9 The One-Dimensional Harmonic Oscillator

We are now ready to study in detail one of the most theoretically interesting and useful physical systems: the harmonic oscillator (HO). The HO occurs in the quantum case in a similar way to the classical case, whenever a potential can be approximated by a parabolic curve in the region of a minimum. It is therefore generally applicable to low-energy oscillations around a potential minimum, such as regularly occur in atoms or molecules, for example. Moreover, the frequent use of Fourier analysis to study complex systems in terms of elementary oscillators makes the HO an important problem in theoretical physics, in addition to its methodological interest due to the fact that it can be solved exactly.

The problem we will tackle first, solving the time-dependent Schrödinger equation, is more complicated than determining the oscillator's eigenstates and energy spectrum. However, it will give us a valuable opportunity to appreciate the similarities and differences between the dynamics of the classical and quantum oscillators. As a second step we will study the stationary solutions of the HO, which is one of the most important orthogonal sets of quantum eigenfunctions because of its many applications, properties, and relative simplicity. Further, the use of raising and lowering (or creation and annihilation) operators is shown to be a powerful way of dealing with both material and field oscillators in general. Finally, the problem of two coupled oscillators is used to generalize the Schrödinger equation to the case of more than one particle.

To simplify the treatment, we will concentrate throughout the chapter on the 1D case, which has no degeneracy; the HO in more than one dimension requires angular-momentum theory for a complete treatment, and this naturally leads to degeneracy.

9.1 A Maximally Coherent Oscillating Packet with Minimal Dispersion

We start with the study of a packet of HO, which we choose to be as mathematically simple as possible, since our interest is focused on the physics of the system. Thus, without sacrificing the physics, we focus on a Gaussian packet with both maximum coherence and minimum dispersion, a case of great interest in quantum optics today.

The potential of a 1D quantum HO is given by the usual expression

$$V(x) = \tfrac{1}{2}m\omega^2 x^2, \tag{9.1}$$

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where ω is the frequency of oscillation; its Schrödinger equation is

$$i\hbar\frac{\partial\psi}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} + \tfrac{1}{2}m\omega^2x^2\psi. \tag{9.2}$$

Let us consider a wave packet consisting of oscillators with a *Gaussian distribution* (also known as *normal distribution*) centered at x_0 and allowed to evolve freely from $t = 0$. Due to the linearity of the Schrödinger equation, the packet will retain its Gaussian structure as it evolves, so the time-dependent solution can be written in the general form[1]

$$\psi = Ae^{-\alpha(x-\gamma)^2+f(t)-f(0)}, \quad \alpha(t) > 0, \tag{9.3}$$

where $\alpha = \alpha(t)$ and $\gamma = \gamma(t)$ have initial values

$$\alpha(0) = a, \quad \gamma(0) = x_0, \tag{9.4}$$

so that (9.3) reduces for $t = 0$ to

$$\psi_0(x) \equiv \psi(x,0) = Ae^{-a(x-x_0)^2}, \tag{9.5}$$

which corresponds to an initial normal distribution with dispersion $\sigma^2 = 1/4a^2$; $f(t)$ is a function of time that modulates the Gaussian profile and A is the normalization constant.

We now introduce the proposed (anticipated) solution (9.3) in the Schrödinger equation (9.2); by eliminating the common factor ψ, we obtain

$$-i\hbar\dot{\alpha}(x-\gamma)^2 + 2i\hbar\alpha\dot{\gamma}(x-\gamma) + i\hbar\dot{f} = \frac{\hbar^2\alpha}{m} - \frac{2\hbar^2\alpha^2}{m}(x^2 - 2\gamma x + \gamma^2) + \tfrac{1}{2}m\omega^2x^2. \tag{9.6}$$

This expression contains terms in x^0, x^1 and x^2, which are linearly independent; the respective coefficients must therefore cancel between the right and left sides. The coefficient of x^2 vanishes if

$$-i\hbar\dot{\alpha} + \frac{2\hbar^2}{m}\alpha^2 = \tfrac{1}{2}m\omega^2. \tag{9.7}$$

This equation can be easily solved by writing $\alpha = \lambda\dot{u}/u$ and choosing λ so that the quadratic terms cancel out. The solution,

$$\alpha(t) = -i(m\omega/2\hbar)\cot(\omega t + \beta), \tag{9.8}$$

is a relatively complicated function, since for condition (9.4) to hold with a real, β must be imaginary. The hyperbolic functions that appear due to this expression describe a transient irreversible evolution of the packet, which is added to the periodic motions due to the harmonic terms.

[1] We make use of what is called an *ansatz* (a starting assumption). This is a common technique in physics, mathematics and engineering to solve a problem by anticipating the form of the solution, which should then be verified and refined by introducing it into the equation to be solved, taking into account boundary conditions and other details of the problem.

[2] A normal (Gaussian) distribution has the form $Ne^{-(x-\bar{x})^2/2\sigma^2}$, where $\bar{x} = \langle x\rangle$ is the average of x, $\sigma^2 = \langle x^2\rangle - \langle x\rangle^2$ is the variance of x, and $N = 1/\sqrt{2\pi}\sigma$.

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Note, however, that there is a simpler particular solution obtained by setting $\dot{\alpha} = 0$ in (9.7), which gives then $\alpha = m\omega/2\hbar$ (the negative solution is inadmissible). In this case the dispersion of x remains constant and the packet as a whole oscillates *without changing its shape*, that is, coherently, as if it were rigid. For this solution to be realized, the initial dispersion given by (9.4) must coincide with the value calculated from (9.7), $\alpha(0) = \alpha = a$. We will limit ourselves here to this simple and important case, assuming that the initial Gaussian packet has been prepared with just the required dispersion of x,

$$a = \alpha = \frac{m\omega}{2\hbar}. \tag{9.9}$$

Further, the condition that the coefficient of the terms in x vanishes gives a relation between $\dot{\gamma}$ and γ; integrating this differential equation and substituting the value of a given by (9.9) gives

$$\gamma = x_0 e^{-i\omega t}. \tag{9.10}$$

Integrating what remains of Eq. (9.6) after substituting the values of a and γ, we obtain

$$f = -\frac{i}{2}\omega t + \frac{m\omega}{4\hbar}x_0^2 e^{-2i\omega t}. \tag{9.11}$$

Substituting the preceding results into Eq. (9.3) and normalizing in the usual way gives

$$\psi(x,t) = \left(\frac{m\omega}{\pi\hbar}\right)^{\frac{1}{4}} \exp\left[-\frac{m\omega}{2\hbar}(x - x_0\cos\omega t)^2 \right.$$
$$\left. -i\left(\tfrac{1}{2}\omega t + \frac{m\omega}{\hbar}x_0 x\sin\omega t - \frac{m\omega}{4\hbar}x_0^2\sin 2\omega t\right)\right]. \tag{9.12}$$

From this wave function we can extract all the available information about the behavior of the packet. In particular, it follows that the particle spatial density is

$$\rho(x,t) = \left(\frac{m\omega}{\pi\hbar}\right)^{\frac{1}{2}} \exp\left(-\frac{m\omega}{\hbar}(x - x_0\cos\omega t)^2\right), \tag{9.13}$$

which is in fact still Gaussian for all t, with the center oscillating around the origin with frequency ω and amplitude x_0,

$$\langle x\rangle = x_0\cos\omega t, \tag{9.14}$$

just like a classical oscillator.

The packet (9.12) is a coherent superposition of eigenstates of the Hamiltonian, a particular realization of the usual superposition $\psi(x,t) = \sum_n c_n e^{-iE_n t/\hbar}\varphi_n(x)$ applied to the case at hand. Once we have the eigenstates $\varphi_n(x)$ of the oscillator's Hamiltonian, we can use them to construct this or any other packet of harmonic oscillators of interest.

Exercise E9.1. Minimum dispersion packet of harmonic oscillators
Show that the preceding solution, Eq. (9.12), describes a packet of minimum dispersion.

Solution. From Eq. (9.13) we obtain for the variance of x,

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$$\langle(\Delta x)^2\rangle = \frac{1}{4a} = \frac{\hbar}{2m\omega}. \tag{9.15}$$

The calculation of $\langle(\Delta p)^2\rangle$ gives (as the student should check)

$$\langle(\Delta p)^2\rangle = a\hbar^2 = \tfrac{1}{2}m\hbar\omega. \tag{9.16}$$

Multiplying the two previous results we verify that the packet has the minimum possible dispersion,

$$\langle(\Delta x)^2\rangle\langle(\Delta p)^2\rangle = \tfrac{1}{4}\hbar^2. \tag{9.17}$$

In Section 10.2.2 we will obtain the expression for the wave packet, Eq. (8.68), by requiring it to have minimum dispersion, here it was obtained indirectly by requiring the oscillations to be coherent. It thus corresponds to a very special packet, that of minimum dispersion (maximum organization) and coherent oscillations.

