Chapter V

The one-dimensional harmonic oscillator

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A. Introduction

A-1. Importance of the harmonic oscillator in physics

This chapter is devoted to the study of a particularly important physical system: the one-dimensional harmonic oscillator.

Quantum Mechanics, Volume I, Second Edition. C. Cohen-Tannoudji, B. Diu, and F. Laloë.

The simplest example of such a system is that of a particle of mass m moving in a potential which depends only on x and has the form:

$$V(x) = \frac{1}{2}kx^2 \tag{A-1}$$

(k is a real positive constant). The particle is attracted towards the $x = 0$ plane [the minimum of $V(x)$, corresponding to positions of stable equilibrium] by a restoring force:

$$F_x = -\frac{\mathrm{d}V}{\mathrm{d}x} = -kx \tag{A-2}$$

which is proportional to the distance x between the particle and the $x = 0$ plane (x is an algebraic variable: $x \lesseqgtr 0$). We know that in classical mechanics, the projection onto Ox of the particle's motion is a sinusoidal oscillation about $x = 0$, of angular frequency:

$$\omega = \sqrt{\frac{k}{m}} \tag{A-3}$$

Actually, a large number of systems are governed (at least approximately) by the harmonic oscillator equations. Whenever one studies the behavior of a physical system in the neighborhood of a stable equilibrium position, one arrives at equations which, in the limit of small oscillations, are those of a harmonic oscillator (see § A-2). The results we shall derive in this chapter are applicable, therefore, to a whole series of important physical phenomena – for example, the vibrations of the atoms of a molecule about their equilibrium position, the oscillations of atoms or ions of a crystalline lattice (phonons)[1].

The harmonic oscillator is also involved in the study of the electromagnetic field. We know that in a cavity, there exist an infinite number of possible stationary waves (normal modes of the cavity). The electromagnetic field can be expanded in terms of these modes and it can be shown, using Maxwell's equations, that each of the coefficients of this expansion (which describe the state of the field at each instant) obeys a differential equation, which is identical to that of a harmonic oscillator whose angular frequency ω is that of the associated normal mode. In other words, the electromagnetic field is formally equivalent to a set of independent harmonic oscillators (*cf.* Complement $\mathrm{K_V}$). The quantization of the field is obtained by quantizing these oscillators associated with the various normal modes of the cavity (*cf.* Chapter XIX). Recall, moreover, that it was the study of the behavior of these oscillators at thermal equilibrium (blackbody radiation) which, historically, led Planck to introduce, for the first time in physics, the constant h which bears his name. We shall see (*cf.* Complement $\mathrm{L_V}$) that the mean energy of a harmonic oscillator in thermodynamic equilibrium at the temperature T is different for classical and quantum mechanical oscillators.

The harmonic oscillator also plays an important role in the description of a set of identical particles which are all in the same quantum mechanical state (they must obviously be bosons, *cf.* Chap. XIV). As we shall see later, this is because the energy levels of a harmonic oscillator are equidistant, the spacing between two adjacent levels being equal to $\hbar\omega$. With the energy level labelled by the integer n (situated at a distance $n\hbar\omega$ above the ground state) can then be associated a set of n identical particles (or

[1]Complement $\mathrm{A_V}$ is devoted to a qualitative study of some physical examples of harmonic oscillators.

quanta), each possessing an energy $\hbar\omega$ (*cf.* Chapter XV). The transition of the oscillator from level n to level $n+1$ or $n-1$ corresponds to the creation or annihilation of a quantum of energy $\hbar\omega$. In this chapter, we shall introduce the operators $a^\dagger$ and a, which enable us to describe this transition from level n to level $n+1$ or $n-1$. These operators, respectively called "creation" and "annihilation" operators[2], are used throughout quantum statistical mechanics and quantum field theory[3].

The detailed study of the harmonic oscillator in quantum mechanics is therefore extremely important from a physical point of view. Moreover, we are dealing with a quantum mechanical system for which the Schrödinger equation can be solved rigorously. Having studied spin 1/2 and two-level systems in Chapter IV, we shall therefore now consider another simple example which illustrates the general formalism of quantum mechanics. We shall show in particular how to solve an eigenvalue equation by dealing only with the operators and the commutation relations (this technique will also be applied to angular momentum). We shall also study in a detailed way the motion of wave packets, particularly at the classical limit (*cf.* Complement G_V on quasi-classical states).

In § A-2, we shall review some results related to the classical oscillator before stating (§ A-3) certain general properties of the eigenvalues of the Hamiltonian H. Then, in §§ B and C, we shall determine these eigenvalues and eigenvectors by introducing creation and annihilation operators and using only the consequences of the canonical commutation relation $[X, P] = i\hbar$, as well as the particular form of H. § D is devoted to a physical study of the stationary states of the oscillator and wave packets formed by linear superpositions of these stationary states.

A-2. The harmonic oscillator in classical mechanics

The potential energy $V(x)$ [formula (A-1)] is shown in Figure 1. The motion of the particle is governed by the dynamical equation:

$$m\frac{\mathrm{d}^2x}{\mathrm{d}t^2} = -\frac{\mathrm{d}V}{\mathrm{d}x} = -kx \tag{A-4}$$

The general solution of this equation is of the form:

$$x = x_M \cos(\omega t - \varphi) \tag{A-5}$$

where ω is defined by (A-3), and the constants of integration x_M and φ are determined by the initial conditions of the motion. The particle therefore *oscillates sinusoidally* about the point O, with an amplitude x_M and an angular frequency ω.

The kinetic energy of the particle is:

$$T = \frac{1}{2}m\left(\frac{\mathrm{d}x}{\mathrm{d}t}\right)^2 = \frac{p^2}{2m} \tag{A-6}$$

[2]Annihilation operators are also often called "destruction operators".

[3]The aim of quantum field theory is to describe interactions between particles in the relativistic domain, especially the interactions between electrons, positrons and photons. It is clear that creation and annihilation operators should play an important role, since such processes are indeed observed experimentally (absorption or emission of photons, pair creation...). The quantum theory of electromagnetism is introduced in Chapter XIX.

where $p = m\dfrac{\mathrm{d}x}{\mathrm{d}t}$ is the momentum of the particle. The total energy is:

$$E = T + V = \frac{p^2}{2m} + \frac{1}{2}m\omega^2 x^2 \tag{A-7}$$

Substituting solution (A-5) into this equation, we find:

$$E = \frac{1}{2}m\omega^2 x_M^2 \tag{A-8}$$

The energy of the particle is therefore time-independent (this is a general property of conservative systems) and can take on any positive (or zero) value, since x_M is *a priori* arbitrary.

If we fix the total energy E, the limits of the classical motion $x = \pm x_M$ can be determined from Figure 1 by taking the intersection of the parabola with the line parallel to Ox of ordinate E. At these points $x = \pm x_M$, the potential energy is at a maximum and equal to E, and the kinetic energy is zero. On the other hand, at $x = 0$, the potential energy is zero and the kinetic energy is maximum.

Comment:

Consider an arbitrary potential $V(x)$ which has a minimum at $x = x_0$ (Fig. 2). Expanding the function $V(x)$ in a Taylor's series in the neighborhood of x_0, we obtain:

$$V(x) = a + b(x - x_0)^2 + c(x - x_0)^3 + ... \tag{A-9}$$

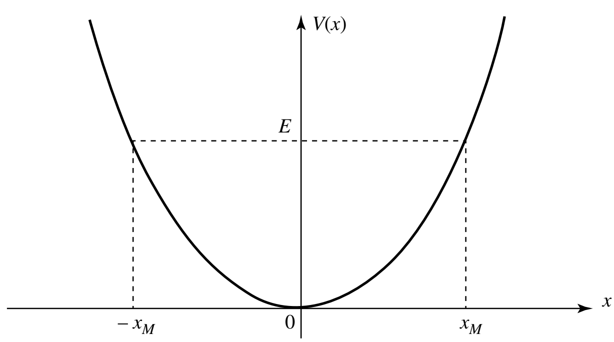

Figure 1: The potential energy $V(x)$ of a one-dimensional harmonic oscillator. The amplitude of the classical motion of energy E is x_M.

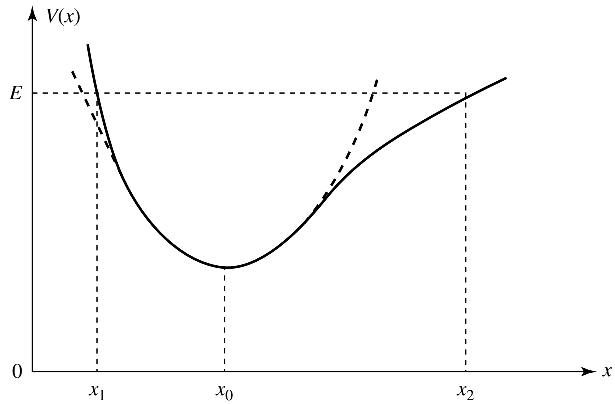

Figure 2: In the neighborhood of a minimum, any potential $V(x)$ can be approximated by a parabolic potential (dashed line). In the potential $V(x)$, a classical particle of energy E oscillates between x_1 and x_2.

