

2. The Quantum Harmonic Oscillator

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2.1 The Dawn of the Quantum Physics

We have in the former chapter discussed the classical theory of the harmonic oscillator. The results from the theory are in good agreement with measured facts as long as the oscillator is macroscopic, that is, of substantial size. When the oscillator is of atomic size, as it is in the case of the diatomic molecule, the agreement with experiments is not good at all. For example we can in the classical theory have any energy, and also very small oscillations where energy is nearly zero, and the oscillator can entirely stand still in zero oscillation energy. Oscillators of molecular size do not at all follow these classical results, which became clear due time. The lowest possible oscillation energy is in fact greater than zero, and the possible oscillation energies over that lowest "zero-point energy" come in discrete steps.

A theoretical problem appeared in the classical theory of radiation, which more or less initiated the quantum era. In classical physics can any amount of energy go with all frequencies, also very high frequencies. And when the oscillation frequency increases then the energy increases even more. Because there are tremendously many small molecular oscillators in the world, this would lead to that most of the energy available in the world would at end be absorbed by the molecular oscillators in very high frequencies. This situation was catastrophic, not for the world, such energy absorption into high frequencies was not observed at all, but it was catastrophic for the classical physics, because the prediction was terribly wrong. It was called "the ultraviolet catastrophe" because the frequency of ultraviolet light was the highest known at that time (in about year 1900).

In reality it was found that energy that goes to higher frequencies increases first rapidly, but reaches soon a maximum and then gradually decreases again. The maximum of the energy curve depends on the temperature. This is called the "black body" radiation curve. (An "absolutely black body" is a non-colored idealized object, an aid for theoretical calculations, but real objects in most part behave very similarly.) Investigation of this radiation curve led Max Planck (German physicist, 1858 - 1947) to suggest a solution in form of a quantization rule.

Planck's rule was first assumed only as tentative, it was based on fitting theoretical curve forms on experimental results. It says: energy E of an oscillator comes in bunches bound to the frequency ν by a constant h :

$$E = h \nu \tag{2.1}$$

This Planck's constant is very small, which explains why energy in macroscopic oscillators appear to be (nearly) continuous. It is necessary for energy to reach the amount $E=h$ in order to be absorbed (or emitted).

Because this amount, even if it is very small for low frequencies, becomes substantially high for higher frequencies, it makes it easier for energy go in lower frequencies, and exceedingly difficult for higher energies. Consequently the absorption rate goes first up and then down again after a certain maximum. The "catastrophe" is thus avoided. What is said of absorption also holds other way round, for emission of energy: big chunks of energy are not so easy to get rid off, and very small amounts do not give off much effect, so the maximum energy emission rate is somewhere mid between. By making the assumption (2.1) and substituting it to already known formulas of energy density in statistical arrays of oscillators, Planck found (he was an expert of statistical physics) the formula now called the "Planck's radiation formula":

$$E_{\text{density}} = \frac{8 \pi h}{c^3} \frac{\nu^3}{e^{h\nu/kT} - 1} \tag{2.2}$$

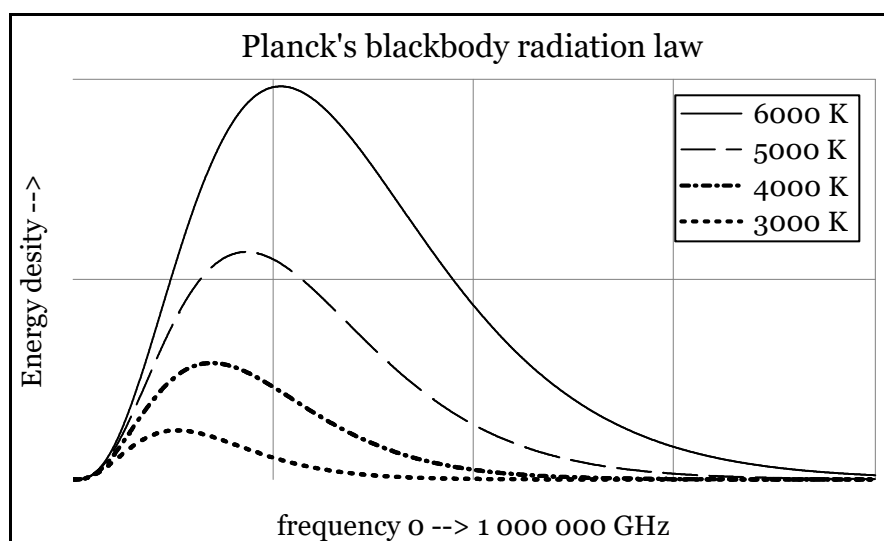
It gives the energy density per unit volume and frequency for a black body object of surface temperature T in degrees Kelvin (K, degrees from absolute zero -273.16 °C).