Note that the mean energy associated with the packet (9.12),

$$\langle\widehat{E}\rangle = \langle i\hbar\frac{\partial}{\partial t}\rangle = \tfrac{1}{2}\hbar\omega + \tfrac{1}{2}m\omega^2 x_0^2, \tag{9.18}$$

consists of two terms: the second term is the classical oscillation energy $\frac{1}{2}m\omega^2 x_0^2$, which may acquire any positive value and goes to zero with the oscillation amplitude x_0. The first term $\frac{1}{2}\hbar\omega$ represents the minimum energy of the system. This is the *zero-point energy* (ZPE) of the HO that remains at absolute zero temperature, when the packet is "frozen" (i.e., $x_0 = 0$). The origin and meaning of this term can be understood as follows. Even when the temperature of the system is brought down toward absolute zero, the random motion of the oscillators is maintained by the action of the ZPF. As we will see in the next chapter, the energy associated with these fluctuations is balanced by the ZPE of the field at the oscillation frequency, which is exactly $\frac{1}{2}\hbar\omega$.

This inevitable presence of fluctuations (an example of quantum fluctuations) means that we cannot simultaneously build a stationary packet of oscillators with arbitrarily small widths in x and p, since this would imply an arbitrary reduction of the initial energy, while the equilibrium energy is bounded from below at the zero point. In other words, the Heisenberg equality (9.17) is a direct consequence of the fact that the energy of the zero point is nonzero. We can therefore regard Heisenberg's inequalities as a proof of the existence of fluctuations in any quantum system at any temperature, including $T = 0$, precisely the quantum fluctuations that Heisenberg perceived. This shows that notions such as absolute standstill are incompatible with current physical knowledge. In other words, QM is a proof of the existence of irreducible background fluctuations.

To conclude this section, we should add that the ZPE produces observable effects. For example, Brindley and Wood (1929) reported X-ray scattering results from aluminum crystals that could only be explained by the existence of random motions associated with the ZPE. A second example is liquid helium, where the ZPE is so large that it prevents the liquid from solidifying under its own vapor pressure; another effect is the specific heat of the hydrogen molecule, which cannot be understood without the concept of ZPE.

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9.2 Eigenfunctions and Eigenvalues of the Hamiltonian

We now turn to the study of the eigenstates of the HO. In Chapter 3 we obtained many of its fundamental properties using the Heisenberg matrix description, which happens to be very well suited for such purposes; here we will study it from the perspective offered by the Schrödinger description, based on the wave function. The stationary 1D Schrödinger equation for the HO is

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2}+\tfrac{1}{2}m\omega^2x^2\psi=E\psi. \tag{9.19}$$

Before starting the calculations, it is highly recommended to rewrite the equation in terms of dimensionless variables, to give it a canonical form; this will be seen to have several important advantages. Since the equation is homogeneous there is no need to introduce a dimensionless wave function (since it cancels out), so we start by writing

$$x=\alpha_0\xi, \tag{9.20}$$

with α_0 a constant with dimension of length to be determined, and ξ dimensionless. Substituting in Eq. (9.19) and multiplying by $2m\alpha_0^2/\hbar^2$, we get

$$-\frac{d^2\psi}{d\xi^2}+\frac{m^2\alpha_0^4\omega^2}{\hbar^2}\xi^2\psi=\frac{2m}{\hbar^2}\alpha_0^2E\psi. \tag{9.21}$$

To simplify this expression we choose α_0 so that the coefficient of $\xi^2\psi$ is unity (this is an arbitrary choice and can be changed if convenient),

$$\alpha_0^2=\frac{\hbar}{m\omega}. \tag{9.22}$$

As the dimensionless energy variable we take

$$\epsilon=\frac{2m}{\hbar^2}\alpha_0^2E=\frac{2E}{\hbar\omega}. \tag{9.23}$$

With this choice of parameters, the eigenvalue equation (9.19) becomes (a prime represents a derivation with respect to ξ)

$$-\psi''+\xi^2\psi=\epsilon\psi. \tag{9.24}$$

Note that the procedure of eliminating physical dimensions not only greatly simplifies the differential equation and makes it more transparent and elegant, but something else is gained, which can often be important. You will never find Eq. (9.19) in a textbook on differential equations, but you will find its formal version (9.24). In addition, Eq. (9.22) tells us that the quantum oscillator has a *natural length scale* with the unit $\sqrt{\hbar/m\omega}$, while Eq. (9.23) shows that the oscillator has the quantity $\hbar\omega/2$ as a natural unit of energy. The appearance of such natural scales gives an immediate idea of the order of magnitude of the dynamical properties of the system. Another advantage of the transformation is that it makes it easy to see how many independent parameters the differential equation has. For example, Eq. (9.19) seems at first glance to suggest the presence of two independent parameters; however, Eq. (9.24) corrects this and shows that there is actually only one, namely ϵ. All these advantages (and possibly others)

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make it usually advisable to switch to the dimensionless description before starting to solve a new complicated differential problem.

We are interested in solving the eigenvalue problem associated with Eq. (9.24), rather than finding its general (mathematical) solution, which is a different problem. It is therefore convenient to devise a strategy that guarantees in advance that the solutions satisfy the *physical* conditions of the problem, in particular the boundary conditions. The strategy, conventional since its use by Schrödinger himself, consists in studying the behavior of the solutions at the boundaries, selecting those that are suitable for the problem and eliminating the rest. The application of this method to the present case will help to clarify the procedure to be followed in general.

To solve Eq. (9.24) we first study the behavior of the solution at infinity, ψ_∞. When $\xi \to \infty$, we can approximate this equation as $\psi_\infty'' - \xi^2 \psi_\infty = 0$. We have omitted the energy term, which becomes negligible with respect to the large terms in the limit. The solution of this equation has the form $\psi_\infty = e^{a\xi^2}$. Since

$$\psi_\infty'' = 2a\psi_\infty + 4a^2\xi^2\psi_\infty \approx 4a^2\xi^2\psi_\infty \quad (\text{for } \xi \to \infty), \tag{9.25}$$

with $4a^2 = 1$ the result coincides with the asymptotic equation; therefore $a = \pm\frac{1}{2}$, and the general asymptotic solution reads

$$\psi_\infty = Ae^{\frac{1}{2}\xi^2} + Be^{-\frac{1}{2}\xi^2}. \tag{9.26}$$

The condition $\psi \to 0$ as $|\xi| \to \infty$ requires taking $A = 0$; the physically acceptable solutions of (9.24) can therefore be written in the form

$$\psi = e^{-\frac{1}{2}\xi^2} u(\xi), \tag{9.27}$$

where $u(\xi)$ can be at most a polynomial in ξ, since the asymptotic behavior of ψ is already contained in the exponential factor. Indeed, it is easy to see that if u were an infinite power series, it would diverge for $|\xi| \to \infty$ and the asymptotic behavior would pass from $e^{-\frac{1}{2}\xi^2}$ to $e^{\frac{1}{2}\xi^2}$and ψ would then cease to be square-integrable and finite at all points. Substituting thus (9.27) into (9.24) and simplifying, we obtain the differential equation for the function u,

$$u'' - 2\xi u' + (\epsilon - 1)u = 0. \tag{9.28}$$

This equation and its polynomial solutions are reviewed in Appendix A, Section A.1. It is found that polynomial (and therefore regular) solutions exist if and only if the parameter $\epsilon - 1$ is an even integer,

$$\epsilon - 1 = 2n, \quad n = 0, 1, 2, \ldots \tag{9.29}$$

In this case the equation reduces to the Hermite equation

$$H_n'' - 2\xi H_n' + 2nH_n = 0, \tag{9.30}$$

whose solutions are the Hermite polynomials H_n,

$$u = H_n(\xi). \tag{9.31}$$

Therefore, the energy eigenfunctions are

$$\psi_n = C_n e^{-\frac{1}{2}\xi^2} H_n(\xi), \tag{9.32}$$

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where H_n is the Hermite polynomial of order n and C_n is the normalization constant, to be determined later. The energy eigenvalues are obtained by solving for ϵ in Eq. (9.29) and using (9.23),

$$E = \hbar\omega\left(n + \tfrac{1}{2}\right). \tag{9.33}$$

This result confirms that the energy of the ground state ($n = 0$) corresponds to the zero point, i.e., the athermal fluctuations. Starting from this minimum energy, the energy eigenvalues increase in uniform steps of value $\hbar\omega$.

