Chapter 5

The Quantum Harmonic Oscillator

In this Chapter we start our analysis of a number of simple Hamiltonians that are both practically and conceptually relevant to understand some of the emergent phenomena in quantum mechanics. The main task will be to solve the Schrödinger equation for these Hamiltonians, both in the static and in the time-dependent case.

5.1 Stationary States

We start our analysis with the simple harmonic oscillator in one dimension. The Hamiltonian in this case is given by

$$\hat{H} \;=\; \frac{\hat{p}^2}{2m} \;+\; \frac{1}{2}\, m\omega^2\, \hat{x}^2, \tag{5.1.1}$$

where the first term is the usual kinetic energy and the second one represents the energy of a "spring" connected to the mass m. While this is a highly idealized model, it is often very useful to understand molecular vibrations in solids or even the behavior of diluted atoms confined with light. It is therefore essential, for any physicist, to know how to solve this quantum Hamiltonian and understand its qualitative and quantitative features.

We start determining the eigenstates of the Hamiltonian. There are several techniques to derive them; in this Chapter we will follow the so-called "ladder method." We define for this purpose a pair of so-called annihilation and creation operators (for reasons to be clarified later) with the following form:

$$\hat{a} \;=\; \sqrt{\frac{m\omega}{2\hbar}}\left(\hat{x} \;+\; \frac{i\,\hat{p}}{m\omega}\right), \quad \hat{a}^\dagger \;=\; \sqrt{\frac{m\omega}{2\hbar}}\left(\hat{x} \;-\; \frac{i\,\hat{p}}{m\omega}\right). \tag{5.1.2}$$

These are non-Hermitian operators (thus, they cannot be directly measured); however, they are conceptually very useful to determine the eigenstates of our Hamiltonian. We first notice that

$$\begin{aligned}\left[\hat{a},\,\hat{a}^\dagger\right] &= \frac{m\omega}{2\hbar}\left[\hat{x} + \frac{i\,\hat{p}}{m\omega},\,\hat{x} - \frac{i\,\hat{p}}{m\omega}\right] \\ &= \frac{m\omega}{2\hbar}\,\frac{i}{m\omega}\Big(-\left[\hat{x},\,\hat{p}\right] \;+\; \left[\hat{p},\,\hat{x}\right]\Big) \\ &= \frac{m\omega}{2\hbar}\,\frac{2\,\hbar\, i}{m\omega} \;=\; 1.\end{aligned}$$

We further define the so-called "number operator"

$$\hat{N} \;=\; \hat{a}^\dagger\,\hat{a}, \tag{5.1.3}$$

this is manifestly Hermitian, and it is directly connected to the Hamiltonian. We can see that

$$\begin{aligned}\hat{N} &= \frac{m\omega}{2\hbar}\Big(\hat{x}^2 \;-\; \frac{i}{m\omega}\,\hat{p}\,\hat{x} \;+\; \frac{i}{m\omega}\,\hat{x}\,\hat{p} \;+\; \frac{\hat{p}^2}{m^2\,\omega^2}\Big) \\ &= \frac{m\omega}{2\hbar}\Big(\frac{\hat{p}^2}{m^2\,\omega^2} \;+\; \hat{x}^2 \;-\; \frac{\hbar}{m\omega}\Big) \\ &= \frac{1}{\hbar\,\omega}\Big(\frac{\hat{p}^2}{2m} \;+\; \frac{1}{2}\,m\omega^2\,\hat{x}^2\Big) \;-\; \frac{1}{2} \\ &= \frac{\hat{H}}{\hbar\,\omega} \;-\; \frac{1}{2}.\end{aligned}$$

