A. J. F. Lovie "Applied Quantum Mechanics" 2nd Edition. (Cambridge)

6 The harmonic oscillator

6.1 The harmonic oscillator potential

We know from our experience with classical mechanics that a particle of mass m subject to a linear restoring force $F(x) = -\kappa x$, where κ is the force constant, results in one-dimensional simple harmonic motion with an oscillation frequency. $\omega = \sqrt{\kappa/m}$. The potential the particle moves in is quadratic $V(x) = \kappa x^2/2$, and so in this case the potential has a minimum at position $x = 0$. The idea that a quadratic potential may be used to describe a local minimum in an otherwise more complex potential turns out to be a very useful concept in both classical and quantum mechanics. An underlying reason why it is of practical importance is that a local potential minimum often describes a point of stability in a system. For example, the positions of atoms that form a crystal are stabilized by the presence of a potential that has a local minimum at the location of each atom. If we wish to understand how the vibrational motion of atoms in a crystal determines properties such as the speed of sound and heat transfer, then we need to develop a model that describes the oscillatory motion of an atom about a local potential minimum. The same is true if we wish to understand the vibrational behavior of atoms in molecules.

As a starting point for our investigation of the vibrational properties of atomic systems, let us assume a static potential and then expand the potential function in a power series about the classically stable equilibrium position x_0 of one particular atom. In one dimension,

$$V(x) = \sum_{n=0}^{\infty} \frac{1}{n!} \frac{d^n}{dx^n} V(x)\bigg|_{x=x_0} (x - x_0)^n \tag{6.1}$$

Assuming that higher-order terms in the polynomial expansion are of decreasing importance, we need only keep the first few terms:

$$V(x) = V(x_0) + \frac{d}{dx} V(x)\bigg|_{x=x_0} (x - x_0) + \frac{1}{2} \frac{d^2}{dx^2} V(x)\bigg|_{x=x_0} (x - x_0)^2 + \cdots \tag{6.2}$$

Because the atom position is stabilized by the potential, we know that the potential is at a local minimum, so the term in the first derivative in our series expansion about the equilibrium position x_0 can be set to zero. This leaves us with

$$V(x) = V(x_0) + \frac{1}{2} \frac{d^2}{dx^2} V(x)\bigg|_{x=x_0} (x - x_0)^2 + \cdots \tag{6.3}$$

The first term on the right-hand side of the equation, $V(x_0)$, is a constant, and so it has no impact on the particle dynamics. The second term is just the quadratic potential of a

one-dimensional harmonic oscillator for which the force constant is easily identified as a measure of the curvature of the potential about the equilibrium point:

$$\kappa = \frac{d^2}{dx^2} V(x)\Big|_{x=x_0} \tag{6.4}$$

We now see the importance of the harmonic oscillator in describing the dynamics of a particle in a local potential minimum. Very often a local minimum in potential energy can be approximated by the quadratic function of a harmonic oscillator.

While it is often convenient to visualize the harmonic oscillator in classical terms as illustrated in Fig. (6.1) if we are dealing with atomic scale particles then we will have to solve for the particle motion using quantum mechanics. Let us consider the time-independent Schrödinger equation for a particle of mass m subject to a restoring force $F(x) = -\kappa x$ in one dimension. The equation is

$$\left(\frac{-\hbar^2}{2m}\frac{d^2}{dx^2} + \frac{\kappa}{2}x^2\right)\psi_n(x) = E_n\psi_n(x) \tag{6.5}$$

where the first term in the brackets is the kinetic energy and the second term is the potential energy

$$V(x) = -\int_{x'=0}^{x'=x} F(x')dx' = -\int_{x'=0}^{x'=x} \kappa x' dx' = \frac{\kappa}{2}x^2 \tag{6.6}$$