The calculation of the normalization constant is greatly simplified by making effective use of the properties of Hermite polynomials, in particular, of the Rodrigues formula (A.6)

$$H_n(\xi) = (-1)^n e^{\xi^2}\frac{d^n e^{-\xi^2}}{d\xi^n}. \tag{9.34}$$

The normalization condition is written, using Eq. (9.32), as

$$\int_{-\infty}^{\infty}\psi_n^*\psi_n dx = 1 = \alpha_0\int_{-\infty}^{\infty}\psi_n^*(\xi)\psi_n(\xi)d\xi = \alpha_0|C_n|^2\int_{-\infty}^{\infty}e^{-\xi^2}H_n^2(\xi)d\xi. \tag{9.35}$$

We introduce (9.34) in this expression to eliminate a factor H_n,

$$\alpha_0|C_n|^2(-1)^n\int_{-\infty}^{\infty}H_n(\xi)\frac{d^n e^{-\xi^2}}{d\xi^n}d\xi = 1. \tag{9.36}$$

Integrating by parts n successive times, noting that all integrated terms are zero at the limits $|\xi| = \infty$, we obtain

$$\alpha_0|C_n|^2\int_{-\infty}^{\infty}e^{-\xi^2}\frac{d^n H_n(\xi)}{d\xi^n}d\xi = 1. \tag{9.37}$$

Carrying out now the derivatives indicated in (9.34), one obtains the following explicit expression for the Hermite polynomials, Eq. (A.4),

$$H_n(\xi) = (2\xi)^n - \frac{n(n-1)}{1!}(2\xi)^{n-2} + \frac{n(n-1)(n-2)(n-3)}{2!}(2\xi)^{n-4} - \ldots, \tag{9.38}$$

from which it immediately follows that

$$\frac{d^n H_n(\xi)}{d\xi^n} = 2^n n!. \tag{9.39}$$

Substituting in the normalization condition and calculating the remaining integral, which is immediate, we obtain

$$\alpha_0|C_n|^2 2^n n!\int_{-\infty}^{\infty}e^{-\xi^2}d\xi = \alpha_0|C_n|^2 2^n n!\sqrt{\pi} = 1; \tag{9.40}$$

whence, taking C_n as real and positive,

$$C_n = \left(\sqrt{\pi}\alpha_0 2^n n!\right)^{-\frac{1}{2}}. \tag{9.41}$$

This completely determines the stationary wave functions of the 1D HO.

The wave functions (9.32) decay exponentially with distance from the origin, so the particles are predominantly in the region of small values of ξ, as shown in Fig. 9.1. However, there is a finite probability that the particles will visit the classically forbidden

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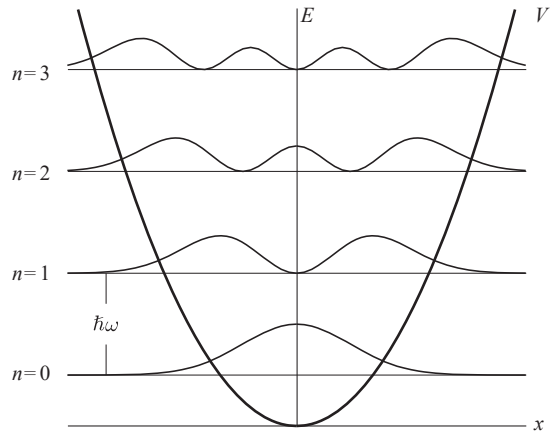


Figure 9.1 Energy levels and probability distribution for the lowest energy states of the harmonic oscillator.

region where the potential exceeds the value of the energy, as can be seen in the same figure. This is a particular example of a general property of quantum systems: the probability of visiting classically forbidden regions may turn out to be very small, but it does not generally vanish. If one adheres strictly to the interpretation of the wave function as a probability amplitude, this is another sign that in no limit does quantum behavior reduce strictly to the classical behavior, as a general rule. For an eigenstate of the Hamiltonian – for example, the ground state – with perfectly fixed energy, in these nonclassical regions the momentum of the particle takes on imaginary values, as happens inside a potential barrier or in any example where tunneling occurs.

The ground state corresponds to a Gaussian distribution centered at the origin and with variance $\langle x^2\rangle = \frac{1}{2}a_0^2 = \hbar/2m\omega$, cf. Eq. (9.15). Since H_n is a polynomial of order n, the wave function (9.32) has n zeros. This result illustrates in a particularly simple way the general rule that the number of nodes increases with n.

Exercise E9.2. The HO in the momentum representation
Solve the problem of the 1D HO in the momentum representation.

Solution. In the momentum representation we have $x^2 = -\hbar^2\partial^2/\partial p^2$ and the Schrödinger equation of the oscillator is therefore

$$\frac{p^2}{2m}\varphi(p) - \tfrac{1}{2}m\omega^2\hbar^2\frac{\partial^2\varphi(p)}{\partial p^2} = E\varphi(p). \tag{9.42}$$

In terms of the dimensionless variable $\xi = p/p_0$, with $p_0 = \sqrt{m\hbar\omega}$, this equation becomes

$$\varphi'' + (\epsilon - \xi^2)\varphi = 0, \tag{9.43}$$

where ϵ is given by Eq. (9.23). Equation (9.43) coincides with (9.24), so the solutions to this eigenvalue problem follow directly from those already obtained with a simple change of notation,

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$$\varphi_n(p) = \frac{1}{\sqrt{2^n n! \sqrt{\pi}\, p_o}} e^{-\frac{1}{2}(p/p_0)^2} H_n\,(p/p_0)\,, \tag{9.44}$$

$$E_n = \hbar\omega\left(n + \tfrac{1}{2}\right). \tag{9.45}$$

These results show that the statistical behavior of the HO in the momentum space is analogous to that in the configuration space.

Exercise E9.3. Landau[3] levels

Consider an electron moving in the xy-plane, subject to a uniform magnetic field B along the z-axis. Find the possible values of the electron's energy and the corresponding wave functions.

Solution. The Hamiltonian of the particle in a magnetic field is

$$H = \frac{1}{2}m\boldsymbol{v}^2 = \frac{1}{2m}(\boldsymbol{p} - e\boldsymbol{A})^2, \tag{9.46}$$

where $\boldsymbol{B} = \nabla \times \boldsymbol{A}$. Since $\boldsymbol{B} = B\hat{\mathbf{k}}$, we may choose $\boldsymbol{A} = Bx\hat{\mathbf{j}}$, so that the Hamiltonian reduces to

$$H = \frac{p_x^2}{2m} + \frac{1}{2m}(p_y - eB)^2, \qquad B = B_z. \tag{9.47}$$

Note that since the operator p_y commutes with H, it can be replaced by its eigenvalue $p_y = \hbar k_y$. We therefore rewrite H in the form

$$H = \frac{p_x^2}{2m} + \frac{1}{2}m\omega^2(x - \frac{\hbar k_y}{m\omega})^2, \tag{9.48}$$

where $\omega = |eB/m|$ is the Larmor frequency. This is exactly the Hamiltonian for the quantum harmonic oscillator with the minimum of the potential shifted in the x-direction by $x_0 = \hbar k_y/m\omega$. The total energy is then given by

$$H = \hbar\omega(n + \frac{1}{2}), \quad n \geq 0. \tag{9.49}$$

This result shows that the energies of the electronic motion on the xy-plane are quantized. Each set of wave functions with the same value of n,

$$\psi_n(x, y, z) = e^{ik_y y}\phi_n(x - x_0), \tag{9.50}$$

where ϕ_n are harmonic oscillator eigenstates, is called a *Landau level*. These functions describe the statistical result of the quantized oscillations on the xy-plane.

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[3] Lev Davidovich Landau (1908–1968) was a Soviet physicist who made fundamental contributions to many areas of theoretical physics, including the foundations of condensed matter physics. He was awarded the Nobel Prize in Physics in 1962 for his development of a theory of superfluidity that explains the properties of liquid helium II at low temperatures.