The coefficients of this expansion are given by:

$$\begin{aligned} a &= V(x_0) \\ b &= \frac{1}{2}\left(\frac{\mathrm{d}^2 V}{\mathrm{d}x^2}\right)_{x=x_0} \\ c &= \frac{1}{3!}\left(\frac{\mathrm{d}^3 V}{\mathrm{d}x^3}\right)_{x=x_0} \end{aligned} \quad \text{(A-10)}$$

and the linear term in $(x - x_0)$ is zero since x_0 corresponds to a minimum of $V(x)$. The force derived from the potential $V(x)$ is, in the neighborhood of x_0:

$$F_x = -\frac{\mathrm{d}V}{\mathrm{d}x} = -2b(x - x_0) - 3c(x - x_0)^2 + ... \quad \text{(A-11)}$$

Since $x = x_0$ represents a minimum, the coefficient b is positive.

The point $x = x_0$ corresponds to a stable equilibrium position for the particle: F_x is zero for $x = x_0$; moreover, for $(x - x_0)$ sufficiently small, F_x and $(x - x_0)$ have opposite signs since b is positive.

If the amplitude of the motion of the particle about x_0 is sufficiently small for the term in $(x - x_0)^3$ of (A-9) [and therefore, the corresponding term in $(x - x_0)^2$ of (A-11)] to be negligible compared to the preceding ones, we have a harmonic oscillator since the dynamical equation can then be approximated by:

$$m\frac{\mathrm{d}^2 x}{\mathrm{d}t^2} \simeq -2b(x - x_0) \quad \text{(A-12)}$$

The corresponding angular frequency ω is related to the second derivative of $V(x)$

at $x = x_0$ by the formula:

$$\omega = \sqrt{\frac{2b}{m}} = \sqrt{\frac{1}{m}\left(\frac{\mathrm{d}^2 V}{\mathrm{d}x^2}\right)_{x=x_0}} \tag{A-13}$$

Since the amplitude of the motion must remain small, the energy of the harmonic oscillator will be low.

For higher energies E, the particle will be in *periodic but not sinusoidal motion* between the limits x_1 and x_2 (Fig. 2). If we expand the function $x(t)$ in a Fourier series giving the position of the particle, we find, not one, but several, sinusoidal terms; their frequencies are integral multiples of the lowest frequency. We then say that we are dealing with an *anharmonic* oscillator. Note also that, in this case, the period of the motion is not generally $2\pi/\omega$, where ω is given by formula (A-13).

A-3. General properties of the quantum mechanical Hamiltonian

In quantum mechanics, the classical quantities x and p are replaced respectively by the observables X and P, which satisfy:

$$[X, P] = i\hbar \tag{A-14}$$

It is then easy to obtain the Hamiltonian operator of the system from (A-7):

$$H = \frac{P^2}{2m} + \frac{1}{2}m\omega^2 X^2 \tag{A-15}$$

Since H is time-independent (conservative system), the quantum mechanical study of the harmonic oscillator reduces to the solution of the eigenvalue equation:

$$H|\varphi\rangle = E|\varphi\rangle \tag{A-16}$$

which is written, in the $\{|x\rangle\}$ representation:

$$\left[-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2}{\mathrm{d}x^2} + \frac{1}{2}m\omega^2 x^2\right]\varphi(x) = E\ \varphi(x) \tag{A-17}$$

Before undertaking the detailed study of equation (A-16), let us indicate some important properties that can be deduced from the form (A-1) of the potential function:

(*i*) *The eigenvalues of the Hamiltonian are positive.* It can be shown that, in general (Complement $\mathrm{M_{III}}$), if the potential function $V(x)$ has a lower bound, the eigenvalues E of the Hamiltonian $H = \dfrac{P^2}{2m} + V(X)$ are greater than the minimum of $V(x)$:

$$V(x) \geq V_m \quad \text{requires} \quad E > V_m \tag{A-18}$$

For the harmonic oscillator we are studying here, we have chosen the energy origin such that V_m is zero.

(*ii*) *The eigenfunctions of H have a definite parity.* This is due to the fact that the potential $V(x)$ is an even function:

$$V(-x) = V(x) \tag{A-19}$$

We can then (*cf.* Complements F_{II} and C_V) look for eigenfunctions of H, in the $\{|x\rangle\}$ representation, amongst the functions which have a definite parity (in fact, we shall see that the eigenvalues of H are not degenerate; consequently, the wave functions associated with the stationary states are necessarily either even or odd).

(*iii*) *The energy spectrum is discrete.* Whatever the value of the total energy, the classical motion is limited to a bounded region of the Ox axis (Fig. 1), and it can be shown (Complement M_{III}) that in this case, the eigenvalues of the Hamiltonian form a discrete set.

We shall derive these properties (in a more precise form) in the following sections. However, it is interesting to note that they can be obtained simply by applying to the harmonic oscillator some general theorems concerning one-dimensional problems.

B. Eigenvalues of the Hamiltonian

We are now going to study the eigenvalue equation (A-16). First of all, using only the canonical commutation relation (A-14), we shall find the spectrum of the Hamiltonian H written in (A-15).

B-1. Notation

We shall begin by introducing some useful notations.

B-1-a. The $\hat{X}$ and $\hat{P}$ operators

The observables X and P obviously have dimensions (those of a length and a momentum, respectively). Since ω has the dimension of the inverse of a time and $\hbar$, of an action (product of an energy and a time), it is easy to see that the observables $\hat{X}$ and $\hat{P}$ defined by:

$$\begin{aligned} \hat{X} &= \sqrt{\frac{m\omega}{\hbar}}X \\ \hat{P} &= \frac{1}{\sqrt{m\hbar\omega}}P \end{aligned} \tag{B-1}$$

are dimensionless.

If we use these new operators, the canonical commutation relation will be written:

$$[\hat{X}, \hat{P}] = i \tag{B-2}$$

and the Hamiltonian can be put in the form:

$$H = \hbar\omega\,\hat{H} \tag{B-3}$$

with:

$$\hat{H} = \frac{1}{2}\left(\hat{X}^2 + \hat{P}^2\right) \tag{B-4}$$

We shall therefore seek the solutions of the eigenvalue equation:

$$\hat{H}|\varphi_\nu^i\rangle = \varepsilon_\nu \; |\varphi_\nu^i\rangle \tag{B-5}$$

where the operator $\hat{H}$ and the eigenvalues ε_ν are dimensionless. The index ν can belong to either a discrete or a continuous set, and the additional index i enables us to distinguish between the various possible orthogonal eigenvectors associated with the same eigenvalue ε_ν.

B-1-b. The a, $a^\dagger$ and N operators

If $\hat{X}$ and $\hat{P}$ were numbers and not operators, we could write the sum $\hat{X}^2 + \hat{P}^2$ appearing in expression (B-4) for $\hat{H}$ in the form of a product of linear terms, and obtain $(\hat{X} - i\hat{P})(\hat{X} + i\hat{P})$. In fact, since $\hat{X}$ and $\hat{P}$ are non-commuting operators, $\hat{X}^2 + \hat{P}^2$ is not equal to $(\hat{X} - i\hat{P})(\hat{X} + i\hat{P})$. We shall show, however, that the introduction of operators proportional to $\hat{X} + i\hat{P}$ and $\hat{X} - i\hat{P}$ enables us to simplify considerably our search for eigenvalues and eigenvectors of $\hat{H}$.

We therefore set[4]:

$$a = \frac{1}{\sqrt{2}}(\hat{X} + i\hat{P}) \tag{B-6a}$$

$$a^\dagger = \frac{1}{\sqrt{2}}(\hat{X} - i\hat{P}) \tag{B-6b}$$

These formulas can immediately be inverted to yield:

$$\hat{X} = \frac{1}{\sqrt{2}}(a^\dagger + a) \tag{B-7a}$$

$$\hat{P} = \frac{i}{\sqrt{2}}(a^\dagger - a) \tag{B-7b}$$

Since $\hat{X}$ and $\hat{P}$ are Hermitian, a and $a^\dagger$ are not (because of the factor i), but are adjoints of each other.

The commutator of a and $a^\dagger$ is easy to calculate from (B-6) and (B-2):

$$\begin{aligned}[a, a^\dagger] &= \frac{1}{2}\left[\hat{X} + i\hat{P}, \hat{X} - i\hat{P}\right] \\ &= \frac{i}{2}\left[\hat{P}, \hat{X}\right] - \frac{i}{2}\left[\hat{X}, \hat{P}\right]\end{aligned} \tag{B-8}$$

that is:

$$[a, a^\dagger] = 1 \tag{B-9}$$

This relation is completely equivalent to the canonical commutation relation (A-14).

[4] Until now, we have designated operators by capital letters. However, to conform to standard usage, we shall use the small letters a and $a^\dagger$ for the operators (B-6).