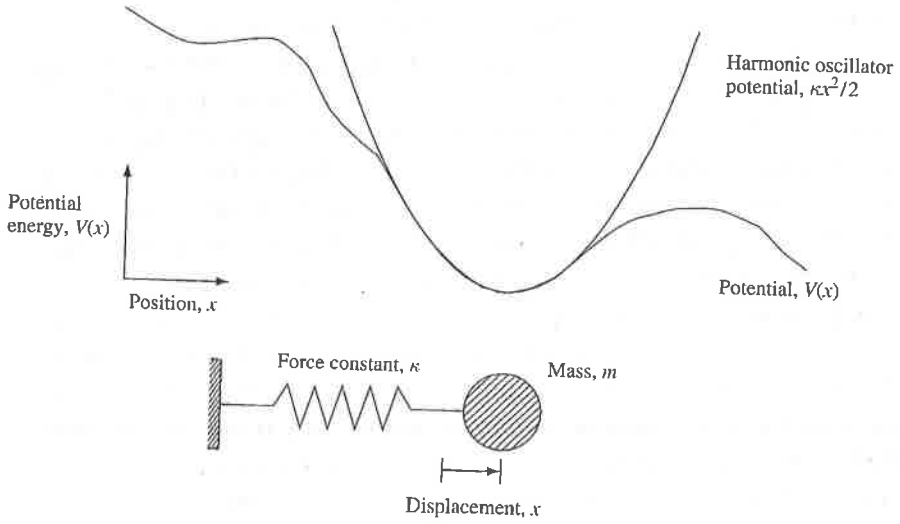

Fig. 6.1 Illustration of a one-dimensional potential with a local minimum that may be approximated by the parabolic potential of a harmonic oscillator. Also shown is a representation of a physical system that has a harmonic potential for small displacement from equilibrium. The classical system consists of a particle of mass m attached to a light spring with force constant κ. The one-dimensional displacement of the particle from its equilibrium position is x.

Note that we have used our definition of a scalar potential that relates force to the potential via $\mathbf{F}(\mathbf{r}) = -\nabla V(\mathbf{r})$.

Our next step is to solve Eq. (6.5). However, before finding the quantized eigenstates and eigenvalues of the harmonic oscillator, we can predict the form of the results using our previous experience developed in Chapter 3. We start by noting that the potential $V(x) = \kappa x^2/2$ has inversion symmetry in such a way that $V(x) = V(-x)$. A consequence of this fact is that the wave functions that describe the bound states of the harmonic oscillator must have definite parity. In addition, we can state that the lowest-energy state of the system (the ground state) will have even parity. With these basic facts in mind, we now turn our effort to finding the quantum mechanical solution for the harmonic oscillator.

6.2 Creation and annihilation operators

In classical mechanics, a particle of mass m moving in the potential $V(x) = \kappa x^2$ oscillates at frequency $\omega = \sqrt{\kappa/m}$, where κ is the force constant. The Hamiltonian for this one-dimensional harmonic oscillator consists of kinetic energy and potential energy terms such that

$$H = T + V = \frac{p_x^2}{2m} + \frac{m\omega^2}{2}x^2 \tag{6.7}$$

where the x-directed particle momentum p_x is $m\ dx/dt$.

In quantum mechanics, the classical momentum p_x is replaced by the operator $\hat{p}_x = -i\hbar\ \partial/\partial x$, so that

$$\hat{H} = \frac{\hat{p}_x^2}{2m} + \frac{m\omega^2}{2}\hat{x}^2 \tag{6.8}$$

Mathematically, this equation is nicely symmetric, since the two operators $\hat{p}_x$ and $\hat{x}$ only appear as simple squares. This immediately suggests that the equation can be factored into two operators which are linear in $\hat{p}_x$ and $\hat{x}$. We define new operators,

$$\hat{b} = \left(\frac{m\omega}{2\hbar}\right)^{1/2}\left(\hat{x} + \frac{i\hat{p}_x}{m\omega}\right) \tag{6.9}$$

$$\hat{b}^\dagger = \left(\frac{m\omega}{2\hbar}\right)^{1/2}\left(\hat{x} - \frac{i\hat{p}_x}{m\omega}\right) \tag{6.10}$$

so that

$$\hat{x} = \left(\frac{\hbar}{2m\omega}\right)^{1/2}(\hat{b} + \hat{b}^\dagger) \tag{6.11}$$

and

$$\hat{p}_x = i\left(\frac{\hbar m\omega}{2}\right)^{1/2}(\hat{b}^\dagger - \hat{b}) \tag{6.12}$$

The Hamiltonian (Eq. (6.8)) expressed in terms of the new operators is (see Problem 6.1)

$$\boxed{\hat{H} = \frac{\hbar\omega}{2}(\hat{b}\hat{b}^\dagger + \hat{b}^\dagger\hat{b})} \tag{6.13}$$

The symmetry of this equation will both help in simplifying problem solving and provide new insight into the quantum-mechanical nature of the harmonic oscillator.