Thus the Hamiltonian is (apart from scaling factors and a constant shift) identical to the number operator:

$$\hat{H} \;=\; \hbar\,\omega\Big(\hat{N} \;+\; \frac{1}{2}\Big), \tag{5.1.4}$$

therefore it is also true that $[\hat{H},\,\hat{N}] = 0$ and that the eigenvalues and eigenvectors of $\hat{N}$ are essentially the same as those of $\hat{H}$. We denote these eigenvalues and eigenvectors with

$$\hat{N}\;|n\rangle \;=\; n\;|n\rangle\,, \tag{5.1.5}$$

and it will be shown in a moment that the eigenvalues n are positive integers. We start showing that $n \geq 0$. Indeed, we use the fact that

$$\|\hat{a}\;|n\rangle\,\|^2 \;\geq\; 0, \tag{5.1.6}$$

and the eigenvalue equation for the number operator

$$\|\hat{a}\;|n\rangle\,\|^2 \;=\; \langle n|\;\hat{a}^\dagger\hat{a}\;|n\rangle \;=\; n \;\geq\; 0. \tag{5.1.7}$$

It is also useful to derive the commutation relations satisfied between the number operator and the creation/annihilation operators:

$$\left[\hat{N},\,\hat{a}^\dagger\right] \;=\; \left[\hat{a}^\dagger\hat{a},\,\hat{a}^\dagger\right] \;=\; \hat{a}^\dagger, \tag{5.1.8}$$

and

$$\left[\hat{N},\,\hat{a}\right] \;=\; \left[\hat{a}^\dagger\hat{a},\,\hat{a}\right] \;=\; -\,\hat{a}. \tag{5.1.9}$$

With these in hand, we are now ready to show that the states $\hat{a}^\dagger |n\rangle$ and $\hat{a}\,|n\rangle$ are eigenstates of $\hat{N}$ with eigenvalues $n+1$ and $n-1$ respectively. We see this directly:

$$\hat{N}\Big(\hat{a}^\dagger |n\rangle\Big) \;=\; \Big[\hat{N},\, \hat{a}^\dagger\Big] |n\rangle \;+\; \hat{a}^\dagger\, \hat{N}\, |n\rangle \;=\; \hat{a}^\dagger |n\rangle \;+\; n\, \hat{a}^\dagger |n\rangle \;=\; (n+1)\, \hat{a}^\dagger |n\rangle\,, \qquad (5.1.10)$$

and

$$\hat{N}\Big(\hat{a}\,|n\rangle\Big) \;=\; \Big[\hat{N},\, \hat{a}\Big] |n\rangle \;+\; \hat{a}\, \hat{N}\, |n\rangle \;=\; -\,\hat{a}\,|n\rangle \;+\; n\, \hat{a}\,|n\rangle \;=\; (n-1)\, \hat{a}\,|n\rangle\,. \qquad (5.1.11)$$

We thus see that

$$\hat{a}^\dagger |n\rangle \;=\; \alpha_n\, |n+1\rangle\,, \qquad \hat{a}\,|n\rangle \;=\; \beta_n\, |n-1\rangle\,, \qquad (5.1.12)$$

where the constants α_n and β_n can be determined by imposing normalization conditions. For example,

$$\langle n+1|n+1\rangle \;=\; \frac{\langle n|\; \hat{a}\, \hat{a}^\dagger\; |n\rangle}{|\alpha_n|^2} \;=\; \frac{\langle n|\; (\hat{N} + [\hat{a},\, \hat{a}^\dagger])\; |n\rangle}{|\alpha_n|^2} \;=\; \frac{n+1}{|\alpha_n|^2}, \qquad (5.1.13)$$

thus $|\alpha_n|^2 \;=\; n+1$. Similarly, one can show $|\beta_n|^2 \;=\; n$. For simplicity we can take $\alpha_n = \sqrt{n+1}$ and $\beta_n = \sqrt{n}$, giving the fundamental equations

$$\hat{a}^\dagger |n\rangle \;=\; \sqrt{n+1}\; |n+1\rangle\,, \qquad \hat{a}\,|n\rangle \;=\; \sqrt{n}\; |n-1\rangle\,. \qquad (5.1.14)$$

These two equations also imply that n must be a nonnegative integer. If this were not the case, by repeated applications of the destruction operator we could find a negative eigenvalue, which is not possible, as we have already demonstrated. If instead $n \geq 0$, then the destruction operator terminates with the null state $|0\rangle$, corresponding to $n = 0$. The sequence of eigenstates is then simply given as

$$|0\rangle\,, \quad |1\rangle \;=\; \hat{a}^\dagger\, |0\rangle\,, \quad |2\rangle \;=\; \frac{(\hat{a}^\dagger)^2}{\sqrt{2}}\; |0\rangle\,, \quad |3\rangle \;=\; \frac{(\hat{a}^\dagger)^3}{\sqrt{6}}\; |0\rangle\,, \quad \ldots \quad |n\rangle \;=\; \frac{(\hat{a}^\dagger)^n}{\sqrt{n!}}\; |0\rangle\,.$$