Finally, we derive some simple formulas which will be useful in the rest of this chapter. We first calculate $a^\dagger a$:

$$\begin{aligned}
a^\dagger a &= \frac{1}{2}(\hat{X} - i\hat{P})(\hat{X} + i\hat{P}) \\
&= \frac{1}{2}(\hat{X}^2 + \hat{P}^2 + i\hat{X}\hat{P} - i\hat{P}\hat{X}) \\
&= \frac{1}{2}(\hat{X}^2 + \hat{P}^2 - 1) \qquad \text{(B-10)}
\end{aligned}$$

Comparing this with expression (B-4), we see that:

$$\hat{H} = a^\dagger a + \frac{1}{2} = \frac{1}{2}(\hat{X} - i\hat{P})(\hat{X} + i\hat{P}) + \frac{1}{2} \qquad \text{(B-11)}$$

Unlike the situation in the classical case, $\hat{H}$ cannot be put in the form of a product of linear terms. The non-commutativity of $\hat{X}$ and $\hat{P}$ is at the origin of the additional term 1/2 that appears on the right-hand side of (B-11). Similarly, it can be shown that:

$$\hat{H} = aa^\dagger - \frac{1}{2} \qquad \text{(B-12)}$$

Let us now introduce the operator N defined by:

$$N = a^\dagger a \qquad \text{(B-13)}$$

This operator is Hermitian since:

$$N^\dagger = a^\dagger (a^\dagger)^\dagger = a^\dagger a = N \qquad \text{(B-14)}$$

Moreover, according to (B-11):

$$\hat{H} = N + \frac{1}{2} \qquad \text{(B-15)}$$

so that *the eigenvectors of $\hat{H}$ are eigenvectors of N, and vice versa.*

Finally, let us calculate the commutators of N with a and $a^\dagger$:

$$\begin{aligned}
[N, a] &= [a^\dagger a, a] = a^\dagger [a, a] + [a^\dagger, a]a = -a \\
[N, a^\dagger] &= [a^\dagger a, a^\dagger] = a^\dagger [a, a^\dagger] + [a^\dagger, a^\dagger]a = a^\dagger \qquad \text{(B-16)}
\end{aligned}$$

that is:

$$[N, a] = -a \qquad \text{(B-17a)}$$

$$[N, a^\dagger] = a^\dagger \qquad \text{(B-17b)}$$

Our study of the harmonic oscillator will be based on the use of the a, $a^\dagger$ and N operators. We have replaced the eigenvalue equation of H, which we first wrote in the form (B-5), by that of N:

$$N|\varphi_\nu^i\rangle = \nu|\varphi_\nu^i\rangle \qquad \text{(B-18)}$$

When this equation is solved, we shall know that the eigenvector $|\varphi_\nu^i\rangle$ of N is also an eigenvector of H with the eigenvalue $E_\nu = (\nu + 1/2)\hbar\omega$ [formulas (B-3) and (B-15)]:

$$H|\varphi_\nu^i\rangle = (\nu + 1/2)\hbar\omega \ |\varphi_\nu^i\rangle \tag{B-19}$$

The solution of equation (B-18) will be based on the commutation relation (B-9), which is equivalent to the initial relation (A-14), and on formulas (B-17), which are consequences of it.

B-2. Determination of the spectrum

B-2-a. Lemmas

α. *Lemma I (property of the eigenvalues of N)*

The eigenvalues ν of the operator N are positive or zero.

Consider an arbitrary eigenvector $|\varphi_\nu^i\rangle$ of N. The square of the norm of the vector $a\,|\varphi_\nu^i\rangle$ is positive or zero:

$$\| \, a|\varphi_\nu^i\rangle \, \|^2 = \langle\varphi_\nu^i|a^\dagger a|\varphi_\nu^i\rangle \geq 0 \tag{B-20}$$

Let us then use definition (B-13) of N:

$$\langle\varphi_\nu^i|a^\dagger a|\varphi_\nu^i\rangle = \langle\varphi_\nu^i|N|\varphi_\nu^i\rangle = \nu\langle\varphi_\nu^i|\varphi_\nu^i\rangle \tag{B-21}$$

Since $\langle\varphi_\nu^i|\varphi_\nu^i\rangle$ is positive, comparison of (B-20) and (B-21) shows that:

$$\nu \geq 0 \tag{B-22}$$

β. *Lemma II (properties of the vector $a\,|\varphi_\nu^i\rangle$)*

Let $|\varphi_\nu^i\rangle$ be a (non-zero) eigenvector of N with the eigenvalue ν.

We shall prove the following:

(i) If $\nu = 0$, the ket $a|\varphi_{\nu=0}^i\rangle$ is zero.

(ii) If $\nu > 0$, the ket $a|\varphi_\nu^i\rangle$ is a non-zero eigenvector of N with the eigenvalue $\nu - 1$.

(i) According to (B-21), the square of the norm of $a|\varphi_\nu^i\rangle$ is zero if $\nu = 0$; now, the norm of a vector is zero if and only if this vector is zero. Consequently, if $\nu = 0$ is an eigenvalue of N, all eigenvectors $|\varphi_0^i\rangle$ associated with this eigenvalue satisfy the relation:

$$a\,|\varphi_0^i\rangle = 0 \tag{B-23}$$

Let us now show that relation (B-23) is characteristic of these eigenvectors. Consider a vector $|\varphi\rangle$ which satisfies:

$$a\,|\varphi\rangle = 0 \tag{B-24}$$

Multiply both sides of this equation from the left by $a^\dagger$:

$$a^\dagger a|\varphi\rangle = N|\varphi\rangle = 0 \tag{B-25}$$

Any vector which satisfies (B-24) is therefore an eigenvector of N with the eigenvalue $\nu = 0$.

(ii) Now let us assume that ν is strictly positive. According to (B-21), the vector $a|\varphi_\nu^i\rangle$ is then non-zero, since the square of its norm is not equal to zero.

Let us show that $a|\varphi_\nu^i\rangle$ is an eigenvector of N. To do this, let us apply the operator relation (B-17a) to the vector $|\varphi_\nu^i\rangle$:

$$\begin{aligned}[N,a]|\varphi_\nu^i\rangle &= -a|\varphi_\nu^i\rangle \\ Na|\varphi_\nu^i\rangle &= aN|\varphi_\nu^i\rangle - a|\varphi_\nu^i\rangle \\ &= a\nu|\varphi_\nu^i\rangle - a|\varphi_\nu^i\rangle\end{aligned} \tag{B-26}$$

Therefore:

$$N\big[a|\varphi_\nu^i\rangle\big] = (\nu-1)[a|\varphi_\nu^i\rangle] \tag{B-27}$$

which shows that $a|\varphi_\nu^i\rangle$ is an eigenvector of N with the eigenvalue $\nu - 1$.

γ. *Lemma III (properties of the vector $a^\dagger|\varphi_\nu^i\rangle$)*

Let $|\varphi_\nu^i\rangle$ be a (non-zero) eigenvector of N of eigenvalue ν.

We shall prove the following:

(i) $a^\dagger|\varphi_\nu^i\rangle$ is always non-zero.

(ii) $a^\dagger|\varphi_\nu^i\rangle$ is an eigenvector of N with the eigenvalue $\nu+1$.

(i) It is easy to calculate the norm of the vector $a^\dagger|\varphi_\nu^i\rangle$, using formulas (B-9) and (B-13):

$$\begin{aligned}\| a^\dagger|\varphi_\nu^i\rangle \|^2 &= \langle\varphi_\nu^i|aa^\dagger|\varphi_\nu^i\rangle \\ &= \langle\varphi_\nu^i|(N+1)|\varphi_\nu^i\rangle \\ &= (\nu+1)\langle\varphi_\nu^i|\varphi_\nu^i\rangle\end{aligned} \tag{B-28}$$

Since, according to lemma I, ν is positive or zero, the ket $a^\dagger|\varphi_\nu^i\rangle$ always has a non-zero norm and, consequently, is never zero.

(ii) The proof of the fact that $a^\dagger|\varphi_\nu^i\rangle$ is an eigenvector of N is analogous to that of lemma II; starting from relation (B-17b) between operators, we obtain:

$$\begin{aligned}[N,a^\dagger]\;|\varphi_\nu^i\rangle &= a^\dagger|\varphi_\nu^i\rangle \\ Na^\dagger|\varphi_\nu^i\rangle &= a^\dagger N|\varphi_\nu^i\rangle + a^\dagger|\varphi_\nu^i\rangle = (\nu+1)a^\dagger|\varphi_\nu^i\rangle\end{aligned} \tag{B-29}$$

B-2-b. The spectrum of N is composed of non-negative integers

Consider an arbitrary eigenvalue ν of N and a non-zero eigenvector $|\varphi_\nu^i\rangle$ associated with this eigenvalue.

According to lemma I, ν is necessarily positive or zero. First, let us assume ν to be non-integral. We are now going to show that such a hypothesis contradicts lemma I and must consequently be excluded. If ν is non-integral, we can always find an integer $n \geq 0$ such that:

$$n < \nu < n+1 \tag{B-30}$$

Now let us consider the series of vectors:

$$|\varphi_\nu^i\rangle, \quad a|\varphi_\nu^i\rangle \; ... \; a^n|\varphi_\nu^i\rangle \tag{B-31}$$

According to lemma *II*, each of the vectors $a^p|\varphi_\nu^i\rangle$ of this series (with $0 \leq p \leq n$) is non-zero and an eigenvector of N with the eigenvalue $\nu - p$ (*cf.* Fig. 3). The proof is by iteration: $|\varphi_\nu^i\rangle$ is non-zero by hypothesis; $a|\varphi_\nu^i\rangle$ is non-zero (since $\nu > 0$) and corresponds to the eigenvalue $\nu-1$ of N ...; $a^p|\varphi_\nu^i\rangle$ is obtained when a acts on $a^{p-1}|\varphi_\nu^i\rangle$, an eigenvector of N with the strictly positive eigenvalue $\nu - p + 1$, since $p \leq n$ and $\nu > n$ [*cf.* (B-30)].