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9.3 Transitions Between States: Selection Rules for the Harmonic Oscillator

As mentioned in Section 3.5 and will be studied in detail in Sections 10.4.3 and 17.2, the interaction of a bound particle (e.g., an atomic electron) with the radiation field induces transitions between stationary states. The most prominent (and simplest) of these transitions are the electric dipole ones, when the interaction is proportional to the dipole moment, $e\boldsymbol{r}$. This means that when the dipole matrix element $\langle n'|e\boldsymbol{r}|n\rangle$ is different from zero, electric dipole transitions occur between the states n, n'.

We will use this information to derive the selection rules (i.e., the rules that apply to these transitions) for the 1D HO, which amounts to calculating

$$x_{n'n} = \langle n'|x|n\rangle = \int_{-\infty}^{\infty} \psi_{n'}^* x \psi_n dx. \tag{9.51}$$

The explicit calculation of this integral provides another opportunity to show how an efficient handling of the properties of special functions can greatly simplify the task. Using Eq. (9.32), we first rewrite the integral in the following form

$$x_{n'n} = \alpha_0^2 C_{n'} \int_{-\infty}^{\infty} e^{-\frac{1}{2}\xi^2} \xi H_{n'}(\xi)\psi_n(\xi)d\xi. \tag{9.52}$$

This has been done in order to use the recurrence relation of the Hermite polynomials

$$\xi H_n(\xi) = nH_{n-1}(\xi) + \tfrac{1}{2}H_{n+1}(\xi), \tag{9.53}$$

which allows us to write

$$x_{n'n} = \alpha_0^2 C_{n'} \int_{-\infty}^{\infty} \left(n' H_{n'-1} + \tfrac{1}{2} H_{n'+1}\right) e^{-\frac{1}{2}\xi^2} \psi_n(\xi)d\xi. \tag{9.54}$$

We now express each polynomial in the integrand in terms of the corresponding wave function, again using Eq. (9.32),

$$x_{n'n} = \alpha_0^2 \int_{-\infty}^{\infty} \left(\frac{n' C_{n'}}{C_{n'-1}} \psi_{n'-1}^* + \frac{C_{n'}}{2C_{n'+1}} \psi_{n'+1}^*\right) \psi_n d\xi, \tag{9.55}$$

so that taking into account the orthonormality of the wave functions, we get

$$x_{n'n} = \alpha_0 \left(\frac{n' C_{n'}}{C_{n'-1}} \delta_{n'-1,n} + \frac{C_{n'}}{2C_{n'+1}} \delta_{n'+1,n}\right). \tag{9.56}$$

This expression is different from zero only for $n' - 1 = n$ and $n' + 1 = n$, i.e., for transitions characterized by $|\Delta n| = 1$, which correspond to changes in the energy by the amount $\hbar\omega$. Spontaneous transitions (in the absence of external radiation) occur only for $n' < n$, so only the term with $n' + 1 = n$ contributes when there is no external field,

$$x_{n-1,n} = \frac{\alpha_0 C_{n-1}}{2C_n}. \tag{9.57}$$

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Inserting the values of $C_n,\ C_{n-1}$ given by Eq. (9.41) and taking into account that the matrix x is Hermitian, we get (with $\alpha_0 = \sqrt{\hbar/m\omega}$)

$$x_{n-1,n} = x_{n,n-1} = \alpha_0\sqrt{\frac{n}{2}}. \tag{9.58}$$

By substituting $n \to n+1$, we obtain the remaining nonzero matrix elements for upward (induced) transitions,

$$x_{n,n+1} = x_{n+1,n} = \alpha_0\sqrt{\frac{n+1}{2}}. \tag{9.59}$$

Note that the results obtained here by solving the Schrödinger equation are in complete agreement with those obtained in Section 3.5 using the Heisenberg matrix method.

9.4 Raising and Lowering Operators

We now study the problem of the HO from a different perspective, still using the Schrödinger approach. The present procedure is a fundamental part of quantum theory and serves as an introduction to an extremely useful method for dealing with more complicated problems.

From Eq. (9.38) it is easy to show that

$$H_n' = 2nH_{n-1}, \tag{9.60}$$

from where it follows, using (9.32), (9.41), and (9.53), that

$$\frac{1}{\sqrt{2}}\left(\xi + \frac{\partial}{\partial\xi}\right)\psi_n = \sqrt{n}\,\psi_{n-1}, \tag{9.61}$$

$$\frac{1}{\sqrt{2}}\left(\xi - \frac{\partial}{\partial\xi}\right)\psi_n = \sqrt{n+1}\,\psi_{n+1}. \tag{9.62}$$

Introducing the dimensionless operator $\widehat{p}_\xi$

$$\widehat{p}_\xi \equiv -i\frac{\partial}{\partial\xi} = \frac{1}{\sqrt{m\hbar\omega}}\widehat{p}_x, \tag{9.63}$$

we define the (*non-Hermitian*) operators

$$\widehat{a} \equiv \tfrac{1}{\sqrt{2}}(\xi + \partial_\xi) = \tfrac{1}{\sqrt{2}}(\xi + i\,\widehat{p}_\xi) \tag{9.64}$$

$$\widehat{a}^\dagger \equiv \tfrac{1}{\sqrt{2}}(\xi - \partial_\xi) = \tfrac{1}{\sqrt{2}}(\xi - i\,\widehat{p}_\xi). \tag{9.65}$$

In terms of the canonical variables these operators are

$$\widehat{a} = \frac{1}{\sqrt{2m\hbar\omega}}(m\omega x + i\,\widehat{p}), \tag{9.66}$$

$$\widehat{a}^\dagger = \frac{1}{\sqrt{2m\hbar\omega}}(m\omega x - i\,\widehat{p}), \tag{9.67}$$

in coincidence with Eqs. (3.72, 3.73).

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Equations (9.61, 9.62) then take the simple form

$$\widehat{a}\psi_n = \sqrt{n}\psi_{n-1} \tag{9.68}$$

$$\hat{a}^\dagger\psi_n = \sqrt{n+1}\psi_{n+1}. \tag{9.69}$$

We therefore identify the operator $\hat{a}^\dagger$ as the raising operator and $\widehat{a}$ as the lowering operator for the HO introduced in Section 3.5. By successively applying $a^\dagger$ to ψ_0 we get

$$\begin{aligned}
\widehat{a}^\dagger\psi_0 &= \sqrt{1}\psi_1, \\
\widehat{a}^\dagger(\widehat{a}^\dagger\psi_0) = (\widehat{a}^\dagger)^2\psi_0 &= \sqrt{1}\widehat{a}^\dagger\psi_1 = \sqrt{1\cdot 2}\psi_2, \\
\widehat{a}^\dagger(\widehat{a}^\dagger)^2\psi_0 = (\widehat{a}^\dagger)^3\psi_0 &= \sqrt{1\cdot 2}\widehat{a}^\dagger\psi_2 = \sqrt{1\cdot 2\cdot 3}\psi_3,
\end{aligned} \tag{9.70}$$

and so on. From this we see that by applying $a^\dagger$ to ψ_0 n times, we obtain an important expression for the normalized wave function of state n in terms of the normalized wave function of the ground state,

$$\psi_n = \frac{1}{\sqrt{n!}}(\widehat{a}^\dagger)^n\psi_0. \tag{9.71}$$

Taking now $n = 0$ in (9.68), we obtain

$$\widehat{a}\psi_0 = 0, \tag{9.72}$$

which, with the introduction of the differential expression of the operator $\widehat{a}$, Eq. (9.64), gives a *first-order* differential equation for the ground state,

$$\left(\xi + \frac{\partial}{\partial\xi}\right)\psi_0 = 0. \tag{9.73}$$

The normalized solution of this equation is

$$\psi_0 = C_0 e^{-\frac{1}{2}\xi^2}, \tag{9.74}$$

where C_0 is given by Eq. (9.41) with $n = 0$. From this ψ_0 we obtain ψ_n by simple successive algebraic and differentiation processes using (9.71). Note in particular that the equation $\widehat{a}\psi_0 = 0$, which *defines* the ground state, *already contains* the correct boundary condition $\psi_0(\xi) \to 0$ for $|\xi| \to \infty$, which guarantees, via Eq. (9.71), that *all* ψ_n generated with this formalism are square integrable. How this was possible can be seen by proceeding as follows. The Schrödinger equation (9.24) for the HO can be factored interchangeably in the following two forms,

$$\tfrac{1}{2}\hbar\omega\left(\xi + \frac{\partial}{\partial\xi}\right)\left(\xi - \frac{\partial}{\partial\xi}\right)\psi = \left(E + \tfrac{1}{2}\hbar\omega\right)\psi, \tag{9.75}$$

$$\tfrac{1}{2}\hbar\omega\left(\xi - \frac{\partial}{\partial\xi}\right)\left(\xi + \frac{\partial}{\partial\xi}\right)\psi = \left(E - \tfrac{1}{2}\hbar\omega\right)\psi. \tag{9.76}$$

The second of these expressions vanishes for the ground state with $E = \hbar\omega/2$; then we can *define* the ground state through the condition (9.73) whose solution (9.74) automatically satisfies the boundary condition $\psi_0 \underset{\xi\to\infty}{\to} 0$. The alternative possibility that follows from Eq. (9.75),

$$\left(\xi - \frac{\partial}{\partial\xi}\right)\psi = 0, \tag{9.77}$$

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leads to a function $C_0 e^{+\frac{1}{2}\xi^2}$ that is not square integrable.[4] Thus we see that the definition of the ground state given by Eq. (9.72) is a simple way to guarantee the correct boundary condition at infinity and an energy spectrum that is bounded from below. Incidentally, these results are at the root of method of quantization by factorization, which is used in many applications.