The eigenvalues of the Hamiltonian are instead simply

$$E(n) \;=\; \hbar\,\omega\Big(n \;+\; \frac{1}{2}\Big), \qquad (5.1.15)$$

thus since n is an integer, we see once more a quantization of the energy levels, whereas in the classical case we would expect the internal energy of the harmonic oscillator to be continuous.

5.1.1 Eigenstates in real space

We have now determined the full spectrum of eigenvalues and eigenvectors of the harmonic oscillator Hamiltonian, but we have not explicitly found the functional form for the eigenstates. To do so, we need to specify a convenient basis. We now consider the position basis, since it is quite natural to reason in terms of position amplitudes, at least to start developing some intuition about quantum behavior. Consider, for example, the ground-state amplitude

$$\langle x\,|0\rangle \;=\; \phi_0(x). \qquad (5.1.16)$$

We can solve for the function $\phi_0(x)$ using the fact that

$$\hat{a}\;|0\rangle \;=\; 0, \tag{5.1.17}$$

and recalling the definition of the destruction operator in terms of position and momentum operators:

$$\hat{a} \;=\; \sqrt{\frac{m\omega}{2\,\hbar}}\Big(\hat{x} \;+\; \frac{i\,\hat{p}}{m\omega}\Big),$$

thus

$$\langle x|\hat{a}\,|0\rangle \;=\; \sqrt{\frac{m\omega}{2\,\hbar}}\Big(x \;+\; \frac{\hbar}{m\,\omega}\,\frac{d}{dx}\Big)\phi_0(x) \;=\; 0. \tag{5.1.18}$$

Define a convenient length scale $x_0 = \sqrt{\hbar/(m\,\omega)}$, and explicitly solve this differential equation. It is easily verified that the normalized ground-state wave function that solves it reads

$$\phi_0(x) \;=\; \frac{1}{\pi^{1/4}\,\sqrt{x_0}}\,\exp\Big[-\frac{1}{2}\Big(\frac{x}{x_0}\Big)^2\Big], \tag{5.1.19}$$

which is a special case of the Gaussian wave packet.

Uncertainty product

In that context, we have already evaluated expectation values of physical quantities over this type of wave function, but it is also interesting to see how one can compute expectation values of functions of $\hat{x}$ and $\hat{p}$ using the creation and annihilation operators $\hat{a}$ and $\hat{a}^\dagger$. Considering again their definitions,

$$\hat{a} \;=\; \sqrt{\frac{1}{2\,x_0^2}}\Big(\hat{x} \;+\; \frac{i\,\hat{p}}{m\omega}\Big), \quad \hat{a}^\dagger \;=\; \sqrt{\frac{1}{2\,x_0^2}}\Big(\hat{x} \;-\; \frac{i\,\hat{p}}{m\omega}\Big). \tag{5.1.20}$$

we have

$$\hat{x} \;=\; \sqrt{\frac{x_0^2}{2}}\Big(\hat{a} \;+\; \hat{a}^\dagger\Big), \quad \hat{p} \;=\; -\,i\,\sqrt{\frac{\hbar^2}{2\,x_0^2}}\Big(\hat{a} \;-\; \hat{a}^\dagger\Big). \tag{5.1.21}$$

