a_k^\dagger e^{-ik(R_n+d/2)} \right) \end{aligned}$$

The potential energy is then:

$$U = \frac{1}{2} K \sum_n (x_n - x_{n+1})^2 = -\frac{K}{2NM} \sum_k \frac{4 \sin^2\left(\frac{kd}{2}\right)}{2\omega_k} \left[-a_k^\dagger a_{-k}^\dagger - a_k^\dagger a_k - a_k a_{-k} - a_k a_k^\dagger \right]$$

(where we used the same identities for the sum of exponential and the fact that $\sin\left(\frac{kd}{2}\right) \sin\left(\frac{hd}{2}\right) \delta_{k,-h} = \sin^2\left(\frac{kd}{2}\right)$). By summing the potential and kinetic energy and imposing as before:

$$\omega_k = 2\omega_0 \left| \sin\left(\frac{kd}{2}\right) \right|$$

(with $\omega_0^2 = \frac{K}{M}$) we can simplify the Hamiltonian to:

$$\mathcal{H} = \frac{1}{2} \sum_k \omega_k \left(a_k^\dagger a_k + a_k a_k^\dagger \right) = \sum_k \omega_k \left(a_k^\dagger a_k + \frac{1}{2} \right)$$

The operators a_k, a_k^\dagger do diagonalize the Hamiltonian. The number operator $n_k = a_k^\dagger a_k$ describes the excitation number of a normal mode of the ion vibration. Instead of talking of excitations, we can introduce quasi particles, called **phonons**. The number of phonons then corresponds to the number of excitations. Thus the operators a_k, a_k^\dagger can create or annihilate a phonon of mode k .

9.4.3 Thermal energy density and Specific Heat

We want to first calculate the thermal energy density $u = E/V$ and then the specific heat, $c_V = \frac{\partial u}{\partial T}$ for a crystal at thermal equilibrium.

The thermal energy is given by the lattice vibration. Thus we want to calculate:

$$\langle E \rangle = \text{Tr} \{ \rho \mathcal{H} \}$$

with the Hamiltonian given above. The system in thermal equilibrium is described by the usual distribution:

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

Notice that $\langle E \rangle = -\frac{\partial \ln Z}{\partial \beta}$. We thus need to calculate the partition function. Computing the trace in the number state basis, we have:

$$\begin{aligned} Z &= \text{Tr} \left\{ \exp \left[-\beta \sum_k \omega_k \left(a_k^\dagger a_k + \frac{1}{2} \right) \right] \right\} = \text{Tr} \left\{ \prod_k \exp \left[-\beta \omega_k \left(a_k^\dagger a_k + \frac{1}{2} \right) \right] \right\} \\ &= \prod_k e^{-\beta \omega_k / 2} \sum_n (e^{-\beta \omega_k})^n = \prod_k \frac{e^{-\beta \omega_k / 2}}{1 - e^{-\beta \omega_k}} \end{aligned}$$

Taking the derivative of the logarithm, we find:

$$u = -\frac{1}{V} \partial_\beta (\ln Z) = \frac{1}{V} \sum_k \frac{\omega_k}{2} \coth \left(\frac{\omega_k \beta}{2} \right)$$

This can also be written in terms of the average phonon number for the mode k ,

$$\begin{aligned} \langle n_k \rangle &= n(k) = \text{Tr} \left\{ a_k^\dagger a_k \rho \right\} = [e^{\beta \omega_k} - 1]^{-1} : \\ u &= \frac{1}{V} \sum_k \omega_k \left[n(k) + \frac{1}{2} \right] \end{aligned}$$

The specific heat is then:

$$c_V = \frac{\partial u}{\partial T} = \sum_k \frac{\omega_k^2}{4V k_b T^2 \sinh^2 \left(\frac{\omega_k}{2k_b T} \right)}$$

Note that at high temperature (small β) this is approximated by $c_V \approx \sum_k \frac{k_b}{V} = N \frac{k_b}{V}$, which is the classical Dulong-Petit law, stating that the specific heat is independent of the temperature and given by the density $n = N/V$ and the system's dimension D , $c_V = D n k_b$.

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