Now let a act on the ket $a^n|\varphi_\nu^i\rangle$. Since $\nu - n > 0$ according to (B-30), the action of a on $a^n|\varphi_\nu^i\rangle$ (an eigenvector of N with the eigenvalue $\nu - n > 0$) yields a non-zero vector (lemma *II*). Moreover, again according to lemma *II*, $a^{n+1}|\varphi_\nu^i\rangle$ is an eigenvector of N with the eigenvalue $\nu - n - 1$, which is strictly negative according to (B-30). If ν is non-integral, we can therefore construct a non-zero eigenvector of N with a strictly negative eigenvalue. Since this is impossible, according to lemma *I*, the hypothesis of non-integral ν must be rejected.

What now happens if:

$$\nu = n \tag{B-32}$$

with n a positive integer or zero? In the series of vectors (B-31), $a^n|\varphi_n^i\rangle$ is non-zero and an eigenvector of N with the eigenvalue 0. According to lemma *II* (§ (i)), we therefore have:

$$a^{n+1}|\varphi_n^i\rangle = 0 \tag{B-33}$$

The series of vectors obtained by repeated action of the operator a on $|\varphi_n^i\rangle$ is therefore limited when n is integral. It is then never possible to obtain a non-zero eigenvector of N which corresponds to a negative eigenvalue.

In conclusion, ν can only be a non-negative integer.

Lemma *III* can then be used to show that the spectrum of N indeed includes all positive or zero integers. We have already constructed an eigenvector of N with an eigenvalue of zero ($a^n|\varphi_n^i\rangle$). All we must do is let $(a^\dagger)^k$ act on such a vector in order to obtain an eigenvector of N of eigenvalue k, where k is an arbitrary positive integer.

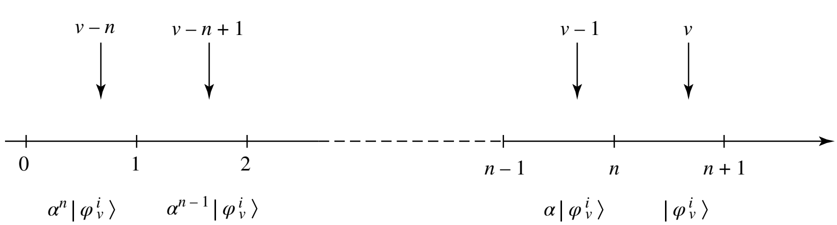

Figure 3: Letting a act several times on the ket $|\varphi_\nu^i\rangle$, we can construct eigenvectors of N with eigenvalues $\nu - 1$, $\nu - 2$ etc...

If we then refer to formula (B-19), we conclude that the eigenvalues of H are of the form:

$$E_n = \left(n + \frac{1}{2}\right)\hbar\omega \tag{B-34}$$

with $n = 0, 1, 2, ...$ Therefore, in quantum mechanics, *the energy of the harmonic oscillator is quantized* and cannot take on any arbitrary value. Note also that the smallest value (the ground state) is not zero, but $\hbar\omega/2$ (see § D-2 below).

B-2-c. Interpretation of the a and $a^\dagger$ operators

If we start with an eigenstate $|\varphi_n^i\rangle$ of H corresponding to the eigenvalue $E_n = (n + 1/2)\hbar\omega$, application of the operator a yields an eigenvector associated with the eigenvalue $E_{n-1} = (n + 1/2)\hbar\omega - \hbar\omega$, and application of $a^\dagger$ yields, in the same way, the energy $E_{n+1} = (n + 1/2)\hbar\omega + \hbar\omega$.

For this reason, $a^\dagger$ is said to be a *creation operator* and a an *annihilation operator* (or destruction operator); their action on an eigenvector of N makes an energy quantum $\hbar\omega$ appear or disappear.

B-3. Degeneracy of the eigenvalues

We now show that the energy levels of the one-dimensional harmonic oscillator, given by equation (B-34), are not degenerate.

B-3-a. The ground state is non-degenerate

The eigenstates of H associated with the eigenvalue $E_0 = \hbar\omega/2$, that is, the eigenstates of N associated with the eigenvalue $n = 0$, according to lemma *II* of § B-2-a-β, must all satisfy the equation:

$$a|\varphi_0^i\rangle = 0 \tag{B-35}$$

To find the degeneracy of the E_0 level, all we must do is see how many linearly independent kets satisfy (B-35).

Using definition (B-6a) of a and relations (B-1), we can write (B-35) in the form:

$$\frac{1}{\sqrt{2}}\left[\sqrt{\frac{m\omega}{\hbar}}X + \frac{i}{\sqrt{m\hbar\omega}}P\right]|\varphi_0^i\rangle = 0 \tag{B-36}$$

In the $\{|x\rangle\}$ representation, this relation becomes:

$$\left(\frac{m\omega}{\hbar}x + \frac{\mathrm{d}}{\mathrm{d}x}\right)\varphi_0^i(x) = 0 \tag{B-37}$$

where:

$$\varphi_0^i(x) = \langle x|\varphi_0^i\rangle \tag{B-38}$$

Therefore we must solve a first-order differential equation. Its general solution is:

$$\varphi_0^i(x) = c\,\mathrm{e}^{-\frac{1}{2}\frac{m\omega}{\hbar}x^2} \tag{B-39}$$

where c is the constant of integration. The various solutions of (B-37) are all proportional to each other. Consequently, to within a multiplicative factor, there exists only one ket $|\varphi_0\rangle$ that satisfies (B-35): the ground state $E_0 = \hbar\omega/2$ is not degenerate.

B-3-b. All the states are non-degenerate

We have just seen that the ground state is not degenerate. Let us show by recurrence that this is also the case for all the other states.

All we need prove is that, if the level $E_n = (n + 1/2)\hbar\omega$ is not degenerate, the level $E_{n+1} = (n + 1 + 1/2)\hbar\omega$ is not either. Let us therefore assume that there exists, to within a constant factor, only one vector $|\varphi_n\rangle$ such that:

$$N|\varphi_n\rangle = n|\varphi_n\rangle \tag{B-40}$$

Then consider an eigenvector $|\varphi^i_{n+1}\rangle$ corresponding to the eigenvalue $n + 1$:

$$N|\varphi^i_{n+1}\rangle = (n + 1)|\varphi^i_{n+1}\rangle \tag{B-41}$$

We know that the ket $a|\varphi^i_{n+1}\rangle$ is not zero and that it is an eigenvector of N with the eigenvalue n (*cf.* lemma *II*). Since this ket is not degenerate by hypothesis, there exists a number c^i such that:

$$a|\varphi^i_{n+1}\rangle = c^i|\varphi_n\rangle \tag{B-42}$$

It is simple to invert this equation by applying $a^\dagger$ to both sides:

$$a^\dagger a|\varphi^i_{n+1}\rangle = c^i a^\dagger|\varphi_n\rangle \tag{B-43}$$

that is, taking (B-13) and (B-41) into account:

$$|\varphi^i_{n+1}\rangle = \frac{c^i}{n + 1} a^\dagger|\varphi_n\rangle \tag{B-44}$$

We already knew that $a^\dagger|\varphi_n\rangle$ was an eigenvector of N with the eigenvalue $(n + 1)$; we see here that all kets $|\varphi^i_{n+1}\rangle$ associated with the eigenvalue $(n + 1)$ are proportional to $a^\dagger|\varphi_n\rangle$. They are therefore proportional to each other: the eigenvalue $(n + 1)$ is not degenerate.

Thus, since the eigenvalue $n = 0$ is not degenerate (see § B-3-a), the eigenvalue $n = 1$ is not either, nor is $n = 2$, etc...: all the eigenvalues of N and, consequently, all those of H, are non-degenerate. This enables us to write simply $|\varphi_n\rangle$ for the eigenvector of H associated with the eigenvalue $E_n = (n + 1/2)\hbar\omega$.

C. Eigenstates of the Hamiltonian

In this section, we are going to study the principal properties of the eigenstates of the operator N and of the Hamiltonian H.

C-1. The $\{|\varphi_n\rangle\}$ representation

We shall assume that N and H are observables, meaning their eigenvectors constitute a basis in the space $\mathcal{E}_x$, the state space of a particle in a one-dimensional problem (this could be proved by considering the wave functions associated with the eigenstates of N, which we shall calculate in § C-2 below). Since none of the eigenvalues of N (or of H) is degenerate (see § B-3), N (or H) alone constitutes a C.S.C.O. in $\mathcal{E}_x$.