We have here the constants:

Planck's constant $h = 6.620688 \times 10^{-34} \text{ J s}$

velocity of light $c = 2.99792458 \times 10^8 \frac{\text{m}}{\text{s}}$

and Boltzmann constant $k = 1.380650 \times 10^{-23} \frac{\text{J}}{\text{K}}$



The plot above shows energy density as it varies with increasing frequency. The curves are for different blackbody temperatures from 3000 K to 6000 K. They are also called the "blackbody radiation curves" for the given temperatures. (It is not unusual drawing them with wavelength as argument, which turns them left to right.)

The formula (2.2) has found to be correct, although it was originally based on semi-classical and not even entirely correct assumptions. This Planck energy curve is continuous, although strictly bound to the frequency. According to Planck's rule energy is quantized in that extent that radiation of a certain frequency can only appear in packets of certain amounts of energy.

Next stage of the quantum idea was due to Albert Einstein, who explained the photoelectric effect using the Planck's rule (2.1). Einstein was the first to set forward the concept "quantum of light" or "quantum of energy". Now it became clear that Planck's law was not a property of the oscillators, but a property of the radiation itself (and we are still talking about electromagnetic radiation, the early quantum mechanics was only concerned on that). Nevertheless, there is also a quantization of the oscillators themselves, so that they can only absorb, and emit, certain distinct levels of energy, as will be seen below.

Although the energy quantization was first only a tentative idea, it was soon realized that quantum physics was here to stay. One thing logically lead to an other, and in end most of the physics got to be rewritten into the modern quantum language. Not only is energy quantized, but almost everything in physics.

2.2 The Simple Quantum Harmonic Oscillator

Consider an microscopic one-dimensional harmonic oscillator e.g. a diatomic molecule. We take from the classical case the basic constituents. We need the reduced mass m , and the angular velocity, which is simply related to the oscillation frequency $\omega = 2\pi \nu$, and in stead of velocity we are going to use the linear momentum $p = m v$.

$$\text{Potential energy:} \quad V(x) = \frac{1}{2} k x^2 = \frac{1}{2} m \omega^2 x^2 \quad (2.3)$$

$$\text{Kinetic energy:} \quad T = \frac{1}{2} m v^2 = \frac{p^2}{2m} \quad (2.4)$$

Hamiltonian function, from the total energy:

$$H(p, x) = T + V = \frac{p^2}{2m} + \frac{1}{2} m \omega^2 x^2 \quad (2.5)$$

2.3 The Correspondence Principle

We now go over to a quantum mechanical system using the "correspondence principle", which means that going from macroscopic to microscopic objects, the numerical algebra of classical mechanics is taken over by operator algebra in quantum mechanics. These operators are differential operators. Operator algebra appears sometimes also in classical mechanics. This kind of mathematical tools are often used in solving of differential equations, and also the equation (1.8) of the harmonic oscillator is a differential equation. We will now construct quantum operators using the correspondence principle:

1. The position x becomes the position operator, which simply consist of a multiplication with the value x . This is a very elementary operator, but formally we need to call it an operator.

$$\mathbf{x} = x \quad (2.6)$$

2. The linear momentum p becomes the differential operator.

$$\mathbf{p} = -i \hbar \frac{\partial}{\partial x} \quad (2.7)$$

The mathematical logic of operators needs to use imaginary numbers, i denotes the imaginary unit: $i = \sqrt{-1}$. It is customary to use the "h-bar" symbol, the Dirac constant, in stead of Plank's constant h . This shortens up the expressions somewhat in many cases

$$\hbar = \frac{h}{2\pi} \quad (2.8)$$

3. The Hamiltonian function H becomes now the Hamiltonian operator \mathbf{H} :

$$\mathbf{H} = \frac{\mathbf{p}^2}{2m} + \frac{1}{2} m \omega^2 \mathbf{x}^2 = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + \frac{1}{2} m \omega^2 x^2 \quad (2.9)$$