The commutation relations for the operators $\hat{b}^\dagger$ and $\hat{b}$ can be found by writing out the differential form and operating on a dummy wave function. However, we do not have to use a dummy wave function to find the commutator if we express $\hat{b}^\dagger$ and $\hat{b}$ in terms of the operators $\hat{x}$ and $\hat{p}_x$. For example, to find the commutation relation $[\hat{b}, \hat{b}^\dagger] = \hat{b}\hat{b}^\dagger - \hat{b}^\dagger\hat{b}$

$$\begin{aligned}[\hat{b}, \hat{b}^\dagger] &= \hat{b}\hat{b}^\dagger - \hat{b}^\dagger\hat{b} \\ &= \left(\frac{m\omega}{2\hbar}\right)\left(\hat{x} + \frac{i\hat{p}_x}{m\omega}\right)\left(\hat{x} - \frac{i\hat{p}_x}{m\omega}\right) - \left(\frac{m\omega}{2\hbar}\right)\left(\hat{x} - \frac{i\hat{p}_x}{m\omega}\right)\left(\hat{x} + \frac{i\hat{p}_x}{m\omega}\right)\end{aligned} \tag{6.14}$$

$$\begin{aligned}[\hat{b}, \hat{b}^\dagger] = &\left(\frac{m\omega}{2\hbar}\right)\left(\hat{x}^2 + \frac{i\hat{p}_x\hat{x}}{m\omega} - \frac{i\hat{x}\hat{p}_x}{m\omega} + \frac{\hat{p}_x^2}{m^2\omega^2}\right) \\ &- \left(\frac{m\omega}{2\hbar}\right)\left(\hat{x}^2 - \frac{i\hat{p}_x\hat{x}}{m\omega} + \frac{i\hat{x}\hat{p}_x}{m\omega} + \frac{\hat{p}_x^2}{m^2\omega^2}\right)\end{aligned} \tag{6.15}$$

$$[\hat{b}, \hat{b}^\dagger] = \left(\frac{im\omega}{\hbar}\right)\left(\frac{\hat{p}_x\hat{x}}{m\omega} - \frac{\hat{x}\hat{p}_x}{m\omega}\right) = \frac{i}{\hbar}(\hat{p}_x\hat{x} - \hat{x}\hat{p}_x) = \frac{i}{\hbar}[\hat{p}_x, \hat{x}] = i(-i\hbar) = 1 \tag{6.16}$$

where we have used the commutation relation $[\hat{p}_x, \hat{x}] = -i\hbar$ (see Eq. (5.54)).

One can now go through the same process and obtain all the commutation relations for the operators $\hat{b}$ and $\hat{b}^\dagger$. The result is

$$\boxed{[\hat{b}, \hat{b}^\dagger] = \hat{b}\hat{b}^\dagger - \hat{b}^\dagger\hat{b} = 1} \tag{6.17}$$

$$\boxed{[\hat{b}^\dagger, \hat{b}] = \hat{b}^\dagger\hat{b} - \hat{b}\hat{b}^\dagger = -1} \tag{6.18}$$

$$\boxed{[\hat{b}, \hat{b}] = \hat{b}\hat{b} - \hat{b}\hat{b} = 0} \tag{6.19}$$

$$\boxed{[\hat{b}^\dagger, \hat{b}^\dagger] = \hat{b}^\dagger\hat{b}^\dagger - \hat{b}^\dagger\hat{b}^\dagger = 0} \tag{6.20}$$

Thus, the Hamiltonian given by Eq. (6.13) may be rewritten as

$$\hat{H} = \frac{\hbar\omega}{2}(\hat{b}\hat{b}^\dagger + \hat{b}^\dagger\hat{b}) = \frac{\hbar\omega}{2}(\hat{b}\hat{b}^\dagger - \hat{b}^\dagger\hat{b} + 2\hat{b}^\dagger\hat{b}) = \frac{\hbar\omega}{2}(1 + 2\hat{b}^\dagger\hat{b}) \tag{6.21}$$

Notice that we made use of the fact that $[\hat{b}, \hat{b}^\dagger] = \hat{b}\hat{b}^\dagger - \hat{b}^\dagger\hat{b} = 1$.

Hence, the Hamiltonian is

$$\boxed{\hat{H} = \hbar\omega\left(\hat{b}^\dagger\hat{b} + \frac{1}{2}\right)} \tag{6.22}$$

The commutation relations, the Hamiltonian, and the constraint that a lowest energy (ground state) exists *completely* specify the harmonic oscillator in terms of operators. What remains, of course, is to find the condition that expresses the fact that a ground state exists.