C-1-a. The basis vectors in terms of $|\varphi_0\rangle$

The vector $|\varphi_0\rangle$ associated with $n = 0$ is the vector of $\mathcal{E}_x$ that satisfies:

$$a|\varphi_0\rangle = 0 \tag{C-1}$$

It is defined to within a constant factor; we shall assume $|\varphi_0\rangle$ to be normalized, so the indeterminacy is reduced to a global phase factor of the form $\mathrm{e}^{i\theta}$, with θ real.

According to lemma *III* of § B-2-a, the vector $|\varphi_1\rangle$ which corresponds to $n = 1$ is proportional to $a^\dagger|\varphi_0\rangle$:

$$|\varphi_1\rangle = c_1 a^\dagger|\varphi_0\rangle \tag{C-2}$$

We shall determine c_1 by requiring $|\varphi_1\rangle$ to be normalized and choosing the phase of $|\varphi_1\rangle$ (relative to $|\varphi_0\rangle$) such that c_1 is real and positive. The square of the norm of $|\varphi_1\rangle$, according to (C-2), is equal to:

$$\begin{aligned}\langle\varphi_1|\varphi_1\rangle &= |c_1|^2\langle\varphi_0|aa^\dagger|\varphi_0\rangle \\ &= |c_1|^2\langle\varphi_0|(a^\dagger a + 1)|\varphi_0\rangle\end{aligned} \tag{C-3}$$

where (B-9) has been used. Since $|\varphi_0\rangle$ is a normalized eigenstate of $N = a^\dagger a$ with the eigenvalue zero, we find:

$$\langle\varphi_1|\varphi_1\rangle = |c_1|^2 = 1 \tag{C-4}$$

With the preceding phase convention, we have $c_1 = 1$ and, consequently:

$$|\varphi_1\rangle = a^\dagger|\varphi_0\rangle \tag{C-5}$$

Similarly, we can construct $|\varphi_2\rangle$ from $|\varphi_1\rangle$:

$$|\varphi_2\rangle = c_2\, a^\dagger|\varphi_1\rangle \tag{C-6}$$

We require $|\varphi_2\rangle$ to be normalized and choose its phase such that c_2 is real and positive:

$$\begin{aligned}\langle\varphi_2|\varphi_2\rangle &= |c_2|^2\langle\varphi_1|aa^\dagger|\varphi_1\rangle \\ &= |c_2|^2\langle\varphi_1|(a^\dagger a + 1)|\varphi_1\rangle \\ &= 2|c_2|^2 = 1\end{aligned} \tag{C-7}$$

Therefore:

$$|\varphi_2\rangle = \frac{1}{\sqrt{2}}a^\dagger|\varphi_1\rangle = \frac{1}{\sqrt{2}}(a^\dagger)^2|\varphi_0\rangle \tag{C-8}$$

if we take (C-5) into account.

This procedure can easily be generalized. If we know $|\varphi_{n-1}\rangle$ (which is normalized), then the normalized vector $|\varphi_n\rangle$ is written:

$$|\varphi_n\rangle = c_n a^\dagger|\varphi_{n-1}\rangle \tag{C-9}$$

Since:

$$\begin{aligned}\langle\varphi_n|\varphi_n\rangle &= |c_n|^2\langle\varphi_{n-1}|aa^\dagger|\varphi_{n-1}\rangle \\ &= n|c_n|^2 = 1\end{aligned} \tag{C-10}$$

we choose, with the same phase conventions as above:

$$c_n = \frac{1}{\sqrt{n}} \tag{C-11}$$

With these successive phase choices, we can obtain all the $|\varphi_n\rangle$ from $|\varphi_0\rangle$:

$$\begin{aligned}|\varphi_n\rangle &= \frac{1}{\sqrt{n}}a^\dagger|\varphi_{n-1}\rangle = \frac{1}{\sqrt{n}}\frac{1}{\sqrt{n-1}}(a^\dagger)^2|\varphi_{n-2}\rangle = ... \\ &= \frac{1}{\sqrt{n}}\frac{1}{\sqrt{n-1}}...\frac{1}{\sqrt{2}}(a^\dagger)^n|\varphi_0\rangle\end{aligned} \tag{C-12}$$

that is:

$$|\varphi_n\rangle = \frac{1}{\sqrt{n!}}(a^\dagger)^n|\varphi_0\rangle \tag{C-13}$$

C-1-b. Orthonormalization and closure relations

Since H is Hermitian, the kets $|\varphi_n\rangle$ corresponding to different values of n are orthogonal. Since each of them is also normalized, they satisfy the orthonormalization relation:

$$\langle\varphi_{n'}|\varphi_n\rangle = \delta_{nn'} \tag{C-14}$$

In addition, H is an observable (we shall assume this here without proof); the set of the $|\varphi_n\rangle$ therefore constitutes a basis in $\mathcal{E}_x$. This is expressed by the closure relation:

$$\sum_n |\varphi_n\rangle\langle\varphi_n| = 1 \tag{C-15}$$

Comment:

It can be verified directly from expression (C-13) that the kets $|\varphi_n\rangle$ are orthonormal:

$$\langle\varphi_{n'}|\varphi_n\rangle = \frac{1}{\sqrt{n!n'!}}\langle\varphi_0|a^{n'}\,a^{\dagger n}|\varphi_0\rangle \tag{C-16}$$

But:

$$\begin{aligned}a^{n'}\,a^{\dagger n}|\varphi_0\rangle &= a^{n'-1}(aa^\dagger)a^{\dagger n-1}|\varphi_0\rangle \\ &= a^{n'-1}(a^\dagger a+1)a^{\dagger n-1}|\varphi_0\rangle \\ &= n\,a^{n'-1}a^{\dagger n-1}|\varphi_0\rangle\end{aligned} \tag{C-17}$$

(using the fact that ${a^\dagger}^{n-1}|\varphi_0\rangle$ is an eigenstate of $N = a^\dagger a$ with the eigenvalue $n-1$). Thus can we reduce the exponents of a and $a^\dagger$ by iteration. We obtain, finally:

$$\text{if} \quad n < n' : \langle\varphi_0|a^{n'}{a^\dagger}^n|\varphi_0\rangle = n \times (n-1) \times ...2 \times 1 \langle\varphi_0|a^{n'-n}|\varphi_0\rangle \tag{C-18a}$$

$$\text{if} \quad n > n' : \langle\varphi_0|a^{n'}{a^\dagger}^n|\varphi_0\rangle = n \times (n-1)...(n-n'+1)\langle\varphi_0|(a^\dagger)^{n-n'}|\varphi_0\rangle \tag{C-18b}$$

$$\text{if} \quad n = n' : \langle\varphi_0|a^{n'}{a^\dagger}^n|\varphi_0\rangle = n \times (n-1) \times ...2 \times 1 \langle\varphi_0|\varphi_0\rangle \tag{C-18c}$$

The expression (C-18a) is zero because $a|\varphi_0\rangle = 0$. Similarly, (C-18b) is equal to zero because $\langle\varphi_0|(a^\dagger)^{n-n'}|\varphi_0\rangle$ can be considered to be the scalar product of $|\varphi_0\rangle$ and the bra associated with $a^{n-n'}|\varphi_0\rangle$, which is zero if $n > n'$. Finally, if we substitute (C-18c) into (C-16), we see that $\langle\varphi_n|\varphi_n\rangle$ is equal to 1.

C-1-c. Action of the various operators

The observables X and P are linear combinations of the operators a and $a^\dagger$ [formulas (B-1) and (B-7)]. Consequently, all physical quantities can be expressed in terms of a and $a^\dagger$. Now, the action of a and $a^\dagger$ on the $|\varphi_n\rangle$ vectors is especially simple [see equations (C-19) below]. In most cases, it is therefore desirable to use the $\{|\varphi_n\rangle\}$ representation to calculate the matrix elements and mean values of the various observables.

With the phase conventions introduced in § C-1-a above, the action of the a and $a^\dagger$ operators on the vectors of the $\{|\varphi_n\rangle\}$ basis is given by:

$$a^\dagger|\varphi_n\rangle = \sqrt{n+1}\ |\varphi_{n+1}\rangle \tag{C-19a}$$

$$a|\varphi_n\rangle = \sqrt{n}\ |\varphi_{n-1}\rangle \tag{C-19b}$$

We have already proved (C-19a): it suffices to replace n by $n+1$ in equations (C-9) and (C-11). To obtain (C-19b), multiply both sides of (C-9) on the left by the operator a and use (C-11):

$$a|\varphi_n\rangle = \frac{1}{\sqrt{n}}\ aa^\dagger|\varphi_{n-1}\rangle = \frac{1}{\sqrt{n}}(a^\dagger a + 1)|\varphi_{n-1}\rangle = \sqrt{n}\ |\varphi_{n-1}\rangle \tag{C-20}$$

Comment:

The adjoint equations of (C-19a) and (C-19b) are:

$$\langle\varphi_n|a = \sqrt{n+1}\ \langle\varphi_{n+1}| \tag{C-21a}$$

$$\langle\varphi_n|a^\dagger = \sqrt{n}\ \langle\varphi_{n-1}| \tag{C-21b}$$

Note that a decreases or increases n by one unit depending on whether it acts on the ket $|\varphi_n\rangle$ or on the bra $\langle\varphi_n|$. Similarly, $a^\dagger$ increases or decreases n by one unit, depending on whether it acts on the ket $|\varphi_n\rangle$ or on the bra $\langle\varphi_n|$.