The operators operate on a function, of historical reasons called the "wave equation". Formally mathematically it is a generating function, because operating on it gives the physical quantities the operators represent. The correspondence principle and going over to differential operators is not that far-fetched as it might look at first sight, also the classical theoretical physics could be, and had been, formulated using operators and generating functions. These two operators above obey canonical correspondence principle (position and linear momentum are what is called "canonical conjugates" in the classical theory):

$$\begin{aligned}
 (\mathbf{x} \mathbf{p} - \mathbf{p} \mathbf{x}) \Psi &= \mathbf{x} \left(-i \hbar \frac{\partial \Psi}{\partial \mathbf{x}} \right) - \left[-i \hbar \frac{\partial}{\partial \mathbf{x}} (\mathbf{x} \Psi) \right] = \dots \\
 \dots &= -i \hbar \mathbf{x} \frac{\partial \Psi}{\partial \mathbf{x}} + i \hbar \mathbf{x} \frac{\partial \Psi}{\partial \mathbf{x}} \Psi + i \hbar \frac{\partial \mathbf{x}}{\partial \mathbf{x}} \Psi = i \hbar \Psi
 \end{aligned}
 \tag{2.10}$$

and so the commutator (customarily denoted with the square parenthesis) gives

$$[\mathbf{x}, \mathbf{p}] = \mathbf{x} \mathbf{p} - \mathbf{p} \mathbf{x} = i \hbar
 \tag{2.11}$$

2.4. The Schrödinger Equation

Erwin Schrödinger (German physicist 1887 - 1961) was the first to suggest a method setting up the quantization condition. If we have a system that does not change in time (other than periodic changed, that is oscillations) we have the time-independent form of the Schrödinger equation (otherwise there is a time derivative of Ψ too in the equation). The method consists of using the Hamiltonian operator and claiming that there should be a constant, the total energy, that gives same result as operating with the Hamiltonian operator. The Hamiltonian operator \mathbf{H} is the one with the property that it produces the energy values E in that way, by operating on the wave-function.

$$\mathbf{H} \Psi = E \Psi
 \tag{2.12}$$

The Schrödinger method always gives a differential equation to solve. The Schrödinger equation for the harmonic oscillator is a differential equation in such time-independent form:

$$-\frac{\hbar^2}{2m} \frac{\partial^2 \Psi}{\partial x^2} + \frac{1}{2} m \omega^2 x^2 \Psi = E \Psi
 \tag{2.13}$$

where E is the oscillators total energy. This is a second grade differential equation, and such equations also appear in classical theory of wave movement (like waves in water). Of this formal reason (it is no more mystical) the function Ψ is called the "wave function".

The differential equation (2.13) can be solved using some standard method for solving of differential equations, like the power series method (found in mathematical books, it is interesting mathematically but somewhat tedious, therefore only the result is given here). The resulting quantum mechanical "wave function", is a quantized function, meaning that it depends on a parameter that can only take a discrete set of values (integers 0,1, ... in this case). The wave function for the harmonic oscillator becomes (this is in normalized form)

$$\Psi_n(x) = A e^{-\frac{(\alpha x)^2}{2}} H_n(\alpha x)
 \tag{2.14}$$

where
$$\alpha = \sqrt{\frac{m \omega}{\hbar}} \tag{2.15}$$

and the normalizing constant is (explained below)

$$A = \sqrt{\frac{\alpha}{2^n n! \sqrt{\pi}}} \tag{2.16}$$

and the Hermite polynomial which appears in the expression (2.14) is defined as

$$H_n(x) = (-1)^n e^{x^2} \frac{d^n}{dx^n} (e^{-x^2}) \tag{2.17}$$

(Not to be confused with the Hamiltonian, there are many H:s in different forms here.)

It is a polynomial function which is part of the function Ψ , which we in (2.14) denote Ψ_n , because there is more than one possible solution. In fact there is a solution corresponding every nonnegative integer n. Because n can only take discrete values, integers, it is a quantum number. For every possible value for n there is a corresponding quantized energy (not proved here, but we do it later on):

$$E_n = \left(\frac{1}{2} + n \right) \hbar \omega \quad n = 0, 1, 2, \dots \tag{2.18}$$

2.5. Heisenberg's Uncertainty Principle

Werner Heisenberg (German physicist 1901-1976) developed an other method (independently and somewhat earlier than Schrödinger) called the matrix method. Heisenberg set up an equation with the formal appearance like (2.12), but the operator there is a matrix operator \mathbf{H} that operates a vector Ψ . A Heisenberg matrix is a formal mathematical object, a quadratic table of numbers, with special multiplication rules, that operating on vectors gives the desired quantized energy values. This kind of matrix equation is called an eigenvalue (German for own-value or specific value) equation. The corresponding vector Ψ is called the **eigenvector** or **state vector**. Matrices were used before Heisenberg in solving of groups of linear equations, but Heisenberg, not knowing of it, in effect reinvented the matrices for quantum mechanical purposes. (Some matrices are given here in the last chapter.)

