Chapter 3
THE HARMONIC OSCILLATOR

We now consider an extended example which allows us to apply the theoretical apparatus constructed in previous sections. The example we choose, that of a particle subjected to a linear restoring force - the so-called harmonic oscillator - is important for several reasons. First, it is one of the relatively small number of quantum mechanical problems that can be solved exactly and completely. In addition, the problem provides a basis for our understanding of many important physical problems, including molecular vibrations, the vibrational excitations of solids (i.e., phonons), and the quantization of the electromagnetic field (photons). In a real sense, the one-dimensional harmonic oscillator is the main building block of a great deal of quantum field theory.

3.1 Statement of the Problem

We consider a particle of mass m subject to a linear restoring force $F = -kx$, corresponding to the quadratic potential

$$V(x) = \frac{1}{2}kx^2 = \frac{1}{2}m\omega^2 x^2 \tag{3.1}$$

where $\omega = \sqrt{k/m}$. In the Hamiltonian description of classical mechanics, the system is described by the dynamical variables $\{x, p\}$, and the evolution is governed by the Hamiltonian

$$H = T + V = \frac{p^2}{2m} + \frac{1}{2}m\omega^2 x^2. \tag{3.2}$$

Hamilton's equations of motion

$$\dot{x} = \frac{\partial H}{\partial p} = \frac{p}{m} \tag{3.3}$$

$$\dot{p} = -\frac{\partial H}{\partial x} = -m\omega^2 x \tag{3.4}$$

are, upon taking a second derivative, equivalent to the familiar Newtonian equations

$$\ddot{x} + \omega^2 x = 0 \qquad\qquad \ddot{p} + \omega^2 p = 0 \tag{3.5}$$

whose solutions lead to the familiar oscillatory behavior

$$x(t) = A\sin(\omega t + \delta) \tag{3.6}$$

$$p(t) = Am\omega\cos(\omega t + \delta). \tag{3.7}$$

In passing from a classical treatment to a quantum mechanical one, the dynamical variables are replaced by operators

$$\begin{aligned} x &\to X \\ p &\to P = \hbar K \end{aligned} \tag{3.8}$$

which obey the canonical commutation relations

$$[X, P] = i\hbar. \tag{3.9}$$

Evolution of the quantum mechanical system is governed by the associated Hamiltonian operator

$$H = \frac{P^2}{2m} + \frac{1}{2}m\omega^2 X^2. \tag{3.10}$$

Since the system is conservative ($\partial H/\partial t = 0$), this evolution is best considered in the basis of the eigenstates $|\phi_n\rangle$ of the Hamiltonian, which are assumed to span the space of a single particle moving in one-dimension, and which obey the energy eigenvalue equation

$$(H - E_n)|\phi_n\rangle = 0. \tag{3.11}$$

As with any eigenvalue problem, we need an initial representation in which to work. In the $|x\rangle$ representation, associated with the eigenstates of the position operator X, this becomes a differential equation

$$-\frac{\hbar^2}{2m}\frac{d^2\phi_n}{dx^2} + \left[\frac{1}{2}m\omega^2 x^2 - E_n\right]\phi_n(x) = 0 \tag{3.12}$$

for the eigenfunctions $\phi_n(x) = \langle x|\phi_n\rangle$. The notation that we have introduced suggests a discrete spectrum, and, indeed it can be anticipated that all of the eigenstates of the harmonic potential must be bound states. This follows from the observation that the potential energy of the oscillator becomes infinite as $|x| \to \infty$. As a result, the wave function must go to zero at large distances from the origin in order for the energy of the system to remain finite. Thus, the above equation is to be solved with the boundary condition $\phi_n(x) \to 0$ as $|x| \to \infty$, characteristic of a bound state solution.

Of course, it is also possible to solve the eigenvalue equation in the wave vector or momentum representation. Indeed, in the $|k\rangle$ basis, the eigenvalue equation for the harmonic oscillator is *also* a second order differential equation

$$\left[\frac{\hbar^2 k^2}{2m} - E_n\right]\phi_n(k) - \frac{1}{2}m\omega^2\frac{d^2\phi_n}{dk^2} = 0, \tag{3.13}$$

due to the fact that $x = id/dk$ is a differential operator in that representation. Again, this eigenvalue equation is to be solved under the requirement that the solution vanish as $|k| \to \infty$, so that the energy of the system (in this case the kinetic energy) be finite.

A traditional approach commonly taken to solve either of these equations is the so-called power series method, the basic steps of which we enumerate for the spatial eigenfunctions below:

1. Determine for large x that the solution has the asymptotic form $\phi(x) \sim A(x)e^{-\alpha x^2}$, where $\alpha = m\omega/2\hbar$, and $A(x)$ is slowly varying in x. This asymptotic form follows since for large x the differential equation can be written [cf. Eq. (3.12)] in the simpler form
$$\frac{d^2\phi_n}{dx^2} - \frac{m^2\omega^2}{\hbar^2}x^2\phi_n(x) = 0. \tag{3.14}$$
2. Assume a power series solution of the form
$$\phi(x) = e^{-\alpha x^2}\sum_k a_k x^k \tag{3.15}$$
to describe the slowly-varying function $A(x)$, obtaining a recursion relation for the coefficients a_k.
3. Show that if the series does not terminate, the series produced will yield a solution that *diverges* exponentially as $\mathrm{e}^{\alpha x^2}$ for large x. Deduce, thereby, that the solutions corresponding to physically acceptable solutions must have series which terminate, i.e., for which $A(x)$ is a polynomial in x.
4. Deduce the values of energy E_n for which the series terminates, thereby solving the eigenvalue problem.

In what follows we take a different approach, due to Dirac, that allows us ultimately to obtain all eigenfunctions from the solution to a simple first-order differential equation. This *algebraic method* uses the fundamental commutation relations to directly deduce the spectrum and degeneracy of the harmonic oscillator Hamiltonian.