9.4.1 Eigenvalue equations for ψ_n

By applying $\widehat{a}^\dagger$ to Eq. (9.68) from the left and using (9.69), we get $\widehat{a}^\dagger\widehat{a}\psi_n = \sqrt{n}\widehat{a}^\dagger\psi_{n-1} = n\psi_n$. The result,

$$\widehat{a}^\dagger\widehat{a}\psi_n = n\psi_n, \tag{9.78}$$

shows that ψ_n is an eigenfunction of the operator $\widehat{a}^\dagger\widehat{a}$ with eigenvalue n. If we reverse the order of the operations, we get similarly

$$\widehat{a}\,\widehat{a}^\dagger\psi_n = (n+1)\psi_n, \tag{9.79}$$

i.e., ψ_n is also an eigenfunction of the operator $\widehat{a}\,\widehat{a}^\dagger$, but with eigenvalue $n+1$. Adding and subtracting these two results gives

$$(\widehat{a}\,\widehat{a}^\dagger + \widehat{a}^\dagger\widehat{a})\psi_n = (2n+1)\psi_n \tag{9.80}$$

and

$$(\widehat{a}\,\widehat{a}^\dagger - \widehat{a}^\dagger\widehat{a})\psi_n = \psi_n. \tag{9.81}$$

These expressions are valid for all ψ_n, so the latter is equivalent to the commutation rule obtained in Section 3.5,

$$[\widehat{a}, \widehat{a}^\dagger] = 1. \tag{9.82}$$

In turn, (9.80) suggests that the operator $\widehat{a}\,\widehat{a}^\dagger + \widehat{a}^\dagger\widehat{a}$ is proportional to the Hamiltonian. Indeed, in terms of the dimensionless variables ξ and p_ξ the Hamiltonian is

$$\widehat{H} = \frac{\widehat{p}^2}{2m} + \tfrac{1}{2}m\omega^2 x^2 = \tfrac{1}{2}\hbar\omega(\widehat{p}_\xi^2 + \xi^2). \tag{9.83}$$

For its part, from the definitions (9.64, 9.65, 9.66, 9.67) it follows that

$$\widehat{a}\,\widehat{a}^\dagger + \widehat{a}^\dagger\widehat{a} = \tfrac{1}{2}(\xi + i\,\widehat{p}_\xi)(\xi - i\,\widehat{p}_\xi) + \tfrac{1}{2}(\xi - i\,\widehat{p}_\xi)(\xi + i\,\widehat{p}_\xi) = \widehat{p}_\xi^2 + \xi^2, \tag{9.84}$$

so that

$$\widehat{H} = \tfrac{1}{2}\hbar\omega(\widehat{a}\,\widehat{a}^\dagger + \widehat{a}^\dagger\widehat{a}). \tag{9.85}$$

Eliminating from here the product $\widehat{a}\,\widehat{a}^\dagger$ by means of the commutation relation between $\widehat{a}$ and $\widehat{a}^\dagger$, we obtain a very important alternative expression for the Hamiltonian of the HO,

$$\widehat{H} = \hbar\omega\left(\widehat{a}^\dagger\widehat{a} + \tfrac{1}{2}\right). \tag{9.86}$$

[4] In this alternative ($E = -\hbar\omega/2$) the energy of the "ground" state is negative (which cannot be the case for a harmonic oscillator); since all the energy values obtained from this state by subtracting the quantity $k\hbar\omega$ are negative, there is no lower bound. This would mean that the system could spontaneously decay to an energy $-\infty$, which makes the solution physically inadmissible.

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The eigenvalues of the Hamiltonian now follow from Eqs.(9.85) and (9.80), or from (9.86) and (9.78),

$$E = \langle n|\widehat{H}|n\rangle = \hbar\omega\left(n + \tfrac{1}{2}\right). \tag{9.87}$$

These results show that using the operators $\widehat{a}$ and $\widehat{a}^\dagger$ one can study the HO problem with advantage. In this alternate description, an oscillator of frequency ω is simply a system *defined* by the trio of equations

$$\widehat{H} = \hbar\omega\widehat{a}^\dagger\widehat{a} + \tfrac{1}{2}\hbar\omega, \qquad [\widehat{a}, \widehat{a}^\dagger] = 1, \qquad \widehat{a}|0\rangle = 0, \tag{9.88}$$

$|0\rangle$ being its ground (or vacuum) state.

These equations coincide with Eqs. (3.74) and (3.75) of Chapter 3 and, as mentioned there, they are applicable to any quantum oscillator. In particular, they can be used to describe radiation field oscillators, see Section 17.5. When applied to quantized fields, the method is conventionally called *second quantization*, and $\widehat{a}^\dagger$, $\widehat{a}$ are then called *creation* and *annihilation* operators, respectively, as they increase and decrease the number of field quanta (see Section 17.6). When applied to QM, as we have just done, it is often called the *factorization method*, referring to the fact that the Hamiltonian of the excitations $\widehat{H}_{\text{eff}} \equiv \widehat{H} - \frac{1}{2}\hbar\omega$ is written as $\hbar\omega\widehat{a}^\dagger\widehat{a}$; in this case $\widehat{a}^\dagger, \widehat{a}$ are called raising and lowering operators, for the reasons explained above.

9.4.2 Algebraic construction of eigenstates and eigenvalues

The formalism introduced in the previous section lends itself to an algebraic procedure for the construction of the eigenstates and eigenvalues of the Hamiltonian, by using Eqs. (9.88). From these equations we can obtain the commutators of $\widehat{a}$ and $\widehat{a}^\dagger$ with $\widehat{H}$ (and therefore with the number operator $\widehat{a}^\dagger\widehat{a}$). For example,

$$[\widehat{H}, \widehat{a}] = \hbar\omega\left[\widehat{a}^\dagger\widehat{a}, \widehat{a}^\dagger\right] = \hbar\omega\left[\widehat{a}^\dagger\widehat{a}\,\widehat{a}^\dagger - \widehat{a}^{\dagger 2}\widehat{a}\right] = \hbar\omega\widehat{a}^\dagger\left[\widehat{a}\,\widehat{a}^\dagger - \widehat{a}^\dagger\widehat{a}\right]. \tag{9.89}$$