From these expressions it immediately follows that

$$\langle 0|\hat{x}|0\rangle \;=\; 0, \quad \langle 0|\hat{p}|0\rangle \;=\; 0, \tag{5.1.22}$$

since, in general, only expectations of operators containing products of an equal number of $\hat{a}$ and $\hat{a}^\dagger$ will be different from zero. The situation is different for higher orders of the particle coordinates and momenta, since

$$\hat{x}^2 \;=\; \frac{x_0^2}{2}\Big(\hat{a}\,\hat{a} \;+\; \hat{a}^\dagger\,\hat{a}^\dagger \;+\; \hat{a}\,\hat{a}^\dagger \;+\; \hat{a}^\dagger\,\hat{a}\Big), \tag{5.1.23}$$

yielding

$$\langle 0|\hat{x}^2|0\rangle \;=\; \frac{x_0^2}{2}\langle 0|\hat{a}\,\hat{a} \;+\; \hat{a}^\dagger\,\hat{a}^\dagger \;+\; \hat{a}\,\hat{a}^\dagger \;+\; \hat{a}^\dagger\,\hat{a}|0\rangle \;=\; \frac{x_0^2}{2}\langle 0|\hat{a}\,\hat{a}^\dagger|0\rangle \tag{5.1.24}$$

$$=\; \frac{x_0^2}{2}\langle 0|\Big(\mathbf{1} + \hat{N}\Big)|0\rangle \;=\; \frac{x_0^2}{2}, \tag{5.1.25}$$

as expected, x_0 plays the role of the variance of the density distribution. Similarly,

$$\hat{p}^2 \;=\; -\,\frac{\hbar^2}{2\,x_0^2}\Big(\hat{a}\,\hat{a} \;+\; \hat{a}^\dagger\,\hat{a}^\dagger \;-\; \hat{a}\,\hat{a}^\dagger \;-\; \hat{a}^\dagger\,\hat{a}\Big), \tag{5.1.26}$$

thus

$$\langle 0|\hat{p}^2|0\rangle \;=\; -\,\frac{\hbar^2}{2\,x_0^2}\langle 0|\hat{a}\,\hat{a} \;+\; \hat{a}^\dagger\,\hat{a}^\dagger \;-\; \hat{a}\,\hat{a}^\dagger \;-\; \hat{a}^\dagger\,\hat{a}|0\rangle \;=\; \frac{\hbar^2}{2\,x_0^2}\langle 0|\hat{a}\,\hat{a}^\dagger|0\rangle \tag{5.1.27}$$

$$=\; \frac{\hbar^2}{2\,x_0^2}\langle 0|\Big(\mathbf{1}+\hat{N}\Big)|0\rangle \;=\; \frac{\hbar^2}{2\,x_0^2} \;=\; \frac{1}{2}\,\hbar\,m\omega. \tag{5.1.28}$$

It then follows that

$$\langle 0|\Delta x^2|0\rangle\;\langle 0|\Delta p^2|0\rangle \;=\; \frac{\hbar^2}{4}, \tag{5.1.29}$$

thus the ground state of the harmonic oscillator is also the state with minimum uncertainty.

5.1.2 Excited States

With the explicit form of the ground-state wave function given by Eq. (5.1.19), we can use the creation operators to generate also explicit expressions for the excited (higher-energy) states. For example,

$$\phi_1(x) \;=\; \langle x|\hat{a}^\dagger\,|0\rangle \;=\; \sqrt{\frac{m\omega}{2\,\hbar}}\Big(x \;-\; x_0^2\,\frac{d}{dx}\Big)\phi_0(x). \tag{5.1.30}$$

Carrying out the derivative leads to a first excited state $\phi_1(x)$ that is proportional to $x\,e^{-x^2/(2\,x_0^2)}$. More generally,

$$\phi_n(x) \;=\; \langle x|\frac{(\hat{a}^\dagger)^n}{\sqrt{n!}}|0\rangle \;=\; \frac{1}{\sqrt{n!}}\Big(\hat{a}^\dagger\Big)^n\,\phi_0(x). \tag{5.1.31}$$

One arrives at the well-known solutions expressed in terms of Hermite polynomials.