3.1.1 Algebraic Approach to the Quantum Harmonic Oscillator

To facilitate our study we begin by introducing some simplifying notation. We observe first that the classical harmonic oscillator possesses a natural frequency ω. Quantum mechanically this implies the existence of a natural energy scale $\varepsilon_0 = \hbar\omega$. Thus, the Hamiltonian, which itself has units of energy, can be written in the form

$$H = \frac{P^2}{2m} + \frac{1}{2}m\omega^2X^2 = \frac{\hbar\omega}{2}\left[\frac{1}{\hbar\omega}\frac{P^2}{m} + \frac{1}{\hbar\omega}m\omega^2X^2\right] \tag{3.16}$$
$$= \frac{\hbar\omega}{2}\left[\frac{P^2}{m\hbar\omega} + \frac{m\omega X^2}{\hbar}\right] \tag{3.17}$$

or more simply

$$H = \frac{\hbar\omega}{2}(p^2 + q^2) \tag{3.18}$$

in which

$$p = \frac{P}{\sqrt{m\hbar\omega}} \tag{3.19}$$

and

$$q = \sqrt{\frac{m\omega}{\hbar}}X \tag{3.20}$$

represent *dimensionless* momentum and position operators, respectively. (Note that we are relaxing our convention of representing operators by capital letters.) It is readily verified that these new operators obey a dimensionless form

$$[q, p] = i \tag{3.21}$$

of the canonical commutation relations, and apart from a slightly different normalization, the eigenstates $\{|q\rangle\}$ and $\{|p\rangle\}$ of these operators are essentially those of their dimensionally correct counterparts $\{|x\rangle\}$ and $\{|k\rangle\}$. There is a representation associated with each set of states, so that

$$\int dq\ |q\rangle\langle q| = \mathbf{1} = \int dp\ |p\rangle\langle p| \tag{3.22}$$

$$\langle q|q'\rangle = \delta(q-q') \qquad\qquad \langle p|p'\rangle = \delta(p-p')$$

in terms of which we can expand and arbitrary state of the system (which is that of a particle moving in one-dimension). Thus, we can write

$$|\psi\rangle = \int_{-\infty}^{\infty} dq\ \psi(q)|q\rangle = \int_{-\infty}^{\infty} dp\ \psi(p)|p\rangle, \tag{3.23}$$

which define convenient position and momentum wavefunctions, $\psi(q)$ and $\psi(p)$, respectively. We can, moreover, expand each basis ket in terms of the basis vectors of the other representation just as we can for the normal states of the position and wavevector representations:

$$\begin{aligned} |p\rangle &= (2\pi)^{-1/2} \int_{-\infty}^{\infty} dq\ e^{ipq}|q\rangle \\ |q\rangle &= (2\pi)^{-1/2} \int_{-\infty}^{\infty} dp\ e^{-ipq}|p\rangle. \end{aligned} \tag{3.24}$$

Finally, it is straightforward to show that in the $|q\rangle$ representation p acts like a differential operator, i.e.,

$$p\psi(q) \to -i\frac{d\psi(q)}{dq} \tag{3.25}$$

and in the $|p\rangle$ representation q acts like a differential operator

$$q\psi(p) \to i\frac{d\psi(p)}{dp}. \tag{3.26}$$

To proceed, it is useful to note that the Hamiltonian for the corresponding classical problem is factorizable, i.e., if q and p were classical variables we could write

$$H = \frac{\hbar\omega}{2}(q^2+p^2) = \frac{1}{2}\hbar\omega(q+ip)(q-ip). \qquad \text{(in the classical limit).} \tag{3.27}$$

The fact that q and p do not commute renders this factorization invalid, but it does lead us to consider the non-Hermitian operators

$$a = \frac{1}{\sqrt{2}}(q+ip) \qquad\qquad a^+ = \frac{1}{\sqrt{2}}(q-ip) \tag{3.28}$$

in terms of which our original operators q and p can be written

$$q = \frac{1}{\sqrt{2}}(a^+ + a) \qquad\qquad p = \frac{i}{\sqrt{2}}(a^+ - a). \tag{3.29}$$

The product of a^+ and a is easily evaluated:

$$a^+a = \frac{1}{2}(q-ip)(q+ip) = \frac{1}{2}[q^2+p^2+i(qp-pq)]. \tag{3.30}$$

Recognizing the commutator $[q,p]=i$ in this last expression we find that

$$a^+a=\frac{1}{2}(q^2+p^2)-\frac{1}{2}. \tag{3.31}$$

This identity allows us to express the harmonic oscillator Hamiltonian in the form

$$H=\frac{\hbar\omega}{2}(p^2+q^2)=\hbar\omega(a^+a+\frac{1}{2}). \tag{3.32}$$

Introducing one further bit of simplifying notation, we denote by

$$N=a^+a \tag{3.33}$$

the operator product of a^+ and a. Thus, the Hamiltonian H can be written in the following simple and suggestive form

$$H=(N+\frac{1}{2})\hbar\omega. \tag{3.34}$$

It is obvious that the eigenstates of the (manifestly Hermitian) operator $N=a^+a$ are also eigenstates of the harmonic oscillator Hamiltonian. Indeed, if we can find a complete set of eigenstates $|n\rangle$ such that

$$N|n\rangle=n|n\rangle, \tag{3.35}$$

then these states will also be eigenstates of the Hamiltonian, i.e.,

$$H|n\rangle=(N+\frac{1}{2})\hbar\omega|n\rangle=(n+\frac{1}{2})\hbar\omega|n\rangle=E_n|n\rangle \tag{3.36}$$

where $E_n=(n+\frac{1}{2})\hbar\omega$. Thus, we change our original notation for the energy eigenstates so that $|n\rangle=|\phi_n\rangle$. It is important to stress that, at this point, we haven't really done anything, since we don't know what values are in the spectrum of the operator $N=a^+a$. We have simply transferred the eigenvalue problem that we have to solve to that of the operator N, rather than the operator H. We will refer to the operator N as **the number operator**, because, as we will see, it counts the number of energy quanta, in units of $\hbar\omega$, associated with the system. Our goal in what follows is to use the *commutation relations* obeyed by the *new* operators a, a^+, and $N=a^+a$, to deduce the structure of the energy eigenstates of this system.