Thus,

$$\left[\widehat{H}, \widehat{a}^\dagger\right] = \hbar\omega\widehat{a}^\dagger, \tag{9.90}$$

and similarly,

$$[\widehat{H}, \widehat{a}] = -\hbar\omega\widehat{a}. \tag{9.91}$$

Now let $|E\rangle$ be an eigenstate of $\widehat{H}$ with eigenvalue E, $\widehat{H}|E\rangle = E|E\rangle$. Using (9.91) we get

$$\widehat{H}\widehat{a}|E\rangle = (\widehat{a}\widehat{H} - \hbar\omega\widehat{a})|E\rangle = (E - \hbar\omega)\widehat{a}|E\rangle, \tag{9.92}$$

whence $\widehat{a}|E\rangle$ is also an eigenstate of $\widehat{H}$, with eigenvalue $E - h\omega$. Successively applying the operator $\widehat{a}$ in the same way, we conclude that $\widehat{H}$ has the eigenvalues E, $E - \hbar\omega$, $E - 2\hbar\omega, \ldots, E - n\hbar\omega, \ldots$ On the other hand, we can write for the energy expectation value (recall that $\langle\widehat{F}^\dagger\widehat{F}\rangle \geq 0$ for any $\widehat{F}$)

$$E = \langle\widehat{H}\rangle = \hbar\omega\left(\langle\widehat{a}^\dagger\widehat{a}\rangle + \tfrac{1}{2}\right) \geq \tfrac{1}{2}\hbar\omega, \tag{9.93}$$

so that the minimum energy satisfies

$$E_{\min} \equiv E_0 \geq \tfrac{1}{2}\hbar\omega > 0. \tag{9.94}$$

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The process of lowering the energy with the $\widehat{a}$ operator, illustrated in Eq. (9.92), must come to an end, since $E_{\min} > 0$. This is achieved only by requiring that

$$\widehat{a}|E_0\rangle = 0, \tag{9.95}$$

so that states of lower energy can no longer be created by applying the operator $\widehat{a}$. Applying $\widehat{H}$ given to the ground state $|E_0\rangle$ then gives

$$\widehat{H}|E_0\rangle = \hbar\omega\left(\widehat{a}^\dagger\widehat{a} + \tfrac{1}{2}\right)|E_0\rangle = \tfrac{1}{2}\hbar\omega|E_0\rangle = E_0|E_0\rangle = E_{\min}|E_0\rangle. \tag{9.96}$$

Since this minimum energy is reached from E after n steps of value $\hbar\omega$, it follows that

$$E_n = \tfrac{1}{2}\hbar\omega + n\hbar\omega. \tag{9.97}$$

By iterating, it is not difficult to show that

$$|E_n\rangle = \frac{(\widehat{a}^\dagger)^n}{\sqrt{n!}}|E_0\rangle. \tag{9.98}$$

We thus verify that Eqs. (9.88) completely define a quantum HO of frequency ω.

9.4.3 The displacement operator

A displacement operator in QM effects displacements in phase space: it can change the position or the momentum or both. This operator is particularly useful in quantum optics for describing the state of radiation field modes, which are treated as quantum HOs. Similar to how the creation operator $\widehat{a}^\dagger$ generates (by successive application) the occupation number state $|n\rangle$, the displacement operator $\widehat{D}(\alpha)$ generates the *coherent state* $|\alpha\rangle$,

$$|\alpha\rangle = \widehat{D}(\alpha)\,|0\rangle\,. \tag{9.99}$$

Alternative expressions for $\widehat{D}(\alpha)$ are

$$\widehat{D}(\alpha) = e^{\alpha\widehat{a}^\dagger - \alpha^*\widehat{a}} \tag{9.100}$$

and

$$\widehat{D}(\alpha) = e^{-\frac{1}{2}|\alpha|^2} e^{\alpha\widehat{a}^\dagger} e^{-\alpha^*\widehat{a}}, \tag{9.101}$$

where α is a complex number. By applying this operator to the vacuum state, one obtains after some algebra the following expression for a coherent state in terms of number states,

$$|\alpha\rangle = e^{-\frac{1}{2}|\alpha|^2}\sum_{n=0}^{\infty}\frac{\alpha^n}{\sqrt{n!}}\,|n\rangle\,. \tag{9.102}$$

In quantum optics, coherent states are produced by a laser, which is the most coherent source of oscillations currently available (thermal light, by contrast, can be described as a statistical mixture of coherent states). Coherent states more generally have become a major topic in mathematical physics and in applied mathematics, with applications ranging from quantization to signal processing and image processing.

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Exercise E9.4. The displacement operator applied to the HO
Using (9.101) for $\widehat{D}(\alpha)$, show that this operator displaces both the $\widehat{a}$ and $\widehat{a}^\dagger$ operators. Further, show that the coherent state is an eigenstate of the annihilation operator.

Solution. To show that $\widehat{D}(\alpha)$ given by (9.101) is a displacement operator of $\widehat{a}$, we write it in the form

$$\widehat{D}(\alpha) = e^{\alpha\widehat{a}^\dagger} e^{-\frac{1}{2}|\alpha|^2 - \alpha^*\widehat{a}} \equiv e^{\alpha\widehat{a}^\dagger} F_0(\widehat{a}). \tag{9.103}$$

Using the property

$$[\widehat{a}, (\widehat{a}^\dagger)^n] = n(\widehat{a}^\dagger)^{n-1} \tag{9.104}$$

allows us to write

$$\widehat{a}\widehat{D}(\alpha) = \widehat{a}\sum \frac{\alpha^n}{n!}(\widehat{a}^\dagger)^n F_0(\widehat{a}) = \sum \frac{\alpha^n}{n!}[(\widehat{a}^\dagger)^n\widehat{a} + n(\widehat{a}^\dagger)^{n-1}]F_0(\widehat{a}). \tag{9.105}$$

Since $F_0(\widehat{a})$ and $\widehat{a}$ commute, we can write

$$\widehat{a}\widehat{D}(\alpha) = \widehat{D}(\alpha)\widehat{a} + \alpha\sum \frac{\alpha^{n-1}}{(n-1)!}(\widehat{a}^\dagger)^{n-1} F_0(\widehat{a}) = \widehat{D}(\alpha)\widehat{a} + \alpha\widehat{D}(\alpha), \tag{9.106}$$

that is,

$$\widehat{a}\widehat{D}(\alpha) = \widehat{D}(\alpha)(\widehat{a} + \alpha). \tag{9.107}$$

Multiplying by D^{-1} from the left gives

$$\widehat{D}^{-1}(\alpha)\widehat{a}\widehat{D}(\alpha) = \widehat{a} + \alpha, \tag{9.108}$$

which is the requested result. Similarly,

$$\widehat{D}^{-1}(\alpha)\widehat{a}^\dagger\widehat{D}(\alpha) = \widehat{a}^\dagger + \alpha^*. \tag{9.109}$$

This is why the $\widehat{D}(\alpha)$ operator is called the (Glauber)[5] displacement operator.

Applying Eq. (9.107) to the vacuum state $|0\rangle$ and using (9.99), we get

$$\hat{a}\,|\alpha\rangle = \alpha\,|\alpha\rangle\,, \tag{9.110}$$

which shows that the coherent state $|\alpha\rangle$ is an eigenstate of the annihilation operator, with eigenvalue α. Alternatively, one can use Eqs. (9.68) and (9.102) for the same purpose. In fact, a coherent state is *defined* as an eigenstate of the annihilation operator, as in Eq. ((9.110)).

To conclude, we note that the operator $\widehat{D}(\alpha)$ can be expressed in terms of the variables $\hat{x}$ and $\widehat{p}$, using (9.100). With $\widehat{a} = \frac{1}{\sqrt{2}}(\frac{\hat{x}}{\alpha_0} + i\frac{\alpha_0}{\hbar}\widehat{p}), \widehat{a}^\dagger = \frac{1}{\sqrt{2}}(\frac{\hat{x}}{\alpha_0} - i\frac{\alpha_0}{\hbar}\widehat{p}), \alpha_0 = \sqrt{\hbar/m_0\omega}$, we get

[5] Roy Jay Glauber (1925)–(2018) was a US-born theoretical physicist, best known for his work on optical coherence and his model of photodetection. He was awarded the Nobel Prize in 2005 for his pioneering contributions to quantum optics.

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$$\alpha\hat{a}^\dagger - \alpha^*\hat{a} = i(k\hat{x} - r\hat{p}),$$
$$k = \frac{\sqrt{2}}{\alpha_0}\mathrm{Im}\alpha, \quad r = \sqrt{2}\alpha_0\,\mathrm{Re}\,\alpha, \tag{9.111}$$

whence

$$\hat{D}(\alpha) = e^{i(k\hat{x} - r\hat{p})}. \tag{9.112}$$

The fact that this operator depends on both the $\hat{x}$ and $\hat{p}$ operators can be used to construct a specific quantum description in phase space.