It was soon found out that there were a logical connection between Schrödinger's and Heisenberg's methods. It was possible to express the differential operators as matrices in respect to the energy values in similar manners, and the results from the both theories were identical. These two methods therefore are now seen as two sides of one and the same mathematical reality. They are still, of historical reasons, often called the "wave mechanics" (Schrödinger's) and the "matrix mechanics" (Heisenberg's). This is also called the "complementarily principle", or the "wave-matrix-complementarily".

The commutation rule (2.11) also holds for matrix operators. Starting from it Heisenberg deduced the uncertainty relations

$$\Delta p \Delta x \geq \frac{1}{2} \hbar \tag{2.19}$$

$$\Delta E \Delta t \geq \frac{1}{2} \hbar \tag{2.20}$$

This leads to the probabilistic nature of predicted measurements in quantum physics. A measurement is given as an expectation value. In the commonplace mathematical statistics an expectation value is defined as the integral:

$$\langle f(x) \rangle = \int_{x_0}^{x_1} f(x) P(x) dx \quad (2.21)$$

where $P(x)$ is the probability distribution function for the statistical variable x .

This is for real valued functions P . In quantum mechanics we have in stead the complex valued wave function Ψ , and a physical "observable" represented by an operator $f(x)$. The expectation value, which still must be real valued:

$$\langle f(x) \rangle = \int_{x_0}^{x_1} \Psi^* f \Psi dx \quad (2.22)$$

Here Ψ^* is the complex conjugate of Ψ .

The expectation values for position, momentum, and energy become respectively:

$$\langle x \rangle = \int_{x_0}^{x_1} \Psi^* x \Psi dx = \int_{x_0}^{x_1} \Psi^* \cdot x \Psi dx = \int_{x_0}^{x_1} x |\Psi|^2 dx \quad (2.23)$$

$$\langle p \rangle = \int_{x_0}^{x_1} \Psi^* p \Psi dx = \int_{x_0}^{x_1} \Psi^* \cdot \frac{\hbar}{i} \frac{\partial}{\partial x} \Psi dx \quad (2.24)$$

$$\langle E \rangle = \frac{(\langle p \rangle)^2}{2m} = \int_{x_0}^{x_1} \Psi^* p^2 \Psi dx = \int_{x_0}^{x_1} \Psi^* \cdot \frac{-\hbar^2}{2m} \frac{\partial^2}{\partial x^2} \Psi dx \quad (2.25)$$

Integrated over the values of separation x from the smallest possible value x_0 to the greatest value x_1 , which (formally mathematically) might limit to infinity. The definition (2.21) from mathematical statistics is a special case of the quantum mechanical (2.22), where the operation is simply a multiplication with a real number, like it is in (2.23). We see then that the probability distribution corresponds to the square of the wave function

$$P(x) = \Psi^* \Psi = |\Psi|^2 \quad (2.26)$$

Such a distribution must be normalized to one, saying that the distribution covers all possible cases, but no more than that. Also the normalizing constant (2.16) above was based to such condition, that is, if the condition below is not met the function is multiplied with a suitable constant in order to make it meet the condition:

$$\int_{x_0}^{x_1} \Psi^* \Psi dx = 1 \quad (2.27)$$

This makes clear the point that the wave function Ψ (more precisely, its square) is an expression of the probability distribution for the measured physical value.

In the Heisenberg's formulation of quantum mechanics Ψ is a (formal mathematical) vector, the quantum state vector, and probability density is the square length of this (formal) vector. Note also that the mathematical structure of quantum mechanics is that of a linear algebra, a general mathematical theory that can be used as well for matrix and vector calculus as for solving of many kind differential equations.