The commutation relations that we will need are easily obtained. We note, first, that

$$[a,a^+]=\frac{1}{2}[q+ip,q-ip]=\frac{1}{2}(i[p,q]-i[q,p])=\frac{-i}{2}([q,p]+[q,p]) \tag{3.37}$$

which the canonical commutation relations reduce to

$$[a,a^+]=1. \tag{3.38}$$

One consequence of this relation is that $aa^+=a^+a+1$, so that we can write

$$aa^+=N+1. \tag{3.39}$$

Next, we evaluate the commutator

$$[N,a]=[a^+a,a]=a^+[a,a]+[a^+,a]a \tag{3.40}$$

which our previous result reduces to

$$[N, a] = -a. \tag{3.41}$$

Finally, we evaluate

$$[N, a^+] = [a^+a, a^+] = a^+[a, a^+] + [a^+, a^+]a \tag{3.42}$$

which reduces to

$$[N, a^+] = a^+. \tag{3.43}$$

Combining these relations, we have the following closed *algebra* of commutation relations

$$[a, a^+] = 1 \qquad [N, a] = -a \qquad [N, a^+] = a^+. \tag{3.44}$$

3.1.2 Spectrum and Eigenstates of the Number Operator N

Using the commutation relations obtained above, we now deduce a number of basic properties associated with the eigenstates of the number operator N and, hence, of the eigenstates of the harmonic oscillator Hamiltonian H. In what follows, we begin by simply assuming the existence of at least one *nonzero* eigenvector $|n\rangle$ of the observable N. This is a trivial assumption, since N is a simple function of the observable H, and is therefore an observable of the system. This assumption then allows us to prove the following:

1.) *Positivity of eigenvalues:* If $|n\rangle$ is a nonzero eigenvector of the operator N, and n is the associated eigenvalue, then $n \geq 0$. In other words, the eigenvalues of N are positive definite.
Proof: This just follows from the obvious positivity of the operator $N = a^+a$, which implies that if $N\ |n\rangle = n|n\rangle$ then

$$\langle n|N|n\rangle = n\langle n|n\rangle = \langle n|a^+a|n\rangle = ||a|n\rangle||^2 \tag{3.45}$$

so that

$$n = \frac{||a|n\rangle||^2}{\langle n|n\rangle} \geq 0. \tag{3.46}$$

which proves the assertion.

2.) *Action of a^+ on eigenvectors of N:* If $|n\rangle$ is an eigenvector of the operator N with eigenvalue n, then the vector

$$|n_+\rangle = a^+|n\rangle \tag{3.47}$$

is an eigenvector of N with eigenvalue $n + 1$.
Proof: We consider the action of N on the state $|n_+\rangle$, and use the commutation relation $[N, a^+] = a^+$, to deduce that $Na^+ = a^+N + a^+ = a^+(N + 1)$, and hence

$$N|n_+\rangle = Na^+|n\rangle = a^+(N + 1)|n\rangle = a^+(n + 1)|n\rangle = (n + 1)(a^+|n\rangle) \tag{3.48}$$

so that

$$N|n_+\rangle = (n + 1)|n_+\rangle \tag{3.49}$$

showing that $|n_+\rangle$ obeys the eigenvalue equation. Note that the vector $|n_+\rangle$ is nonzero, since

$$\langle n_+|n_+\rangle = \langle n|aa^+|n\rangle = \langle n|N + 1|n\rangle = (n + 1)\langle n|n\rangle > 0 \tag{3.50}$$

As a corollary, it follows that if there exists one nonzero eigenvector $|n\rangle$, then there necessarily exists an infinite sequence of eigenvectors $\{|n\rangle, a^+|n\rangle, (a^+)^2|n\rangle, \cdots\}$ associated with a corresponding increasing sequence $\{n, n+1, n+2, \cdots\}$ of eigenvalues that can be obtained by repeated application of the operator a^+ to the state $|n\rangle$. For this reason, the operator a^+ is often referred to as the **raising operator** or the **creation operator**, because, as we will see, it acts to create quanta of energy in the system.

3.) *Action of a on eigenvectors of N:* If $|n\rangle$ is an eigenvector of N with eigenvalue n, and if $|n_-\rangle$ is defined through the relation

$$|n_-\rangle = a|n\rangle \tag{3.51}$$

then there are two possibilities, one of which must be true, either: *(i)* the ket $|n_-\rangle$ is the null vector, in which case $n = 0$, or *(ii)* the ket $|n_-\rangle$ is an eigenvector of N with eigenvalue $n-1$.
Proof of (i): We note first that if $|n_-\rangle = 0$, then

$$\langle n_-|n_-\rangle = 0 = \langle n|a^+a|n\rangle = \langle n|N|n\rangle = n\langle n|n\rangle \tag{3.52}$$

showing that $n = 0$, since $|n\rangle$ is by assumption nonzero. Conversely, if $n = 0$, the same expression read from right to left shows that $\langle n_-|n_-\rangle = 0$, which implies that $|n_-\rangle$ is the null vector. As a consequence, we see that any eigenvector $|0\rangle$ of N with eigenvalue $n = 0$ obeys the equation

$$a|0\rangle = 0.$$

Proof of (ii): If $n \neq 0$, then the argument above shows that $|n_-\rangle$ is not the null vector, since then $\langle n_-|n_-\rangle = n\langle n|n\rangle \neq 0$. We then consider the action of N on $|n_-\rangle$ and use the commutation relation $[N, a] = -a$, to deduce that $Na = aN - a = a(N-1)$, so that

$$N|n_-\rangle = Na|n\rangle = a(N-1)|n\rangle = a(n-1)|n\rangle = (n-1)(a|n\rangle) \tag{3.53}$$

and thus

$$N|n_-\rangle = (n-1)|n_-\rangle. \tag{3.54}$$

This last equation shows that $|n_-\rangle$ is a nonzero eigenvector of N with eigenvalue smaller by one than that of the eigenvector $|n\rangle$. This implies, as a corollary, that if there exists one nonzero eigenvector $|n\rangle$ then there exists a sequence of eigenvectors $\{|n\rangle, a|n\rangle, a^2|n\rangle, \cdots\}$ associated with a corresponding sequence of decreasing eigenvalues $\{n, n-1, n-2, \cdots\}$, which can be obtained by repeated application of the operator a. For this reason, the operator a is often referred to as the **lowering operator** or **annihilation operator**, because it acts to annihilate or reduce the number of energy quanta in the system.