Starting with (C-19) and using (B-1) and (B-7), we immediately find the expressions for the kets $X|\varphi_n\rangle$ and $P|\varphi_n\rangle$:

$$X|\varphi_n\rangle = \sqrt{\frac{\hbar}{m\omega}}\frac{1}{\sqrt{2}}\,(a^\dagger + a)|\varphi_n\rangle = \sqrt{\frac{\hbar}{2m\omega}}\left[\sqrt{n+1}\;|\varphi_{n+1}\rangle + \sqrt{n}\;|\varphi_{n-1}\rangle\right] \tag{C-22a}$$

$$P|\varphi_n\rangle = \sqrt{m\hbar\omega}\frac{i}{\sqrt{2}}(a^\dagger - a)|\varphi_n\rangle = i\sqrt{\frac{m\hbar\omega}{2}}\;\left[\sqrt{n+1}\;|\varphi_{n+1}\rangle - \sqrt{n}\;|\varphi_{n-1}\rangle\right] \tag{C-22b}$$

The matrix elements of the a, $a^\dagger$, X and P operators in the $\{|\varphi_n\rangle\}$ representation are therefore:

$$\langle\varphi_{n'}|a|\varphi_n\rangle = \sqrt{n}\;\delta_{n',n-1} \tag{C-23a}$$

$$\langle\varphi_{n'}|a^\dagger|\varphi_n\rangle = \sqrt{n+1}\;\delta_{n',n+1} \tag{C-23b}$$

$$\langle\varphi_{n'}|X|\varphi_n\rangle = \sqrt{\frac{\hbar}{2m\omega}}\left[\sqrt{n+1}\;\delta_{n',n+1} + \sqrt{n}\;\delta_{n',n-1}\right] \tag{C-23c}$$

$$\langle\varphi_{n'}|P|\varphi_n\rangle = i\sqrt{\frac{m\hbar\omega}{2}}\left[\sqrt{n+1}\;\delta_{n',n+1} - \sqrt{n}\;\delta_{n',n-1}\right] \tag{C-23d}$$

The matrices representing a and $a^\dagger$ are indeed Hermitian conjugates of each other, as can be seen from their explicit expressions:

$$(a) = \begin{pmatrix} 0 & \sqrt{1} & 0 & 0 & .. & 0 & .. \\ 0 & 0 & \sqrt{2} & 0 & .. & 0 & .. \\ 0 & 0 & 0 & \sqrt{3} & .. & 0 & .. \\ 0 & 0 & 0 & 0 & .. & 0 & .. \\ .. & .. & .. & .. & .. & \sqrt{n} & .. \\ 0 & 0 & 0 & 0 & 0 & 0 & .. \\ .. & .. & .. & .. & .. & .. & .. \end{pmatrix} \tag{C-24a}$$

and:

$$(a^\dagger) = \begin{pmatrix} 0 & 0 & 0 & 0 & .. & 0 & .. \\ \sqrt{1} & 0 & 0 & 0 & .. & 0 & .. \\ 0 & \sqrt{2} & 0 & 0 & .. & 0 & .. \\ 0 & 0 & \sqrt{3} & 0 & .. & 0 & .. \\ .. & .. & .. & .. & .. & 0 & .. \\ 0 & 0 & 0 & 0 & \sqrt{n+1} & 0 & .. \\ .. & .. & .. & .. & .. & .. & .. \end{pmatrix} \tag{C-24b}$$

As for the matrices representing X and P, they are both Hermitian: the matrix associated with X is, to within a constant factor, the sum of the two preceding ones; the matrix associated with P is proportional to their difference, but the presence of the factor i in (C-22b) re-establishes its Hermiticity.

C-2. Wave functions associated with the stationary states

We shall now use the $\{|x\rangle\}$ representation and write the functions $\varphi_n(x) = \langle x|\varphi_n\rangle$ which then represent the eigenstates of the Hamiltonian.

We have already determined the function $\varphi_0(x)$ which represents the ground state $|\varphi_0\rangle$ (*cf.* § B-3-a):

$$\varphi_0(x) = \langle x|\varphi_0\rangle = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} \mathrm{e}^{-\frac{1}{2}\frac{m\omega}{\hbar}x^2} \tag{C-25}$$

The constant that appears before the exponential insures the normalization of $\varphi_0(x)$.

To obtain the functions $\varphi_n(x)$ associated with the other stationary states of the harmonic oscillator, all we need to do is use expression (C-13) for the ket $|\varphi_n\rangle$ and the fact that, in the $\{|x\rangle\}$ representation, $a^\dagger$ is represented by:

$$\frac{1}{\sqrt{2}}\left[\sqrt{\frac{m\omega}{\hbar}}x - \sqrt{\frac{\hbar}{m\omega}}\frac{\mathrm{d}}{\mathrm{d}x}\right]$$

since X is represented by multiplication by x, and P by $\dfrac{\hbar}{i}\dfrac{\mathrm{d}}{\mathrm{d}x}$ [formula (B-6b)]. Thus we obtain:

$$\begin{aligned}\varphi_n(x) = \langle x|\varphi_n\rangle &= \frac{1}{\sqrt{n!}}\langle x|(a^\dagger)^n|\varphi_0\rangle \\ &= \frac{1}{\sqrt{n!}}\frac{1}{\sqrt{2^n}}\left[\sqrt{\frac{m\omega}{\hbar}}x - \sqrt{\frac{\hbar}{m\omega}}\frac{\mathrm{d}}{\mathrm{d}x}\right]^n \varphi_0(x)\end{aligned} \tag{C-26}$$

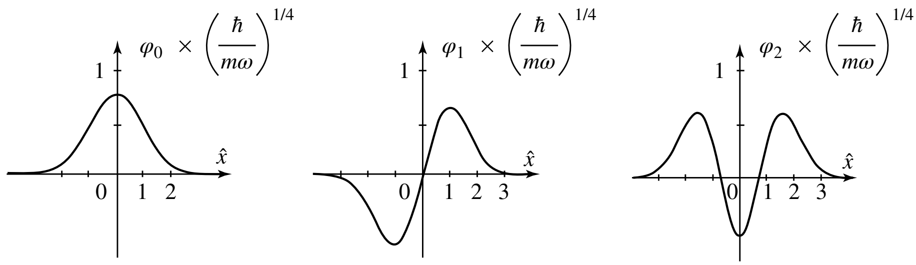

Figure 4: Wave functions associated with the first three levels of a harmonic oscillator.

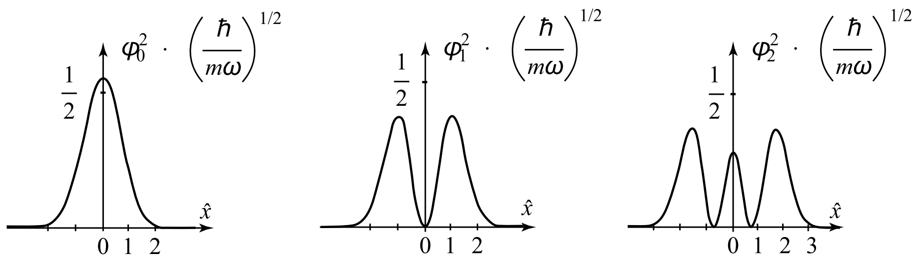

Figure 5: Probability densities associated with the first three levels of a harmonic oscillator.

that is:

$$\varphi_n(x) = \left[\frac{1}{2^n n!}\left(\frac{\hbar}{m\omega}\right)^n\right]^{1/2}\left(\frac{m\omega}{\pi\hbar}\right)^{1/4}\left[\frac{m\omega}{\hbar}x - \frac{\mathrm{d}}{\mathrm{d}x}\right]^n \mathrm{e}^{-\frac{1}{2}\frac{m\omega}{\hbar}x^2} \tag{C-27}$$

It is easy to see from this expression that $\varphi_n(x)$ is the product of $\mathrm{e}^{-\frac{1}{2}\frac{m\omega}{\hbar}x^2}$ and a polynomial of degree n and parity $(-1)^n$, called a *Hermite polynomial* (*cf.* Complements B_V and C_V).

A simple calculation gives the first several functions $\varphi_n(x)$:

$$\varphi_1(x) = \left[\frac{4}{\pi}\left(\frac{m\omega}{\hbar}\right)^3\right]^{1/4} x\,\mathrm{e}^{-\frac{1}{2}\frac{m\omega}{\hbar}x^2}$$
$$\varphi_2(x) = \left(\frac{m\omega}{4\pi\hbar}\right)^{1/4}\left[2\frac{m\omega}{\hbar}x^2 - 1\right]\mathrm{e}^{-\frac{1}{2}\frac{m\omega}{\hbar}x^2} \tag{C-28}$$

These functions are shown in Figure 4, and the corresponding probability densities in Figure 5. Figure 6 gives the shape of the wave function $\varphi_n(x)$ and that of the probability density $|\varphi_n(x)|^2$ for $n = 10$.