2.7. Dirac's Bra-Ket Formulation

Dirac (English physicist 1902 - 1984) set forward a mathematical method that combined Schrödinger's and Heisenberg's methods into one logical structure. For that purpose he invented new mathematical symbols, now known as Dirac's bra-ket formulation. It is today the standard formulation of quantum physics. Starting again from the Schrödinger equation, the quantified solutions and energies written in the equation:

$$\frac{\hbar^2}{2m} \frac{\partial^2 \Psi_n}{\partial x^2} + \frac{1}{2} m \omega^2 x^2 \Psi_n = E_n \Psi_n \quad (2.28)$$

The Schrödinger equation can be represented by operator eigenstate equation. Because we are dealing with energies, we have here the Hamiltonian operator \mathbf{H} , which has energies as eigenvalues. Every one of the wave function solutions corresponds to a state vector in a Hilbert space of functions (a kind of linear algebra). Using the Dirac "bra-ket" notation, written as an eigenvector "ket" $|n\rangle$.

$$\mathbf{H} |n\rangle = E_n |n\rangle \quad (2.29)$$

The wave-function now expresses the probability density function for finding an oscillator with energy state n at position value x :

$$\Psi_n(x) = \langle x | n \rangle \quad (2.30)$$

Note: expressions in form $\langle x | y \rangle$, like that in (2.30) can be treated as inner products in a formal mathematical function space, called Hilbert's space.

There is a freedom what is written inside the Dirac-brackets. It depends what is expected to be informative enough for the reader. In elementary books $|\Psi_n\rangle$ is often used in stead of $|n\rangle$.

The state ket corresponding to the ground state wave function Ψ_0 should be written $|0\rangle$, the next state wave function Ψ_1 corresponds to ket $|1\rangle$, and so on...

The energy eigenvalues for the Hamiltonian operator are

$$E_n = E_0 + n \hbar \omega \quad n = 0, 1, 2, \dots \quad (2.31)$$

where the lowest energy

$$E_0 = \frac{\hbar \omega}{2} \quad (2.32)$$

is the "ground energy" or "zero-point energy": a quantum oscillator always oscillates with a minimum of this energy, it can never "freeze" and stand still in zero energy.

2.8. The Ladder Operator Method

The harmonic oscillator is instructive in many ways. It can be used in demonstrating the most of the mathematical toolbox commonly used in quantum mechanical calculations. A somewhat more abstract but very effective way in solving the problem of eigenstates and eigenvalues is using ladder operators. This formulation has also the advantage that it can be further generalized to Quantum Electrodynamics, and other quantum field theories.

Define an operator expressed in form:

$$\mathbf{a} = A (\mathbf{x} + i B \mathbf{p}) \quad (2.33)$$

where the two constants are defined:

$$A = \sqrt{\frac{m \omega}{2 \hbar}} = \frac{\alpha}{\sqrt{2}} \quad (2.34)$$

$$B = \frac{1}{m \omega} = \frac{1}{\hbar^2 \alpha^2} \quad (2.35)$$

As for a complex number $z = a + i b$ there is the complex conjugate $z^* = a - i b$, quite similarly for an operator there is a corresponding "Hermitian adjoint" or "Hermitian conjugate". It is defined as the corresponding operator that has its eigenvalues complex conjugate to the original one. It can also be effectively defined using the Dirac bra-ket (Q is a complex number):

$$\langle Q x | y \rangle = \langle x | Q^* y \rangle \quad (2.36)$$

For an operator given in form (2.33) the Hermitian conjugate can be written

$$\mathbf{a}^+ = A (\mathbf{x} - i B \mathbf{p}) \quad (2.37)$$

Summing of the operator and its adjoint gives

$$\mathbf{a}^+ + \mathbf{a} = A (\mathbf{x} + i B \mathbf{p}) + A (\mathbf{x} - i B \mathbf{p}) = 2 A \mathbf{x} \quad (2.38)$$

so we see that the displacement operator is now

$$\mathbf{x} = \frac{1}{2 A} (\mathbf{a}^+ + \mathbf{a}) = \sqrt{\frac{\hbar}{2 m \omega}} (\mathbf{a}^+ + \mathbf{a}) \quad (2.39)$$

and subtracting them

$$\mathbf{a}^+ - \mathbf{a} = A (\mathbf{x} + i B \mathbf{p}) - A (\mathbf{x} - i B \mathbf{p}) = -i 2 A B \mathbf{p} \quad (2.40)$$

so we see that the momentum operator is

$$\mathbf{p} = \frac{i}{2 A B} (\mathbf{a}^+ - \mathbf{a}) = \sqrt{\frac{\hbar m \omega}{2}} (\mathbf{a}^+ - \mathbf{a}) \quad (2.41)$$