4.) *The eigenvalues of N are the non-negative integers* - We can now assert that the spectrum of the number operator N consists of the numbers $n = 0, 1, 2, \cdots$. To prove this, assume that there exists a (necessarily positive) eigenvalue $n \geq 0$ of N which is *not* in this set. Given any nonzero eigenvector $|n\rangle$ with this eigenvalue, we could then produce non-null eigenstates of N with negative eigenvalues by repeated application of the lowering operator a. This would violate our proof that N has no negative eigenvalues. On the other hand, if n is a positive integer or zero, then the sequence of eigenvalues terminates at zero before it can produce negative eigenvalues. That is, if $n = 0$, the sequence terminates immediately, with

$$a|0\rangle = 0.$$

(Note that $|0\rangle$ on the left is the eigenvector with eigenvalue 0, while the 0 on the right is the *null vector*.) If n is a positive integer, then the sequence terminates after exactly n steps, i.e., $a^{n-1}|n\rangle$ is an eigenvalue of N with eigenvalue 0, so by our previous result $a^n|n\rangle = 0$. Thus the only possible values for the eigenvalues of n are the non-negative integers. Since one of these is, by assumption, not null, we can produce all those with lower (positive) integer values by application of a and all those with higher integer values by application of a^+. Thus, all values in the set $n = 0, 1, 2, \cdots$ must be eigenvalues of N. This still leaves the question of degeneracy, i.e., the possibility that there may be more than one linearly independent eigenvector for a given eigenvalue n.

5.) *The eigenvalues of N are nondegenerate* - We will first show that *if* the eigenvalue n is nondegenerate, then so is $n+1$. To see this, assume that n is nondegenerate, and let $|\phi_{n+1}\rangle$ and $|\psi_{n+1}\rangle$ be two arbitrary eigenstates of N having eigenvalue $n+1$. From these states we can then produce the states $|\phi_n\rangle = a|\phi_{n+1}\rangle$ and $|\psi_n\rangle = a|\psi_{n+1}\rangle$, which would have to be eigenstates of N associated with the nondegenerate eigenvalue n, and so are linearly dependent. For two vectors, linear dependence implies proportionality, so there exists a constant λ such that $|\phi_n\rangle = \lambda|\psi_n\rangle$. Acting with the raising operator a^+ then reveals that

$$\begin{aligned} a^+|\phi_n\rangle &= a^+a|\phi_{n+1}\rangle = N|\phi_{n+1}\rangle = (n+1)|\phi_{n+1}\rangle \\ &= a^+(\lambda|\psi_n\rangle) = \lambda a^+a|\psi_{n+1}\rangle = \lambda N|\psi_{n+1}\rangle = \lambda(n+1)|\psi_{n+1}\rangle \end{aligned} \tag{3.55}$$

from which we deduce that $|\phi_{n+1}\rangle = \lambda|\psi_{n+1}\rangle$. This shows that $|\phi_{n+1}\rangle$ and $|\psi_{n+1}\rangle$ are necessarily linearly dependent. There is at most one linearly independent eigenvector of N with eigenvalue $n+1$. Hence, if eigenvalue n is nondegenerate, so is $n+1$.

To complete the argument, we now show that there exists, in fact, exactly *one* linearly independent eigenvector $|0\rangle$ of N with eigenvalue $n = 0$, from which it follows that all the eigenvalues of N are nondegenerate. To do this we explicitly construct the corresponding eigenfunction $\phi_0(q) = \langle q|0\rangle$ in the position representation. This is facilitated by the fact, shown above, that *any* eigenstate $|0\rangle$ of N with eigenvalue 0 is annihilated by the lowering operator, i.e., it obeys the equation

$$a|0\rangle = 0. \tag{3.56}$$

Using the relation $a = \frac{1}{\sqrt{2}}(q + ip)$, this implies that

$$\langle q|a|0\rangle = \frac{1}{\sqrt{2}}\langle q|q + ip|0\rangle = \frac{1}{\sqrt{2}}(q + \frac{d}{dq})\phi_0(q) = 0 \tag{3.57}$$

in which we have used the differential form taken by the operator p in the position representation. This *first order* differential equation leads to the relation

$$\frac{d\phi_0}{\phi_0} = -q\, dq, \tag{3.58}$$

which can be integrated from $q = 0$ to obtain

$$\ln[\phi_0(q)/\phi_0(0)] = -\frac{1}{2}q^2 \tag{3.59}$$

or

$$\phi_0(q) = \phi_0(0)\, e^{-\frac{1}{2}q^2}. \tag{3.60}$$

Thus, the eigenfunctions of N with $n = 0$ differ from one another only through an overall multiplicative constant. Thus there is only one linearly independent solution with this eigenvalue. The eigenvalue $n = 0$ is, therefore, nondegenerate as are all the eigenvalues of N.

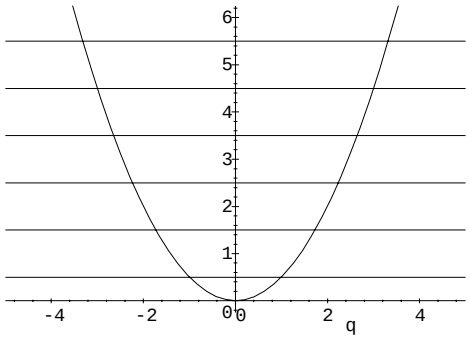
We now summarize the results of the preceding series of arguments. The spectrum of the number operator N is the set of non-negative integers

$$\text{spectrum}(N) = \{0, 1, 2, \cdots\}. \tag{3.61}$$

For each element in this set, there exists exactly one linearly independent eigenstate $|n\rangle$. It follows that the spectrum of the harmonic oscillator Hamiltonian is the set of nondegenerate energies

$$\text{spectrum}(H) = \{E_n = (n + \frac{1}{2})\hbar\omega \,|\, n = 0, 1, 2, \cdots\}. \tag{3.62}$$

Note that the eigenstates of H form a set of equally spaced levels starting at the minimum energy $E_0 = \frac{1}{2}\hbar\omega$, which is often referred to as the zero-point energy of the ground state. The first excited state E_1 is higher in energy than the ground state by one quantum $\Delta E = \hbar\omega$ of energy, and the energy spacing between adjacent levels is a constant. The number operator N, therefore, counts the number of energy quanta that have been added to the system, and the operators a^+ and a can be viewed as creating or annihilating these energy quanta by raising or lowering the value of n.