We see from these figures that when n increases, the region of the Ox axis in which $\varphi_n(x)$ takes on non-negligible values becomes larger. This corresponds to the fact, in classical mechanics, that the amplitude of the particle's motion increases with the energy [*cf.* Fig. 1 and relation (A-8)]. It follows that the mean value of the potential energy grows with n [*cf.* comment (*ii*) of § D-1], since $\varphi_n(x)$, when n is large, takes on non-negligible values in regions of the x-axis where $V(x)$ is large. Moreover, we see in these figures that the number of zeros of $\varphi_n(x)$ is n (*cf.* Complement B_V, where this property is derived). This implies that the mean kinetic energy of the particle increases with n [*cf.* comment (*ii*) of § D-1], since this energy is given by:

$$\frac{1}{2m}\langle P^2\rangle = -\frac{\hbar^2}{2m}\int_{-\infty}^{+\infty} \varphi_n^*(x)\frac{\mathrm{d}^2}{\mathrm{d}x^2}\varphi_n(x)\,\mathrm{d}x \qquad \text{(C-29)}$$

When the number of zeros of $\varphi_n(x)$ increases, the curvature of the wave function increases, and, in (C-29), the second derivative $\frac{\mathrm{d}^2}{\mathrm{d}x^2}\varphi_n(x)$ takes on larger and larger values.

Finally, when n is large, we observe (see, for example, Figure 6) that the probability density $|\varphi_n(x)|^2$ is large for $x \simeq \pm x_M$ [where x_M is the amplitude of the classical motion of energy E_n; *cf.* (A-8)]. This result is related to a feature of the motion predicted by classical mechanics: the classical particle has a zero velocity at $x = \pm x_M$; therefore, on the average, it spends more time in the neighborhood of these two points than in the center of the interval $-x_M \leq x \leq x_M$.

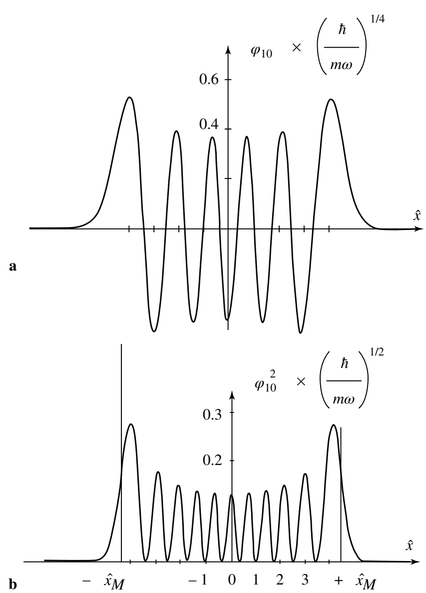

Figure 6: Shape of the wave function (fig. a) and of the probability density (fig. b) for the $n = 10$ level of a harmonic oscillator.

D. Discussion

D-1. Mean values and root mean square deviations of X and P in a state $|\varphi_n\rangle$

Neither X nor P commutes with H, and the eigenstates $|\varphi_n\rangle$ of H are not eigenstates of X or P. Consequently, if the harmonic oscillator is in a stationary state $|\varphi_n\rangle$, a measurement of the observable X or the observable P can, *a priori*, yield any result (since the spectra of X and P include all real numbers). We shall now calculate the mean values of X and P in such a stationary state and then their root mean square deviations ΔX and ΔP, which will enable us to verify the uncertainty relation.

As we indicated in § C-1-c, we shall perform these calculations with the help of the operators a and $a^\dagger$. As far as the mean values of X and P are concerned, the result follows directly from formulas (C-22), which show that neither X nor P has diagonal matrix elements:

$$\begin{aligned} &\langle\varphi_n|X|\varphi_n\rangle = 0 \\ &\langle\varphi_n|P|\varphi_n\rangle = 0 \end{aligned} \tag{D-1}$$

To obtain the root mean square deviations ΔX and ΔP, we must calculate the mean values of X^2 and P^2:

$$\begin{aligned} (\Delta X)^2 &= \langle\varphi_n|X^2|\varphi_n\rangle - (\langle\varphi_n|X|\varphi_n\rangle)^2 = \langle\varphi_n|X^2|\varphi_n\rangle \\ (\Delta P)^2 &= \langle\varphi_n|P^2|\varphi_n\rangle - (\langle\varphi_n|P|\varphi_n\rangle)^2 = \langle\varphi_n|P^2|\varphi_n\rangle \end{aligned} \tag{D-2}$$

Now, according to (B-1) and (B-7):

$$\begin{aligned} X^2 &= \frac{\hbar}{2m\omega}(a^\dagger + a)(a^\dagger + a) \\ &= \frac{\hbar}{2m\omega}(a^{\dagger 2} + aa^\dagger + a^\dagger a + a^2) \\ P^2 &= -\frac{m\hbar\omega}{2}(a^\dagger - a)(a^\dagger - a) \\ &= -\frac{m\hbar\omega}{2}(a^{\dagger 2} - aa^\dagger - a^\dagger a + a^2) \end{aligned} \tag{D-3}$$

The terms in a^2 and $a^{\dagger 2}$ do not contribute to the diagonal matrix elements, since $a^2|\varphi_n\rangle$ is proportional to $|\varphi_{n-2}\rangle$, and $a^{\dagger 2}|\varphi_n\rangle$ to $|\varphi_{n+2}\rangle$; both are orthogonal to $|\varphi_n\rangle$. On the other hand:

$$\begin{aligned} \langle\varphi_n|(a^\dagger a + aa^\dagger)|\varphi_n\rangle &= \langle\varphi_n|(2a^\dagger a + 1)|\varphi_n\rangle \\ &= 2n + 1 \end{aligned} \tag{D-4}$$

Consequently:

$$(\Delta X)^2 = \langle\varphi_n|X^2|\varphi_n\rangle = \left(n + \frac{1}{2}\right)\frac{\hbar}{m\omega} \tag{D-5a}$$

$$(\Delta P)^2 = \langle\varphi_n|P^2|\varphi_n\rangle = \left(n + \frac{1}{2}\right)m\hbar\omega \tag{D-5b}$$

The product $\Delta X.\Delta P$ is therefore equal to:

$$\Delta X.\Delta P = \left(n + \frac{1}{2}\right)\hbar \tag{D-6}$$

We again find (*cf.* Complement C_{III}) that it is greater than or equal to $\hbar/2$. In fact, this lower bound is attained for $n = 0$, that is, for the ground state (§ D-2 below).

Comments:

(*i*) If x_M denotes the amplitude of the classical motion whose energy is given by $E_n = (n + 1/2)\hbar\omega$, it is easy to see, using (A-8) and (D-5a), that:

$$\Delta X = \frac{1}{\sqrt{2}} x_M \tag{D-7}$$

Similarly, if p_M denotes the oscillation amplitude of the corresponding classical momentum:

$$p_M = m\omega\, x_M \tag{D-8}$$

we obtain:

$$\Delta P = \frac{1}{\sqrt{2}} p_M \tag{D-9}$$

It is not surprising that ΔX is of the order of the interval $[-x_M, +x_M]$ over which the classical motion occurs (*cf.* Fig. 1): we saw at the end of § C, that it is approximately inside this interval that $\varphi_n(x)$ takes on non-negligible values. Furthermore, it is easy to understand why, when n increases, so does ΔX. For large n, the probability density $|\varphi_n(x)|^2$ has two symmetric peaks situated approximately at $x = \pm x_M$. The root mean square deviation cannot be much smaller than the distance between these peaks, even if each of them is very sharp (*cf.* Chap. III, § C-5 and the discussion of § 1-b of Complement A_{III}). An analogous argument can be set forth for ΔP (*cf.* Complement D_V).

(*ii*) The mean potential energy of a particle in the state $|\varphi_n\rangle$ is:

$$\langle V(X)\rangle = \frac{1}{2} m\omega^2 \langle X^2\rangle \tag{D-10}$$

that is, since $\langle X\rangle$ is zero [*cf.* (D-1)]:

$$\langle V(X)\rangle = \frac{1}{2} m\omega^2 (\Delta X)^2 \tag{D-11}$$

Similarly, we could find the mean kinetic energy of this particle:

$$\left\langle \frac{P^2}{2m} \right\rangle = \frac{1}{2m}(\Delta P)^2 \tag{D-12}$$

Substituting relations (D-5) into (D-11) and (D-12), we obtain:

$$\langle V(X)\rangle = \frac{1}{2}\left(n+\frac{1}{2}\right)\hbar\omega = \frac{E_n}{2}$$
$$\left\langle \frac{P^2}{2m}\right\rangle = \frac{1}{2}\left(n+\frac{1}{2}\right)\hbar\omega = \frac{E_n}{2} \qquad \text{(D-13)}$$

The mean potential and kinetic energies are therefore equal. This is an illustration of the virial theorem (*cf.* exercise 10 of Complement L_{III}).