Remembering that the operators do not commute, we get

$$\begin{aligned} \mathbf{a}^+ \mathbf{a} &= A (\mathbf{x} - i B \mathbf{p}) A (\mathbf{x} + i B \mathbf{p}) = A^2 (\mathbf{x}^2 + i B \mathbf{x} \mathbf{p} - i B \mathbf{p} \mathbf{x} + B^2 \mathbf{p}^2) = \dots \\ &\dots = A^2 (\mathbf{x}^2 + B^2 \mathbf{p}^2 + i B \cdot [\mathbf{x}, \mathbf{p}]) = A^2 \mathbf{x}^2 + A^2 B^2 \mathbf{p}^2 - A^2 B \hbar \end{aligned} \quad (2.42)$$

and

$$\begin{aligned} \mathbf{a} \mathbf{a}^+ &= A (\mathbf{x} + i B \mathbf{p}) A (\mathbf{x} - i B \mathbf{p}) = A^2 (\mathbf{x}^2 - i B \mathbf{x} \mathbf{p} + i B \mathbf{p} \mathbf{x} + B^2 \mathbf{p}^2) = \dots \\ &\dots = A^2 (\mathbf{x}^2 + B^2 \mathbf{p}^2 - i B \cdot [\mathbf{x}, \mathbf{p}]) = A^2 \mathbf{x}^2 + A^2 B^2 \mathbf{p}^2 + A^2 B \hbar \end{aligned} \quad (2.43)$$

It is easily seen from (2.42) and (2.43) that we have for the constant expressions above

$$A^2 = \frac{m \omega}{2 \hbar} \quad A^2 B^2 = \frac{1}{2 \hbar m \omega} \quad A^2 B = \frac{1}{2 \hbar} \quad (2.44)$$

and substituting these we get

$$\mathbf{a}^+ \mathbf{a} = \frac{m \omega}{2 \hbar} \mathbf{x}^2 + \frac{1}{2 \hbar m \omega} \mathbf{p}^2 - \frac{1}{2} \quad (2.45)$$

$$\mathbf{a} \mathbf{a}^+ = \frac{m \omega}{2 \hbar} \mathbf{x}^2 + \frac{1}{2 \hbar m \omega} \mathbf{p}^2 + \frac{1}{2} \quad (2.46)$$

so the commutator becomes

$$[\mathbf{a}, \mathbf{a}^+] = \mathbf{a} \mathbf{a}^+ - \mathbf{a}^+ \mathbf{a} = 1 \quad (2.47)$$

Now, from the first of the products we get

$$\mathbf{a}^+ \mathbf{a} = \frac{1}{\hbar \omega} \left(\frac{1}{2} m \omega^2 \mathbf{x}^2 + \frac{\mathbf{p}^2}{2 m} \right) - \frac{1}{2} = \frac{1}{\hbar \omega} \mathbf{H} - \frac{1}{2} \quad (2.48)$$

So we can write the Hamiltonian in form

$$\mathbf{H} = \hbar \omega \left(\mathbf{a}^+ \mathbf{a} + \frac{1}{2} \right) \quad (2.49)$$

If the energy eigenstate (to the Hamiltonian operator) with energy E_n is written as the Dirac "ket":

$|n\rangle$, then operating it with the ladder operator \mathbf{a} is written $\mathbf{a} |n\rangle$, and the adjoint of this is expressed as operating the corresponding Dirac "bra" from right with the adjoint operator: $\langle n | \mathbf{a}^+$.

Note: there is a mathematical flaw in the Dirac bra-ket formulation, because the direction of the operation is not explicitly given. This is mostly not a problem, because in most cases the operators of interest are self-adjoint (Hermitian): $\langle x | A | y \rangle = \langle A x | y \rangle = \langle x | A | y \rangle$, and the operation can be performed in either way. But when the operator is not self-adjoint it might lead to confusion.

An inner product of vectors v and u , operated by X and Y , is generally written in the "bra-ket" formulation:

$$(X v, Y u) = \langle v | X^\dagger Y | u \rangle \quad (2.50)$$

For the inner product of the operation above with itself we have

$$(\mathbf{a} | n \rangle, \mathbf{a} | n \rangle) = \langle n | \mathbf{a}^\dagger \mathbf{a} | n \rangle \geq 0 \quad (2.51)$$