Up to this point we have deduced essential features associated with the eigenstates and eigenvalues of the harmonic oscillator Hamiltonian. We now flesh out the analysis by explicitly constructing an ONB of square-normalized energy eigenstates.

3.1.3 The Energy Basis

We have already constructed the eigenstate of N with $n = 0$ by deriving the form of the wave function

$$\langle q|0\rangle = \phi_0(q) = Ae^{-\frac{1}{2}q^2} \tag{3.63}$$

that represents this state in the position representation. To complete the picture we need to specify the normalization constant A. Correct normalization requires that

$$\langle 0|0\rangle = \int_{-\infty}^{\infty} dq\, |\phi_0(q)|^2 = |A|^2 \int_{-\infty}^{\infty} dq\, e^{-q^2} = 1. \tag{3.64}$$

The integral appearing in this condition is well known and has the value $\sqrt{\pi}$, from which we deduce that the correctly normalized ground state wave function has the form

$$\phi_0(q) = \pi^{-1/4} e^{-\frac{1}{2}q^2}. \tag{3.65}$$

It is also possible to express this in terms of the "real" position variable x, rather than the dimensionless variable $q = \sqrt{\frac{m\omega}{\hbar}}x$. This is most easily done by noting that, in general, normalization requires that

$$1 = \int |\phi_n(q)|^2 dq = \int |\phi_n(q(x))|^2 \frac{dq}{dx} dx = \int |\phi_n(x)|^2 dx \tag{3.66}$$

so that

$$\phi_n(x) = \phi_n[q(x)] \sqrt{\frac{dq}{dx}} = \left(\frac{m\omega}{\hbar}\right)^{1/4} \phi_n[q(x)]. \tag{3.67}$$

Making the appropriate substitution gives the ground state wave function

$$\phi_0(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} \exp\left(-\frac{m\omega}{2\hbar}x^2\right). \tag{3.68}$$

The remaining eigenstates can be generated from the ground state by repeated application of the raising operator a^+. Unfortunately, a simple-minded application of a^+ to the ground state does not generate *normalized* eigenstates. To see this, let us denote by $|n\rangle$ and $|n+1\rangle$ the square-normalized eigenstates of N with eigenvalues n and $n+1$, respectively. Now our earlier argument shows that state $a^+|n\rangle$ is also an eigenstate of N with eigenvalue $n+1$, and so must be at least proportional to the state $|n+1\rangle$, since the eigenstates of N are nondegenerate. Thus, there exists a constant λ_n such that

$$a^+|n\rangle = \lambda_n |n+1\rangle \tag{3.69}$$

Taking the norm of this vector reveals that

$$\langle n|aa^+|n\rangle = |\lambda_n|^2 \tag{3.70}$$

or, using the fact that $aa^+ = N + 1$, we see that

$$|\lambda_n|^2 = n + 1. \tag{3.71}$$

Fixing the relative phase of our basis vectors such that λ_n is real and positive, we obtain $\lambda_n = \sqrt{n+1}$, from which we deduce the basic relation

$$a^+|n\rangle = \sqrt{n+1}|n+1\rangle \tag{3.72}$$

between basis vectors with neighboring energy eigenvalues. For the purpose of constructing these states it is useful to write this relation in the equivalent form

$$|n\rangle = \frac{a^+|n-1\rangle}{\sqrt{n}}. \tag{3.73}$$

By recursion, this allows us to express the state $|n\rangle$ in terms of the ground state, i.e.,

$$|n\rangle = \frac{a^+|n-1\rangle}{\sqrt{n}} = \frac{(a^+)^2|n-2\rangle}{\sqrt{n(n-1)}} = \cdots \frac{(a^+)^n|0\rangle}{\sqrt{n!}} \tag{3.74}$$

or

$$|n\rangle = \frac{(a^+)^n|0\rangle}{\sqrt{n!}}. \tag{3.75}$$

To find the wave functions which represent the eigenstates in the position representation we project this onto the basis vectors $|q\rangle$ of that representation

$$\begin{aligned} \phi_n(q) &= \langle q|n\rangle = \frac{\langle q|(a^+)^n|0\rangle}{\sqrt{n!}} \\ &= \frac{1}{\sqrt{2^n n!}}\left(q - \frac{d}{dq}\right)^n \phi_0(q) \end{aligned} \tag{3.76}$$

or using the explicit form for the normalized ground state wave function we find that

$$\phi_n(q) = \frac{\pi^{-1/4}}{\sqrt{2^n n!}}\left(q - \frac{d}{dq}\right)^n e^{-\frac{1}{2}q^2}. \tag{3.77}$$

Thus, we have an explicit prescription for calculating the wave function for the state n in the position representation. Another useful form of this follows from the relation

$$a^+|n\rangle = \sqrt{n+1}|n+1\rangle \tag{3.78}$$

derived earlier, from which it follows that

$$|n+1\rangle = \frac{a^+|n\rangle}{\sqrt{n+1}}, \tag{3.79}$$

which becomes, in the position representation,

$$\langle q|n+1\rangle = \frac{\langle q|a^+|n\rangle}{\sqrt{n+1}} = \frac{1}{\sqrt{n+1}}\frac{1}{\sqrt{2}}\left(q - \frac{d}{dq}\right)\phi_n(q) \tag{3.80}$$

We thus have a recursion relation

$$\phi_{n+1}(q) = \frac{1}{\sqrt{n+1}}\frac{1}{\sqrt{2}}\left(q - \frac{d}{dq}\right)\phi_n(q) \tag{3.81}$$

which allows each wave function to be constructed from the one preceding it.