9.4.4 Time dependence of elementary operators

Applying the Heisenberg equation of motion $i\hbar\dot{\hat{F}} = [\hat{F}, \hat{H}]$ to the operator $\hat{a}$ and using (9.91), we get

$$\dot{\hat{a}} = -i\omega\hat{a}, \tag{9.113}$$

with solution

$$\hat{a} = \hat{a}_0 e^{-i\omega t}, \quad \hat{a}_0 = \hat{a}(0), \tag{9.114}$$

and similarly,

$$\hat{a}^\dagger = \hat{a}_0^\dagger e^{i\omega t}. \tag{9.115}$$

Reversing Eqs. (9.64, 9.65) and using the preceding results, we obtain the expressions that determine the time evolution of $\hat{x}$ and $\hat{p}$,

$$\hat{x}(t) = \frac{\alpha_0}{\sqrt{2}}(\hat{a} + \hat{a}^\dagger) = \sqrt{\frac{\hbar}{2m\omega}}(\hat{a}_0 e^{-i\omega t} + \hat{a}_0^\dagger e^{i\omega t}) \tag{9.116}$$

$$\hat{p}(t) = \frac{\hbar}{i\sqrt{2}\alpha_0}(\hat{a} - \hat{a}^\dagger) = -i\sqrt{\frac{m\omega\hbar}{2}}(\hat{a}_0 e^{-i\omega t} - \hat{a}_0^\dagger e^{i\omega t}), \tag{9.117}$$

or in terms of $\hat{x}_0$ and $\hat{p}_0$,

$$\hat{x} = \hat{x}_0 \cos\omega t + \frac{\hat{p}_0}{m\omega}\sin\omega t, \tag{9.118}$$

$$\hat{p} = \hat{p}_0 \cos\omega t - m\omega\hat{x}_0 \sin\omega t, \tag{9.119}$$

which correspond to the elementary oscillators obtained in Chapter 3. Note that the quantum and classical expressions are formally identical.

Exercise E9.5. Time-dependent commutators

As is clear from Eqs. (9.118, 9.119), operators that commute at equal times do not necessarily commute at different times. Calculate the commutation relations $[\hat{x}(t), \hat{x}_0]$, $[\hat{x}(t), \hat{p}_0]$, and the corresponding Heisenberg inequalities for the HO, for arbitrary t.

Solution. Using Eqs. (9.118, 9.119) and the basic quantum commutators, we get

$$[\hat{x}(t), \hat{x}_0] = \frac{1}{m\omega}[\hat{p}_o, \hat{x}_0]\sin\omega t = \frac{-i\hbar}{m\omega}\sin\omega t,$$
$$[\hat{x}(t), \hat{p}_0] = [\hat{x}_o, \hat{p}_0]\cos\omega t = i\hbar\cos\omega t$$

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$$\Delta\widehat{x}(t)\Delta\widehat{x}_0 \geq \frac{\hbar}{2m\omega}|\sin\omega t|,$$
$$\Delta\widehat{x}(t)\Delta\widehat{p}_0 \geq \tfrac{1}{2}\hbar|\cos\omega t|. \tag{9.120}$$

Note that for the free particle ($\omega \to 0$), the first commutator becomes $[\widehat{x}(t), \widehat{x}_0] = -i\hbar t/m$; the corresponding Heisenberg inequality indicates that in this case the dispersion of x increases linearly with time for not too long times.

9.5 Two Coupled Harmonic Oscillators

The coupled HO problem is interesting from both a physical and a mathematical point of view. Physically, because it allows modeling the small-amplitude oscillations of composite systems, such as the internal oscillations of polyatomic molecules. Mathematically, because it raises a new problem: the need to generalize the Schrödinger equation to the case of more than one particle. We will deal with the latter here specifically for the HO, with more detailed discussions in subsequent chapters.

We write the stationary Schrödinger equation in the form

$$E\psi = \widehat{H}\psi, \tag{9.121}$$

and proceed to the case of more than one particle by writing the total Hamiltonian as the sum of the contribution of each individual Hamiltonian H_i, plus the contributions due to their mutual interactions, that is,[6]

$$\widehat{H} = \sum_i \widehat{H}_i + \sum_{i>j} \widehat{H}_{ij}, \tag{9.122}$$

with $i, j = 1, 2, \ldots, N$,

$$\widehat{H}_i = \frac{\widehat{\boldsymbol{p}}_i^2}{2m_i} + V(\boldsymbol{r}_i) = -\frac{\hbar^2}{2m_i}\nabla_i^2 + V(\boldsymbol{r}_i), \tag{9.123}$$

the Hamiltonian of the particle i, and

$$\widehat{H}_{ij} = V(\boldsymbol{r}_i, \boldsymbol{r}_j) \tag{9.124}$$

the interaction potential between particles i and j. For example, for two harmonically coupled collinear 1D harmonic oscillators of frequencies ω_1 and ω_2, and equal mass m, we have, assuming a bilinear interaction,

$$\widehat{H} = -\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial x_1^2} + \frac{\partial^2}{\partial x_2^2}\right) + \tfrac{1}{2}m\omega_1^2 x_1^2 + \tfrac{1}{2}m\omega_2^2 x_2^2 - m\omega_{12}^2 x_1 x_2. \tag{9.125}$$

Let us solve this problem as an example; the ideas we will use are directly applicable to any number of coupled oscillators, in any number of dimensions.

[6] This procedure is common and, in a sense, shared with classical physics. In neither of these theories are there rules that specify the Hamiltonian; it has to be constructed from empirical principles. In QM, the most common recipe is to start with the corresponding classical Hamiltonian, as is done here, and give it the appropriate quantum avail for the particular case.

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In the corresponding classical problem, the solution is obtained by moving to a new coordinate system y related to the original system x by means of an orthogonal transformation that diagonalizes the matrix of the coupling constants (of the frequencies, in the present notation). In the y-system the variables separate, reducing the problem to that of two decoupled oscillators, each oscillating at its own frequency. For this reason, the y_i are called *normal* coordinates and the characteristic frequencies are the normal modes of oscillation.

We will show that the same separation can be used in the quantum case. The task is simplified by introducing the column matrix x of two components

$$x = \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} \tag{9.126}$$

and the new variables $y_i = \sum_j a_{ij} x_j$ $(i, j = 1, 2)$ also in matrix form,

$$y = ax, \tag{9.127}$$

where y is a column matrix with components y_1, y_2, and a is a 2×2 matrix. Let b correspond to the inverse of a,

$$x = by, \quad b = a^{-1}. \tag{9.128}$$

From (9.127) we have

$$\frac{\partial}{\partial x_i} = \sum_j \frac{\partial y_j}{\partial x_i} \frac{\partial}{\partial y_j} = \sum_j a_{ji} \frac{\partial}{\partial y_j} = \sum_j a^T_{ij} \frac{\partial}{\partial y_j}, \tag{9.129}$$

where a^T is the transpose of a. From this it follows that if $\widehat{p}_x$ is the matrix of the momenta in terms of the variables x, and $\widehat{p}_y$ the corresponding matrix expressed in terms of the variables y, then

$$\widehat{p}_x = a^T \widehat{p}_y. \tag{9.130}$$

We can now write the kinetic energy operator in the form

$$\widehat{T} \equiv \frac{1}{2m} \widehat{p}_x^T \widehat{p}_x = \frac{1}{2m} \widehat{p}_y^T a a^T \widehat{p}_y. \tag{9.131}$$

For the potential energy we get

$$V \equiv \tfrac{1}{2} m x^T \omega^2 x = \frac{m}{2} y^T b^T \omega^2, \quad \text{with } \omega^2 = \begin{pmatrix} \omega_1^2 & -\omega_{12}^2 \\ -\omega_{12}^2 & \omega_2^2 \end{pmatrix}. \tag{9.132}$$

For (9.131) to be reduced to a quadratic form in the variables p_y, we take

$$a a^T = 1, \tag{9.133}$$

which is true if the matrix a is orthogonal, i.e., if

$$a^T = a^{-1} = b. \tag{9.134}$$

On the other hand, for the potential energy to be reduced to a quadratic form in the variables y and for the problem to become separable, it is required that

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$$b^T \omega^2 b = \Omega^2, \tag{9.135}$$

where Ω^2 is a diagonal matrix. With (9.134), this condition takes the form

$$a\omega^2 a^{-1} = \Omega^2, \tag{9.136}$$

that is, a is the matrix that diagonalizes the matrix ω^2. The procedure leads to the normal modes of the system, which are the independent modes. As already mentioned, these results are the same as the classical ones.