Using the result shown earlier we can write

$$\langle n | \frac{1}{\hbar \omega} \mathbf{H} - \frac{1}{2} | n \rangle = \left(\frac{1}{\hbar \omega} E_n - \frac{1}{2} \right) \langle n | n \rangle = \frac{E_n}{\hbar \omega} - \frac{1}{2} \geq 0 \quad (2.52)$$

so that
$$E_n \geq \frac{\hbar \omega}{2} \quad (2.53)$$

For the zero ket $|0\rangle$ (the ground state), we have the lowest energy

$$E_0 = \frac{\hbar \omega}{2} \quad (2.54)$$

Next calculate the commutators with Hamiltonian

$$\begin{aligned} [\mathbf{H}, \mathbf{a}] &= \mathbf{H} \mathbf{a} - \mathbf{a} \mathbf{H} = \left[\left(\mathbf{a}^\dagger \mathbf{a} + \frac{1}{2} \right) \mathbf{a} - \mathbf{a} \left(\mathbf{a}^\dagger \mathbf{a} + \frac{1}{2} \right) \right] \hbar \omega = \dots \\ &\dots = \left(\mathbf{a}^\dagger \mathbf{a} \mathbf{a} + \frac{1}{2} \mathbf{a} - \mathbf{a} \mathbf{a}^\dagger \mathbf{a} - \frac{1}{2} \mathbf{a} \right) \hbar \omega = -\hbar \omega [\mathbf{a}, \mathbf{a}^\dagger] \mathbf{a} = -\hbar \omega \mathbf{a} \end{aligned} \quad (2.55)$$

And similarly can be found

$$[\mathbf{H}, \mathbf{a}^\dagger] = \hbar \omega \mathbf{a}^\dagger \quad (2.56)$$

When $\mathbf{a} | n \rangle$ is not a zero ket

$$\begin{aligned} \mathbf{H}(\mathbf{a} | n \rangle) &= (\mathbf{H} \mathbf{a}) | n \rangle = (\mathbf{H} \mathbf{a} - \mathbf{a} \mathbf{H} + \mathbf{a} \mathbf{H}) | n \rangle = \dots \\ &\dots = ([\mathbf{H}, \mathbf{a}] + \mathbf{a} \mathbf{H}) | n \rangle = (-\hbar \omega \mathbf{a} + \mathbf{a} E_n) | n \rangle = (E_n - \hbar \omega) (\mathbf{a} | n \rangle) \end{aligned} \quad (2.57)$$

Similarly

$$\mathbf{H}(\mathbf{a}^\dagger | n \rangle) = (E_n + \hbar \omega) (\mathbf{a}^\dagger | n \rangle) \quad (2.58)$$

So, taking an energy eigenstate with energy eigenvalue E_n

- the operator \mathbf{a} acting on it lowers it to the nearest lower energy state
- correspondingly the adjoint operator \mathbf{a}^\dagger rises it to the nearest higher energy state

We say that

\mathbf{a} is lowering or annihilation operator, sometimes also written as \mathbf{a}_-
 \mathbf{a}^+ is rising or creation operator, often also written as \mathbf{a}^\dagger

Note: the lowering operator operating on the ground state ket (if it is mathematically allowed) would leave "an empty state", or "empty" ket, meaning "no physical system present", or a "physical vacuum".

$$\mathbf{a} |0\rangle = | \rangle \tag{2.59}$$

The ground state ket $|0\rangle$ itself is not an empty state, but corresponds to the lowest quantum energy state, sometimes called "quantum vacuum", where we have

$$\mathbf{H} |0\rangle = E_0 |0\rangle \tag{2.60}$$

The zero-point (or ground state) energy

$$E_0 = \frac{\hbar \omega}{2} > 0 \tag{2.61}$$

is the energy-eigenvalue corresponding the ground state.

The Number Operator and the Fock-Space

The number operator is often a practical tool, and crucial later in understanding particle fields. It is defined

$$\mathbf{N} = \mathbf{a}^+ \mathbf{a} \tag{2.62}$$

Also important tool is the Fock-space. It is a formal space (Hilbert space) where the base vectors are all the quantum states:

$$|0\rangle, \dots, |n\rangle \tag{2.63}$$

The 0-ket represents the ground state vector, then come the higher quantum states that all represent an independent base vector in the Fock-space. They are the eigenstates of the number operator:

$$\mathbf{N} |n\rangle = n |n\rangle \tag{2.64}$$

The lowering (annihilation) and the rising (creation) operators change these number states down or up. It is easily shown that

$$\mathbf{a} |n\rangle = \sqrt{n} |n-1\rangle \tag{2.65}$$

$$\mathbf{a}^+ |n\rangle = \sqrt{n+1} |n+1\rangle \tag{2.66}$$

Although the number states were defined for use with the lowering and rising operators, they are of course not eigenstates for them (otherwise they would be unusable), but for the number operator. The Hamiltonian operator can now be expressed using the number operator:

$$\mathbf{H} = \left(\mathbf{N} + \frac{1}{2} \right) \hbar \omega \quad (2.67)$$

Any vector of the Fock-space can now be created from the lowest energy state ("quantum vacuum") using successively the creation operator. This is called the "preceding relation", which becomes

$$|n\rangle = \sqrt{n!} (\mathbf{a}^+)^n |0\rangle \quad (2.68)$$

The math here is quite simple, as was seen, but the theory is most powerful and important.