(*iii*) A stationary state $|\varphi_n\rangle$ has no equivalent in classical mechanics: its energy is not zero although the mean values $\langle X\rangle$ and $\langle P\rangle$ are. Nevertheless, there is a certain analogy between the state $|\varphi_n\rangle$ and that of a classical particle whose position is given by (A-5) [where x_M is related to the energy E_n by relation (A-8)], but for which the initial phase φ of the motion is chosen at random (all values included between 0 and 2π have the same probability). The mean values of x and p are then zero, since:

$$\begin{cases} \overline{x}_{cl} = x_M \dfrac{1}{2\pi}\displaystyle\int_0^{2\pi} \cos(\omega t-\varphi)\,\mathrm{d}\varphi = 0 \\ \overline{p}_{cl} = -p_M \dfrac{1}{2\pi}\displaystyle\int_0^{2\pi} \sin(\omega t-\varphi)\,\mathrm{d}\varphi = 0 \end{cases} \qquad \text{(D-14)}$$

Moreover, we find, for the root mean square deviations of the position and the momentum, values identical to those of the state $|\varphi_n\rangle$ [formulas (D-7) and (D-9)]:

$$\overline{x}^2_{cl} = x_M^2 \frac{1}{2\pi}\int_0^{2\pi} \cos^2(\omega t-\varphi)\,\mathrm{d}\varphi = \frac{x_M^2}{2}$$
$$\overline{p}^2_{cl} = p_M^2 \frac{1}{2\pi}\int_0^{2\pi} \sin^2(\omega t-\varphi)\,\mathrm{d}\varphi = \frac{p_M^2}{2} \qquad \text{(D-15)}$$

that is:

$$\delta x_{cl} = \sqrt{\overline{x}^2_{cl} - (\overline{x}_{cl})^2} = \frac{x_M}{\sqrt{2}}$$
$$\delta p_{cl} = \sqrt{\overline{p}^2_{cl} - (\overline{p}_{cl})^2} = \frac{p_M}{\sqrt{2}} \qquad \text{(D-16)}$$

D-2. Properties of the ground state

In classical mechanics, the lowest energy of the harmonic oscillator is obtained when the particle is at rest (zero momentum and kinetic energy) at the x-origin ($x = 0$ and therefore zero potential energy). The situation is completely different in quantum mechanics: the minimum energy state is $|\varphi_0\rangle$, whose *energy is not zero*, and the associated wave function has a certain *spatial extension*, characterized by the root mean square deviation $\Delta X = \sqrt{\hbar/2m\omega}$.

This essential difference between the quantum and classical results can be seen to have its source in the uncertainty relations, which forbid the simultaneous minimization of the kinetic energy and the potential energy. As we pointed out in Complements C_I and M_{III}, the ground state corresponds to a compromise in which the sum of these two energies is as small as possible.

In the special case of a harmonic oscillator, it is possible to state these qualitative considerations semi-quantitatively, and thus find the order of magnitude of the energy and the spatial extension of the ground state. If the distance ξ characterizes this spatial extension, the mean potential energy will be of the order of:

$$\overline{V} \simeq \frac{1}{2} m\omega^2 \xi^2 \tag{D-17}$$

But ΔP is then equal to about $\hbar/\xi$, so the mean kinetic energy is approximately:

$$\overline{T} = \frac{\overline{p^2}}{2m} \simeq \frac{\hbar^2}{2m\xi^2} \tag{D-18}$$

The order of magnitude of the total energy is therefore:

$$\overline{E} = \overline{T} + \overline{V} \simeq \frac{\hbar^2}{2m\xi^2} + \frac{1}{2} m\omega^2 \xi^2 \tag{D-19}$$

The variation of $\overline{T}$, $\overline{V}$ and $\overline{E}$ with respect to ξ is shown in Figure 7. For small values of ξ, $\overline{T}$ prevails over $\overline{V}$; the opposite occurs for large values of ξ. The ground state therefore corresponds approximately to the minimum of the function (D-19); it is easy to see that this minimum occurs at:

$$\xi_m \simeq \sqrt{\frac{\hbar}{m\omega}} \tag{D-20}$$

and is equal to:

$$\overline{E}_m \simeq \hbar\omega \tag{D-21}$$

We again find the correct orders of magnitude of E_0 and ΔX in the state $|\varphi_0\rangle$.

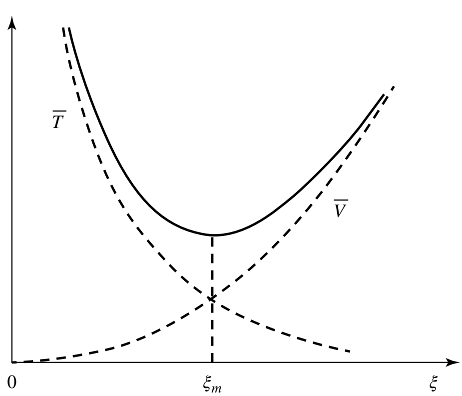

Figure 7: Variation of the potential energy $\overline{V}$ and of the kinetic energy $\overline{T}$ with respect to a parameter ξ characterizing the spatial extension of the wave function about $x = 0$. Since the potential energy is at a minimum at $x = 0$, $\overline{V}$ is a function that increases with $\xi(\overline{V} \propto \xi^2)$. On the other hand, according to Heisenberg's uncertainty relation, the kinetic energy $\overline{T}$ is a decreasing function of ξ. The lowest possible total energy, obtained for $\xi = \xi_m$, results from a compromise in which the sum $\overline{T} + \overline{V}$ (solid line) is at a minimum.

The harmonic oscillator possesses the pecularity that, because of the form of the potential $V(x)$, the product $\Delta X.\Delta P$ actually attains its lower bound, $\hbar/2$, in the ground state $|\varphi_0\rangle$ [formula (D-6)]. This is related to the fact (*cf.* Complement C_{III}) that the wave function of the ground state is Gaussian.

D-3. Time evolution of the mean values

Consider a harmonic oscillator whose state at $t = 0$ is:

$$|\psi(0)\rangle = \sum_{n=0}^{\infty} c_n(0)|\varphi_n\rangle \tag{D-22}$$

($|\psi(0)\rangle$ is assumed to be normalized). Its state $|\psi(t)\rangle$ at t can be obtained by using rule (D-54) of Chapter III:

$$\begin{aligned}|\psi(t)\rangle &= \sum_{n=0}^{\infty} c_n(0)\, \mathrm{e}^{-i\ E_n t/\hbar}|\varphi_n\rangle \\ &= \sum_{n=0}^{\infty} c_n(0)\, \mathrm{e}^{-i\left(n+\frac{1}{2}\right)\omega t}|\varphi_n\rangle \end{aligned}\tag{D-23}$$

The mean value of any physical quantity A is therefore given as a function of time by:

$$\langle\psi(t)|A|\psi(t)\rangle = \sum_{m=0}^{\infty}\sum_{n=0}^{\infty} c_m^*(0)\ c_n(0)\ A_{mn}\,\mathrm{e}^{i(m-n)\omega t} \tag{D-24}$$

with:

$$A_{mn} = \langle\varphi_m|A|\varphi_n\rangle \tag{D-25}$$

Since m and n are integers, the time evolution of the mean values involves only the frequency $\omega/2\pi$ and its various harmonics, which constitute the Bohr frequencies of the harmonic oscillator.

Let us consider, in particular, the mean values of the observables X and P. According to formulas (C-22), the only non-zero matrix elements X_{mn} and P_{mn} are those for which $m = n \pm 1$. Consequently, the mean values of X and P include only terms in $\mathrm{e}^{\pm i\omega t}$; they are sinusoidal functions of time with angular frequency ω. This obviously relates to the classical solution of the harmonic oscillator problem. Moreover, as we pointed out in the discussion of Ehrenfest's theorem (Chap. III, § D-1-d-γ), the form of the harmonic oscillator potential implies that for all $|\psi\rangle$ the mean values of X and P rigorously satisfy the classical equations of motion. Thus, according to general formulas (D-34) and (D-35) of Chapter III:

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle X\rangle = \frac{1}{i\hbar}\langle[X,H]\rangle = \frac{\langle P\rangle}{m} \tag{D-26a}$$

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle P\rangle = \frac{1}{i\hbar}\langle[P,H]\rangle = -m\omega^2\langle X\rangle \tag{D-26b}$$

If we integrate these equations, we obtain:

$$\langle X\rangle(t) = \langle X\rangle(0)\cos\omega t + \frac{1}{m\omega}\langle P\rangle(0)\sin\omega t$$
$$\langle P\rangle(t) = \langle P\rangle(0)\cos\omega t + m\omega\langle X\rangle(0)\sin\omega t \qquad \text{(D-27)}$$

We again find the sinusoidal form indicated by formula (D-24).

Comment:

It is important to note that this analogy with the classical situation appears only when $|\psi(0)\rangle$ is a superposition of states $|\varphi_n\rangle$ of the type of (D-22), where several coefficients $c_n(0)$ are non-zero. If all these coefficients except one are equal to zero, the oscillator is in a stationary state and the mean values of all the observables are constant over time.

It follows that, in a stationary state $|\varphi_n\rangle$, the behavior of a harmonic oscillator is totally different from that predicted by classical mechanics, even if n is very large (the limit of large quantum numbers). If we want to construct a wave packet whose average position oscillates over time, we must superpose different states $|\varphi_n\rangle$ (see Complement G_V).

References and suggestions for further reading:

Dirac (1.13), § 34; Messiah (1.17), Chap. XII.