Suppose we have made the transition to the normal coordinate system y; the Hamiltonian is now

$$\widehat{H} = \widehat{H}_1 + \widehat{H}_2, \tag{9.137}$$

where

$$\widehat{H}_1 = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial y_1^2} + \tfrac{1}{2}m\Omega_1^2 y_1^2, \tag{9.138}$$

and similarly for $\widehat{H}_2$; Ω_1^2 and Ω_2^2 are the eigenvalues of the matrix Ω^2, that is, the solutions of Eq. (9.136). It is left to the student as an exercise to find these solutions. Since $\hat{H}$ is now the sum of two independent terms, the wave function is factorizable in terms of the respective eigenfunctions,

$$\psi(y_1, y_2) = \psi_{n_1}(y_1)\psi_{n_2}(y_2), \tag{9.139}$$

as can be verified by substituting in the Schrödinger equation,

$$\begin{aligned}\widehat{H}\psi &= (\widehat{H}_1 + \widehat{H}_2)\psi_1(1)\psi_2(2) \\ &= (\widehat{H}_1\psi_1)\psi_2 + \psi_1(\widehat{H}_2\psi_2) = E_1\psi_1\psi_2 + E_2\psi_1\psi_2 = (E_1 + E_2)\psi,\end{aligned} \tag{9.140}$$

and the total energy is the sum of the respective energy eigenvalues,

$$E = E_1 + E_2. \tag{9.141}$$

Since $\psi_{n_1}(y_1)$ and $\psi_{n_2}(y_2)$ are the eigenfunctions of the HO in states n_1 and n_2, respectively, the total energy E is

$$E = \hbar\Omega_1\left(n_1 + \tfrac{1}{2}\right) + \hbar\Omega_2\left(n_2 + \tfrac{1}{2}\right). \tag{9.142}$$

The product wave function (9.139) indicates that the oscillators y_i are uncorrelated; this is how the orthogonality of the normal coordinates manifests itself in the quantum case. With respect to the original variables x_i, the oscillators are correlated and the corresponding wave function is not factorizable, since

$$\psi(x_1, x_2) = \psi_{n_1}(a_{11}x_1 + a_{12}x_2)\psi_{n_2}(a_{21}x_1 + a_{22}x_2). \tag{9.143}$$

The total energy, Eq. (9.142), is obtained by solving Eq. (9.136); the fact that this is a quadratic equation for Ω indicates a splitting of the energy levels, due to the coupling of the oscillators. In Section 13.3.2 this problem is revisited to illustrate the application of perturbation theory.

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Problems

P9.1 Derive explicitly Eqs. (9.15) and (9.16) for the minimum-dispersion packet.

P9.2 Show that the stationary states of the harmonic oscillator satisfy the following relations:

$$E_n = m\omega^2 \langle n|x^2|n\rangle; \quad \langle n|\widehat{T}|n\rangle = \langle n|\widehat{V}|n\rangle = \tfrac{1}{2}E_n. \tag{9.144}$$

Discuss these results from the point of view of the virial theorem.

P9.3 Determine the energy eigenvalues for the 1D Schrödinger equation with the potential

$$V(x) = \begin{cases} \frac{1}{2}m\omega^2 x^2, & x > 0; \\ +\infty, & x < 0. \end{cases} \tag{9.145}$$

P9.4 Find the probability that the particles lie within the classically allowed range for the eigenstates of the HO, and determine the value of this probability for the ground state. *Note*: $\mathrm{erf}(1) = 0.8427\ldots$

P9.5 Small-amplitude vibrations in diatomic molecules can be studied using as a model for molecular vibrational potential the potential of the HO, $V(x) = \frac{1}{2}k_f x^2$, with k_f the force constant. For a typical diatomic molecule, $k_f \simeq 1 \times 10^3\ \mathrm{J{\cdot}m^{-2}}$.

a) Use this data to estimate the value of the zero-point vibrational energy.
b) Estimate the spacing, in energy, between two successive states.

P9.6 Solve the 3D HO problem in Cartesian coordinates. Discuss the degeneracy for the isotropic case.

P9.7 A one-dimensional oscillator moves in the external electric field generated by the potential $-e\mathcal{E}x(t)$.

a) State the equations of motion for $\hat{x}(t)$ and $\hat{p}(t)$ and show that they have precisely the form of the corresponding classical equations.
b) Solve for $\hat{x}(t)$ and $\hat{p}(t)$ as a function of $\hat{x}(0)$ and $\hat{p}(0)$.
c) Determine the commutation relations $[x(t_1), x(t_2)]$ for arbitrary $t_1 - t_2$.

P9.8 Consider a HO of frequency ω in its ground state. At time $t = 0$, the oscillation frequency is abruptly reduced to the value $\omega' = \omega/k$, with $1 < k < \infty$. Calculate $\psi(x,t)$ for $t > 0$. Determine:

a) the probability that the system is in the eigenstate with energy E_n at time t;
b) the value of n for which this probability reaches its maximum.

Discuss the results.

P9.9 Derive the evolution equations for $\langle\hat{x}\rangle$ and $\langle\hat{p}\rangle$ for systems with Hamiltonians

$$\widehat{H} = \frac{\hat{p}^2}{2m} + \frac{1}{2}m\left(\omega^2 x^2 + \beta x + \mathcal{E}\right), \tag{9.146}$$

$$\widehat{H} = \frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega^2 x^2 - \frac{A}{x^2}. \tag{9.147}$$

Solve the equations for the first case.

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P9.10 Derive the creation and annihilation operators for the HO, based on the description of the system in momentum space.

P9.11 Calculate the matrix elements x_{nm} and x^2_{nm} for the HO, using $x = \sqrt{\frac{\hbar}{2m\omega}}$ $(\widehat{a} + \widehat{a}^\dagger)$ and Eqs. (9.68, 9.69).

P9.12 Show that

$$e^{\lambda\widehat{a}}\widehat{a}^\dagger e^{-\lambda\widehat{a}} = \widehat{a}^\dagger + \lambda, \tag{9.148}$$

$$e^{\lambda\widehat{a}^\dagger}\widehat{a}e^{-\lambda\widehat{a}^\dagger} = \widehat{a} - \lambda, \tag{9.149}$$

$$e^{\lambda\widehat{a}} f(\widehat{a},\widehat{a}^\dagger)e^{-\lambda\widehat{a}} = f(\widehat{a},\widehat{a}^\dagger + \lambda), \quad \text{and so on.} \tag{9.150}$$

where f represents a function admitting a power series expansion of $\widehat{a}$ and $\widehat{a}^\dagger$.

P9.13 Determine the eigenvalues of the Hamiltonian

$$\widehat{H} = h_0\widehat{a}^\dagger\widehat{a} + h_1(\widehat{a} + \widehat{a}^\dagger). \tag{9.151}$$

Hint: Introduce a new pair of creation and annihilation operators that diagonalize $\widehat{H}$.

P9.14 Show that if $\hat{A} = \hat{A}(t = 0)$ is an operator at time $t = 0$, then $\hat{A}(-t)\psi(x,t) = A\psi(x,t)$, where $\psi(x,0)$ is the eigenstate of $\hat{A}$. Use this result to build the Feynman propagator of the harmonic oscillator. Verify that it approaches the free-particle propagator as $\omega \to 0$. Why does the same happen for ω fixed $(< \infty)$ when $t - t' \to 0$?

P9.15 Prove that if $f(\widehat{a}^\dagger)$ is a polynomial in $\widehat{a}^\dagger$, then

$$\widehat{a} f(\widehat{a}^\dagger)\,|0\rangle = \frac{df(\widehat{a}^\dagger)}{d\widehat{a}^\dagger}\,|0\rangle\,, \tag{9.152}$$

$$e^{\lambda a} f(\widehat{a}^\dagger)\,|0\rangle = f(\widehat{a}^\dagger + \lambda)\,|0\rangle\,. \tag{9.153}$$

P9.16 Prove that

$$e^{\alpha\widehat{a}+\beta\widehat{a}^\dagger} = e^{\alpha\widehat{a}}e^{\beta\widehat{a}^\dagger}e^{-\alpha\beta\hbar/2}. \tag{9.154}$$

P9.17 Calculate the normal frequencies Ω_1 and Ω_2 of the Hamiltonian given by Eq. (9.125).

P9.18 Two particles with masses m_1 and m_2 moving along a straight line interact through the potential $V(x_1,x_2) = a(x_1 - x_2) + b(x_1 - x_2)^2$, $b > 0$. Determine the eigenenergies and the corresponding wave functions.

Bibliographical Notes

The techniques developed in this chapter are widely used in quantum optics. Standard references are Mandel and Wolf (1995), Cohen-Tannoudji et al. (1977), and Scully and Zubairy (1997).

At a more accessible level, chapter 3 of Gerry and Knight (2012) focuses on coherent states in quantum optics.

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