5.2 Time Evolution of the Harmonic Oscillator

In order to evaluate the time evolution induced by the harmonic oscillator Hamiltonian, it is convenient to work in the Heisenberg picture. We have:

$$\frac{d}{dt}\,\hat{x}_H(t) \;=\; \frac{i}{\hbar}\Big[\hat{H},\,\hat{x}_H(t)\Big], \qquad \frac{d}{dt}\,\hat{p}_H(t) \;=\; \frac{i}{\hbar}\Big[\hat{H},\,\hat{p}_H(t)\Big]. \tag{5.2.1}$$

Evaluating the commutators:

$$\begin{aligned}
\Big[\hat{H},\,\hat{x}_H(t)\Big] &= \Big[e^{\frac{i}{\hbar}\,t\,\hat{H}}\,\hat{H}\,e^{-\frac{i}{\hbar}\,t\,\hat{H}},\;e^{\frac{i}{\hbar}\,t\,\hat{H}}\,\hat{x}\,e^{-\frac{i}{\hbar}\,t\,\hat{H}}\Big] \\
&=\; e^{\frac{i}{\hbar}\,t\,\hat{H}}\Big[\hat{H},\,\hat{x}\Big]e^{-\frac{i}{\hbar}\,t\,\hat{H}} \\
&= e^{\frac{i}{\hbar}\,t\,\hat{H}}\Big[\frac{\hat{p}^2}{2\,m},\hat{x}\Big]e^{-\frac{i}{\hbar}\,t\,\hat{H}} \\
&=\; -\,e^{\frac{i}{\hbar}\,t\,\hat{H}}\Big(i\,\frac{\hbar}{m}\,\hat{p}\Big)e^{-\frac{i}{\hbar}\,t\,\hat{H}} \\
&=\; -\,i\,\frac{\hbar}{m}\,\hat{p}_H(t),
\end{aligned}$$

and similarly

$$\left[\hat{H},\, \hat{p}_H(t)\right] = e^{\frac{i}{\hbar}\,t\,\hat{H}}\left[\frac{1}{2}\,m\,\omega^2\,\hat{x}^2, \hat{p}\right]e^{-\frac{i}{\hbar}\,t\,\hat{H}} \;=\; m\,\omega^2\,i\,\hbar\,\hat{x}_H(t). \tag{5.2.2}$$

Thus

$$\frac{d}{dt}\,\hat{x}_H(t) \;=\; \frac{\hat{p}_H(t)}{m}, \qquad \frac{d}{dt}\,\hat{p}_H(t) \;=\; -\,m\,\omega^2\,\hat{x}_H(t). \tag{5.2.3}$$

These equations for the expectation values are completely equivalent to the classical expressions, since in the classical case:

$$\frac{d}{dt}\,x(t) \;=\; \frac{p(t)}{m}, \quad \frac{d}{dt}\,p(t) \;=\; -\frac{\partial}{\partial x}V(x) \;=\; -\,m\,\omega^2\,x(t). \tag{5.2.4}$$

We therefore see that the dynamics of the quantum expectation values is given by expressions that are the same as for the classical values, with oscillations of frequency ω:

$$\langle x(t)\rangle = \langle x(0)\rangle\,\cos(\omega t) \;+\; \frac{\langle p(0)\rangle}{m\,\omega}\,\sin(\omega t), \tag{5.2.5}$$

$$\langle p(t)\rangle = \langle p(0)\rangle\,\cos(\omega t) \;-\; m\,\omega\,\langle x(0)\rangle\,\sin(\omega t). \tag{5.2.6}$$

While these expressions are the same as their classical counterparts, it is important to realize that the expectation values of position and momentum will not always oscillate with frequency ω. For example, analogously to what we have seen for the ground state wave function, for all the eigenstates of the harmonic oscillator we have:

$$\langle n|\hat{x}|n\rangle = 0, \quad \langle n|\hat{p}|n\rangle = 0, \tag{5.2.7}$$

thus if, for example, at time $t = 0$ our system is in one of the eigenstates $|n\rangle$, then the expectation values just stay equal to zero at all times $\langle x\rangle(t) = \langle p\rangle(t) = 0$. In order to see oscillations, one needs to prepare the initial state in, at least, a superposition of two distinct eigenstates. For example:

$$|\psi(0)\rangle \;=\; \frac{1}{\sqrt{2}}\Big(|0\rangle \;+\; |1\rangle\Big). \tag{5.2.8}$$

One can show that in this state,

$$\langle\hat{x}\rangle(0) \;=\; \sqrt{\frac{\hbar}{2\,m\,\omega}}, \quad \langle\hat{p}\rangle(0) \;=\; 0,$$

and hence

$$\langle x(t)\rangle \;=\; \sqrt{\frac{\hbar}{2\,m\,\omega}}\,\cos(\omega t), \quad \langle p(t)\rangle \;=\; -\sqrt{\frac{\hbar\,m\,\omega}{2}}\,\sin(\omega t). \tag{5.2.9}$$