Examples: We derive below the first three harmonic oscillator wave functions

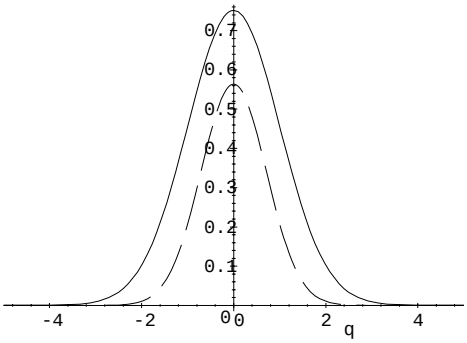
1. For $n = 0$ we have
$$\phi_0(q) = \langle q|0\rangle = \pi^{-1/4}e^{-q^2/2}$$

2. Applying the prescription above we find that for $n = 1$
$$\begin{aligned} \phi_1(q) = \langle q|1\rangle &= \frac{1}{\sqrt{2}}\frac{1}{\sqrt{2}}\left(q - \frac{d}{dq}\right)\left(\pi^{-1/4}e^{-q^2/2}\right) \\ &= \frac{\pi^{-1/4}}{\sqrt{2}}\,(2q)\,e^{-q^2/2} \end{aligned}$$

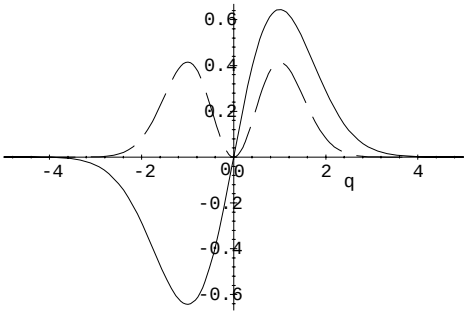
3. For $n = 2$, we have

$$\phi_2(q) = \langle q|2\rangle = \frac{1}{\sqrt{2\cdot 2}}\left(q - \frac{d}{dq}\right)\left(\frac{\pi^{-1/4}}{\sqrt{2}}\,(2q)\,e^{-q^2/2}\right)$$
$$= \frac{\pi^{-1/4}}{\sqrt{2}}\left(2q^2 - 1\right)e^{-q^2/2}$$

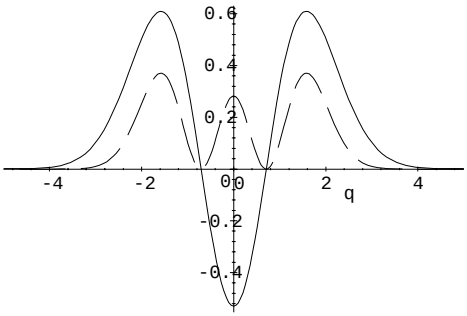
These wave functions are graphed below as solid lines, with the associated probability densities $|\phi_n|^2$ indicated as dashed lines.



$\phi_n(q)$ for $n = 0$.



$\phi_n(q)$ for $n = 1$.



$\phi_n(q)$ for $n = 2$.

The wave function $\phi_n(q)$ is customarily expressed in terms of the nth order Hermite polynomial $H_n(z)$, defined through the relation

$$\begin{aligned} H_n(z) &= e^{z^2/2}\left(z - \frac{d}{dz}\right)^n e^{-z^2/2} \\ &= (-1)^n e^z \frac{d^n}{dz^n} e^{-z} \end{aligned} \tag{3.82}$$

where the latter form follows from the first by simply writing out the powers in the first, inserting factors of unity in the form $1 = e^{-z^2/2}e^{z^2/2}$ between each factor, and performing a little algebra. With this definition, the wave function $\phi_n(q)$ can be written

$$\phi_n(q) = \frac{\pi^{-1/4}}{\sqrt{2^n n!}} H_n(q) e^{-q^2/2}. \tag{3.83}$$

Since the Hamiltonian commutes with the parity operator (the potential is symmetric), and because the harmonic oscillator spectrum is nondegenerate, it follows that the eigenstates of H are also eigenstates of the parity operator, which means that they are either even or odd. The parity of the nth harmonic oscillator state is $(-1)^n$, which makes states with even n symmetric and states of odd n antisymmetric, as suggested by the figures. The probability density $\rho_n(q) = |\phi_n(q)|^2$ associated with each eigenstate is an even function. As a consequence, we can anticipate that the expectation value of the position operator q in each eigenstate vanishes.

By assumption, the basis states of the energy representation, being eigenstates of a Hermitian operator, form a complete ONB for the space of a single particle moving in one dimension. Thus, we can automatically write down the completeness and orthonormality relations appropriate to this set of states

$$\sum_n |n\rangle\langle n| = \mathbf{1} \qquad\qquad \langle n|n'\rangle = \delta_{n,n'} \tag{3.84}$$

This allows us to expand an arbitrary state of the system. Thus an arbitrary state $|\psi\rangle$ of a particle moving in one-dimension can be written in the form

$$|\psi\rangle = \sum_n \psi_n |n\rangle \tag{3.85}$$

and the spatial wave function $\psi(q)$ of such a state can be expanded in the eigenfunctions derived above, i.e.,

$$\psi(q) = \langle q|\psi\rangle = \sum_n \psi_n \langle q|n\rangle = \sum_n \psi_n \phi_n(q), \tag{3.86}$$

with

$$\psi_n = \langle n|\psi\rangle = \int dq\, \phi_n^*(q)\psi(q). \tag{3.87}$$

3.1.4 Action of Various Operators in the Energy Representation

In this section we consider the action and expansion of various operators in the basis of energy eigenstates developed above. We first have the obvious relations encountered during our derivation. For example, the action of the number operator in this representation is particularly simple, since these states are eigenstates of N. Thus,

$$N|n\rangle = n|n\rangle \tag{3.88}$$

so that

$$\langle n'|N|n\rangle = n\langle n'|n\rangle = n\delta_{n',n} \tag{3.89}$$

Hence it follows that

$$N = \sum_{n=0}^{\infty} |n\rangle\ n\ \langle n| \tag{3.90}$$

Similarly, the harmonic oscillator Hamiltonian has the action

$$H|n\rangle = (n + \frac{1}{2})\hbar\omega|n\rangle \tag{3.91}$$

so that

$$\langle n'|H|n\rangle = (n + \frac{1}{2})\hbar\omega\ \delta_{n',n} \tag{3.92}$$

and thus

$$H = \hbar\omega \sum_{n=0}^{\infty} |n\rangle\ (n + \frac{1}{2})\ \langle n| \tag{3.93}$$