Matrix Representation

The matrix representation is originally from Heisenberg. The Dirac bra-ket formulation was originally invented for combining the Schrödinger's method using differential equations and differential operators, and the Heisenberg's method using matrices.

Because the for energies are the eigenvalues of the Hamiltonian operator

$$E_n = \hbar \omega \left(n + \frac{1}{2} \right) \quad (2.69)$$

the Hamiltonian operator for an harmonic oscillator is diagonal in Fock-space :

$$\mathbf{H} = \hbar \omega \begin{pmatrix} \frac{1}{2} & 0 & 0 & 0 & \dots \\ 0 & \frac{3}{2} & 0 & 0 & \dots \\ 0 & 0 & \frac{5}{2} & 0 & \dots \\ 0 & 0 & 0 & \frac{7}{2} & \dots \\ \dots & \dots & \dots & \dots & \dots \end{pmatrix} \quad (2.70)$$

The position and momentum operators become (after some calculations) off-diagonal:

$$\mathbf{x} = \sqrt{\frac{\hbar}{2m\omega}} \begin{pmatrix} 0 & 1 & 0 & 0 & \dots \\ 1 & 0 & \sqrt{2} & 0 & \dots \\ 0 & \sqrt{2} & 0 & \sqrt{3} & \dots \\ 0 & 0 & \sqrt{3} & 0 & \dots \\ \dots & \dots & \dots & \dots & \dots \end{pmatrix} \quad (2.71)$$

$$\mathbf{p} = \sqrt{\frac{m\hbar\omega}{2}} \begin{pmatrix} 0 & -1 & 0 & 0 & \dots \\ 1 & 0 & -\sqrt{2} & 0 & \dots \\ 0 & \sqrt{2} & 0 & -\sqrt{3} & \dots \\ 0 & 0 & \sqrt{3} & 0 & \dots \\ \dots & \dots & \dots & \dots & \dots \end{pmatrix} \quad (2.72)$$

A Dirac ket is now represented by a normalized column vector, and a bra with corresponding row vector. The eigenvalue equation for the Hamiltonian:

$$\mathbf{H} |n\rangle = E_n |n\rangle \quad (2.73)$$

becomes in matrix form, for the n:th vector:

$$\hbar \omega \begin{bmatrix} \frac{1}{2} & 0 & 0 & 0 & \dots \\ \dots & \dots & \dots & \dots & \dots \\ 0 & 0 & n + \frac{1}{2} & 0 & \dots \\ 0 & 0 & 0 & (n+1) + \frac{1}{2} & \dots \\ \dots & \dots & \dots & \dots & \dots \end{bmatrix} \begin{pmatrix} 0 \\ \dots \\ 1 \\ 0 \\ \dots \end{pmatrix} = \hbar \omega \begin{pmatrix} 0 \\ \dots \\ n + \frac{1}{2} \\ 0 \\ \dots \end{pmatrix} \quad (2.74)$$

Bibliography

Herbert Goldstein, Classical Mechanics, Second Edition, 1980, Addison-Wesley Publishing Company, Inc., ISBN 0-201-02969-3

Carl Nordling, Jonny Österman, Physics Handbook for Science and Engineering, Eight Edition, 2008, Studentlitteratur AB, Lund, Sweden, ISBN 978-91-44-04453-8

David J. Griffiths, Quantum Mechanics, Second Edition, 2005, Pearson Education, Inc., ISBN 0-13-191175-9

J. J. Sakurai, Modern Quantum Mechanics, Revised Edition, 1994, Addison-Wesley Publishing Company, Inc., ISBN 0-201-53929-2

E. Elbaz, Quantum The Quantum Theory of Particles, Fields, and Cosmology Springer, 1998, ISBN 3-540-62093-1

Michael Stone, The Physics of Quantum Fields, Springer, 2000, ISBN 0-387-98909-9

Michio Kaku, Quantum Field Theory, A Modern Introduction, Oxford University Press, 1993, ISBN 0-19-509158-2

Franz Gross, Relativistic Quantum Mechanics and Field Theory, John Wiley & Sons, Inc., 1999, ISBN 0-471-35386-8