5.3 Ehrenfest's Theorem

In the previous section we have explicitly solved the Heisenberg's equations of motion, and found out that the dynamics of the expectation values of positions and momenta for the harmonic oscillator follow the classical equations of motion. This result is not a coincidence, and it is actually a consequence of a deeper and more general result. Through Heisenberg's equations of motion we can demonstrate the connection between quantum expectation values and classical equations of motion for a larger class of Hamiltonians. This connection, known as Ehrenfest's Theorem, concerns the time dependence of expectation values of general continuous-space Hamiltonians that depend on momentum and position:

$$\hat{H}(\hat{x},\,\hat{p}) \;=\; \frac{\hat{p}^2}{2\,m} \;+\; V(\hat{x}). \tag{5.3.1}$$

The time-dependent expectation value of the position can be found using Heisenberg's equations of motion we have previously derived:

$$\frac{d}{dt}\langle\hat{x}\rangle \;=\; \frac{i}{\hbar}\langle\big[\hat{H},\,\hat{x}\big]\rangle \;=\; \frac{i}{\hbar}\langle\big[\tfrac{\hat{p}^2}{2\,m},\hat{x}\big]\rangle \;=\; \frac{i}{\hbar}\,\frac{1}{2\,m}\langle\hat{p}\big[\hat{p},\,\hat{x}\big] \;+\; \big[\hat{p},\,\hat{x}\big]\,\hat{p}\rangle. \tag{5.3.2}$$

Using $[\hat{p},\,\hat{x}] = -\,i\,\hbar$, one gets

$$\frac{d}{dt}\langle\hat{x}\rangle \;=\; \frac{\langle\hat{p}\rangle}{m}. \tag{5.3.3}$$

Similarly, one computes

$$\frac{d}{dt}\langle\hat{p}\rangle \;=\; \frac{i}{\hbar}\langle\big[\hat{H},\,\hat{p}\big]\rangle \;=\; \frac{i}{\hbar}\langle\big[V(\hat{x}),\hat{p}\big]\rangle \;=\; -\,\langle\frac{dV}{dx}\rangle, \tag{5.3.4}$$

which completes the proof. Hence, Eqs. (6.3.1) and (6.3.2) are basically the same as Newton's second law for expectation values. This shows that by preparing many identically prepared systems each described by the same state, and measuring their average behavior, one recovers a classical-like motion for the mean values of x and p.

The following commutator relations hold:

$$\big[x^n,\,p\big] \;=\; i\,\hbar\,n\,x^{\,n-1}.$$

Proof. The proof is obtained by recursive application of the elementary commutation relation. Since

$$C^{(n)} \;=\; \big[x^n,\,p\big] \;=\; x^{\,n-1}\big[x,\,p\big] \;+\; \big[x^{\,n-1},\,p\big]\,x,$$

we see then that

$$C^{(n)} \;=\; i\,\hbar\,x^{\,n-1} \;+\; C^{(n-1)}\,x.$$

Repeating this step n times shows $C^{(n)} = i\,\hbar\,n\,x^{\,n-1}$.

Corollary For regular functions $V(x)$, we have $[\,V(\hat{x}),\,\hat{p}\,] = i\,\hbar\,V'(\hat{x})$.
Proof. Consider the Taylor series of $V(x) = \sum_{n=0}^{\infty} g_n\,x^n$, and its derivative $V'(x) = \sum_{n=0}^{\infty} n\,g_n\,x^{n-1}$. Thus

$$\left[\sum_{n=0}^{\infty} g_n\,x^n,\,p\right] \;=\; \sum_{n=0}^{\infty} g_n\big[x^n,\,p\big] \;=\; \sum_{n=0}^{\infty} g_n\,i\,\hbar\,n\,x^{n-1} \;=\; i\,\hbar\,V'(x). \tag{5.3.5}$$

This completes our analysis of the harmonic oscillator. In the next chapters, we will study additional examples and use these techniques to discuss more advanced quantum systems.