The action of the annihilation and creation operators a and a^+ are also easily deduced. We have already derived the relation

$$a^+|n\rangle = \sqrt{n+1}|n+1\rangle \tag{3.94}$$

from which we deduce the matrix elements

$$\langle n'|a^+|n\rangle = \sqrt{n+1}\langle n'|n+1\rangle = \sqrt{n+1}\delta_{n',n+1} \tag{3.95}$$

and so

$$a^+ = \sum_{n=0}^{\infty} |n+1\rangle\ \sqrt{n+1}\ \langle n| \tag{3.96}$$

which is clearly not diagonal, even though it is represented by a single index. Taking the adjoint of this last relation gives an expansion for the annihilation operator

$$a = \sum_{n=0}^{\infty}\ |n\rangle\sqrt{n+1}\ \langle n+1| = \sum_{n=0}^{\infty}\ |n-1\rangle\sqrt{n}\ \langle n|, \tag{3.97}$$

where we have shifted the summation index in the last form. From this it follows that

$$a|n\rangle = \sqrt{n}|n-1\rangle \tag{3.98}$$

which shows that the operator a lowers the state to the next lowest eigenvalue, but multiplies by $\sqrt{n}$ in the process.

From these we can derive relations for the position and momentum operators $q = (a^+ + a)/\sqrt{2}$ and $p = i(a^+ - a)/\sqrt{2}$. Thus, for example, we deduce that

$$q|n\rangle = \frac{1}{\sqrt{2}}(a^+ + a)|n\rangle = \frac{1}{\sqrt{2}}\left[\sqrt{n+1}|n+1\rangle + \sqrt{n}|n-1\rangle\right] \tag{3.99}$$

$$\langle n'|q|n\rangle = \frac{1}{\sqrt{2}}\left[\sqrt{n+1}\ \delta_{n',n+1} + \sqrt{n}\ \delta_{n',n-1}\right] \tag{3.100}$$

$$q = \sum_{n=0}^{\infty} \left[|n+1\rangle \sqrt{n+1}\, \langle n| \quad + \quad |n-1\rangle \sqrt{n}\, \langle n| \right], \tag{3.101}$$

and that

$$p|n\rangle = \frac{i}{\sqrt{2}}(a^+ - a)|n\rangle = \frac{i}{\sqrt{2}} \left[\sqrt{n+1}|n+1\rangle - \sqrt{n}|n-1\rangle \right] \tag{3.102}$$

$$\langle n'|p|n\rangle = \frac{i}{\sqrt{2}} \left[\sqrt{n+1}\, \delta_{n',n+1} - \sqrt{n}\, \delta_{n',n-1} \right] \tag{3.103}$$

$$p = \frac{i}{\sqrt{2}} \sum_{n=0}^{\infty} \left[|n+1\rangle \sqrt{n+1}\, \langle n| \quad - \quad |n-1\rangle \sqrt{n}\, \langle n| \right], \tag{3.104}$$

Thus, the operators N and H are diagonal in the energy representation, while the operators a, a^+, q, and p connect each energy eigenstate to the states immediately above or below it. The matrices representing these operators are straightforward to construct, and appear below

$$N \rightarrow \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & \cdots \\ 0 & 1 & 0 & 0 & 0 & \cdots \\ 0 & 0 & 2 & 0 & 0 & \cdots \\ 0 & 0 & 0 & 3 & 0 & \cdots \\ 0 & 0 & 0 & 0 & 4 & \cdots \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \end{pmatrix}$$

$$H \rightarrow \begin{pmatrix} \hbar\omega/2 & 0 & 0 & 0 & 0 & \cdots \\ 0 & 3\hbar\omega/2 & 0 & 0 & 0 & \cdots \\ 0 & 0 & 5\hbar\omega/2 & 0 & 0 & \cdots \\ 0 & 0 & 0 & 7\hbar\omega/2 & 0 & \cdots \\ 0 & 0 & 0 & 0 & 9\hbar\omega/2 & \cdots \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \end{pmatrix}$$

$$a^+ \rightarrow \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & \cdots \\ \sqrt{1} & 0 & 0 & 0 & 0 & \cdots \\ 0 & \sqrt{2} & 0 & 0 & 0 & \cdots \\ 0 & 0 & \sqrt{3} & 0 & 0 & \cdots \\ 0 & 0 & 0 & \sqrt{4} & 0 & \cdots \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \end{pmatrix}$$

$$a \rightarrow \begin{pmatrix} 0 & \sqrt{1} & 0 & 0 & 0 & \cdots \\ 0 & 0 & \sqrt{2} & 0 & 0 & \cdots \\ 0 & 0 & 0 & \sqrt{3} & 0 & \cdots \\ 0 & 0 & 0 & 0 & \sqrt{4} & \cdots \\ 0 & 0 & 0 & 0 & 0 & \cdots \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \end{pmatrix}$$

$$q \rightarrow \begin{pmatrix} 0 & \sqrt{1/2} & 0 & 0 & 0 & \cdots \\ \sqrt{1/2} & 0 & \sqrt{1} & 0 & 0 & \cdots \\ 0 & \sqrt{1} & 0 & \sqrt{3/2} & 0 & \cdots \\ 0 & 0 & \sqrt{3/2} & 0 & \sqrt{4/2} & \cdots \\ 0 & 0 & 0 & \sqrt{4/2} & 0 & \cdots \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \end{pmatrix}$$

$$p \rightarrow \begin{pmatrix} 0 & -i\sqrt{1/2} & 0 & 0 & 0 & \cdots \\ i\sqrt{1/2} & 0 & -i\sqrt{1} & 0 & 0 & \cdots \\ 0 & i\sqrt{1} & 0 & -i\sqrt{3/2} & 0 & \cdots \\ 0 & 0 & i\sqrt{3/2} & 0 & -i\sqrt{4/2} & \cdots \\ 0 & 0 & 0 & i\sqrt{4/2} & 0 & \cdots \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \end{pmatrix}$$

It is clear from the structure of these last two operators, therefore, that the mean position and momentum associated with any eigenstate vanishes, i.e.,

$$\langle q \rangle = \langle n|q|n\rangle = 0$$

$$\langle p \rangle = \langle n|p|n\rangle = 0,$$

a fact that also follows from the symmetry (and parity) of the wave functions.

It is also interesting to consider the spread of values associated with position or momentum measurements on the system when it is in an energy eigenstate. Thus we consider the mean value of q^2 in the energy eigenstate $|n\rangle$, i.e.,

$$\begin{aligned} \langle q^2 \rangle &= \langle n|q^2|n\rangle = \frac{1}{2}\langle n|(a^+ + a)(a^+ + a)|n\rangle \\ &= \frac{1}{2}\langle n|a^+a^+ + a^+a + aa^+ + aa|n\rangle \end{aligned}$$

We note that in any expression involving the expectation value of a product of a's and a^+'s with respect to an energy eigenstate, the only terms that can survive are those with an equal number of a's and a^+'s

$$\begin{aligned} \langle n|a^+a^+|n\rangle &= \sqrt{n+1}\sqrt{n+2}\langle n|n+2\rangle = 0 \\ \langle n|aa|n\rangle &= \sqrt{n}\sqrt{n-1}\langle n|n-2\rangle = 0 \\ \langle n|aa^+|n\rangle &= \langle n|(N+1)|n\rangle = n+1 \\ \langle n|a^+a|n\rangle &= \langle n|N|n\rangle = n \end{aligned}$$

Thus, we find that

$$\langle q^2 \rangle = \frac{1}{2}[(n+1)+n] = n + \frac{1}{2}$$

so the uncertainty in position

$$\Delta q = \sqrt{\langle q^2 \rangle} = \sqrt{n + \frac{1}{2}}$$

increases with the quantum number n. Putting back the dimensional quantities this can be written

$$\Delta X = \sqrt{\left(n + \frac{1}{2}\right)\frac{\hbar}{m\omega}}$$

Similarly, we can consider the second moment of the momentum

$$\begin{aligned}\langle p^2\rangle &= \langle n|p^2|n\rangle = -\frac{1}{2}\langle n|(a^+ - a)(a^+ - a)|n\rangle \\ &= \frac{1}{2}\langle n|a^+a^+ - a^+a - aa^+ + aa|n\rangle \\ &= n + \frac{1}{2}\end{aligned}$$

so that the uncertainty is

$$\Delta p = \sqrt{\langle p^2\rangle} = \sqrt{n + \frac{1}{2}}$$

or, in terms of the real momentum,

$$\Delta P = \sqrt{\left(n + \frac{1}{2}\right) m\hbar\omega}.$$

The uncertainty product is therefore

$$\Delta q \Delta p = n + \frac{1}{2} \geq \frac{1}{2} = \frac{1}{2}|\langle [q,p]\rangle|$$

in terms of q and p or

$$\Delta X \Delta P = \left(n + \frac{1}{2}\right)\hbar \geq \frac{\hbar}{2} = \frac{1}{2}|\langle [X,P]\rangle|$$

in terms of X and P. In either case we see that for the ground state of the harmonic oscillator, $n = 0$, the lower bound provided by the uncertainty principle becomes an equality.

3.1.5 Time Evolution of the Harmonic Oscillator

Having solved the eigenvalue problem for the time-independent harmonic oscillator Hamiltonian we have essentially solved the time evolution problem as well. For example, we can immediately construct the evolution operator $U(t) = \exp(-iHt/\hbar)$, which is diagonal in the energy representation and in the present problem is given by the relation

$$U(t) = \sum_{n=0}^{\infty} |n\rangle e^{-iE_n t/\hbar}\langle n|$$

where $E_n = (n + \frac{1}{2})\hbar\omega$, so

$$U(t) = e^{-i\omega t/2}\sum_{n=0}^{\infty} |n\rangle e^{-in\omega t}\langle n|.$$

Note that the zero point energy $\frac{1}{2}\hbar\omega$ gives rise to an overall phase factor. If the system is initially in the state $|\psi(0)\rangle$ at time $t = 0$, associated with the wave function $\psi(q,0) = \langle q|\psi(0)\rangle$ then its state at time t is represented by the expansion

$$\begin{aligned}|\psi(t)\rangle &= U(t)|\psi(0)\rangle = e^{-i\omega t/2}\sum_{n=0}^{\infty} |n\rangle e^{-in\omega t}\langle n|\psi(0)\rangle \\ &= e^{-i\omega t/2}\sum_{n=0}^{\infty} \psi_n(0)\, e^{-in\omega t}|n\rangle\end{aligned}$$

and the wave function can be written as an expansion

$$\begin{aligned}\psi(q,t) &= \langle q|\psi(t)\rangle \\ &= e^{-i\omega t/2}\sum_{n=0}^{\infty}\psi_n(0)\,e^{-in\omega t}\langle q|n\rangle \\ &= e^{-i\omega t/2}\sum_{n=0}^{\infty}\psi_n(0)\,e^{-in\omega t}\phi_n(q)\end{aligned}$$

in the harmonic oscillator eigenfunctions derived earlier, with expansion coefficients obtainable through the relation

$$\begin{aligned}\psi_n(0) &= \langle n|\psi(0)\rangle = \int dq\langle n|q\rangle\langle q|\psi(0)\rangle \\ &= \int dq\phi_n(q)\psi(q,0).\end{aligned}$$