6.2.1 The ground state of the harmonic oscillator

To find the ground state wave function and energy of the one-dimensional harmonic oscillator we start with the Schrödinger equation:

$$\hat{H}\psi_n = \hbar\omega\left(\hat{b}^\dagger\hat{b} + \frac{1}{2}\right)\psi_n = E_n\psi_n \tag{6.23}$$

Now we multiply from the *left* by $\hat{b}$ to give

$$\hbar\omega\left(\hat{b}\hat{b}^\dagger\hat{b} + \frac{\hat{b}}{2}\right)\psi_n = E_n\hat{b}\psi_n \tag{6.24}$$

But $[\hat{b}, \hat{b}^\dagger] = \hat{b}\hat{b}^\dagger - \hat{b}^\dagger\hat{b} = 1$, so that $\hat{b}\hat{b}^\dagger = 1 + \hat{b}^\dagger\hat{b}$. Hence, Eq. (6.24) may be written

$$\hbar\omega\left((1 + \hat{b}^\dagger\hat{b})\hat{b} + \frac{\hat{b}}{2}\right)\psi_n = E_n\hat{b}\psi_n \tag{6.25}$$

Factoring out the term $\hat{b}\psi_n$ on the left-hand side of Eq. (6.25) gives

$$\hbar\omega\left((1 + \hat{b}^\dagger\hat{b}) + \frac{1}{2}\right)(\hat{b}\psi_n) = E_n(\hat{b}\psi_n) \tag{6.26}$$

Subtracting the term $\hbar\omega(\hat{b}\psi_n)$ from both sides allows one to write

$$\hbar\omega\left(\hat{b}^\dagger\hat{b} + \frac{1}{2}\right)(\hat{b}\psi_n) = (E_n - \hbar\omega)(\hat{b}\psi_n) \tag{6.27}$$

$$\hbar\omega\left(\hat{b}^\dagger\hat{b} + \frac{1}{2}\right)\psi_{n-1} = E_{n-1}\psi_{n-1} \tag{6.28}$$

This shows that $\psi_{n-1} = (\hat{b}\psi_n)$ is a new eigenfunction with energy eigenvalue $(E_n - \hbar\omega)$. In a similar way, it can be shown that the operator $\hat{b}^\dagger$ acting on eigenfunction ψ_n creates a new eigenfunction ψ_{n+1} with eigenenergy $(E_n + \hbar\omega)$.

We now know enough to define the ground state. Clearly, the operator $\hat{b}$ can only be used to reduce the energy eigenvalue of any eigenstate except the ground state. Notice

that we *assume the existence* of a ground state. Because there are, by definition, no energy eigenstates with energy less than the ground state, the ground state must be defined by

$$\boxed{\hat{b}\psi_0 = 0} \tag{6.29}$$

This, when combined with Eqs. (6.17) to (6.20) and Eq. (6.22), completes our definition of the harmonic oscillator in terms of the operators $\hat{b}^\dagger$ and $\hat{b}$.

It is now possible to use our definition of the ground state to find the ground state wave function. Since

$$\hat{b} = \left(\frac{m\omega}{2\hbar}\right)^{1/2}\left(\hat{x} + \frac{i\hat{p}_x}{m\omega}\right) = \left(\frac{m\omega}{2\hbar}\right)^{1/2}\left(x + \frac{\hbar}{m\omega}\frac{\partial}{\partial x}\right) \tag{6.30}$$

our definition $\hat{b}\psi_0 = 0$ requires

$$\left(\frac{m\omega}{2\hbar}\right)^{1/2}\left(x + \frac{\hbar}{m\omega}\frac{\partial}{\partial x}\right)\psi_0 = 0 \tag{6.31}$$

The solution for the wave function is of Gaussian form

$$\boxed{\psi_0 = A_0 e^{-x^2 m\omega/2\hbar}} \tag{6.32}$$

where the normalization constant A_0 is found in the usual way from the requirement that $\int \psi_0^* \psi_0 dx = 1$. This gives

$$A_0 = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} \tag{6.33}$$

Notice that the ground state wave function ψ_0 for the harmonic oscillator has the even-parity we predicted earlier based solely on symmetry arguments.

To find the eigenenergy of the ground state ψ_0 one substitutes Eq. (6.32) into the Schrödinger equation for the one-dimensional harmonic oscillator:

$$\left(\frac{-\hbar^2}{2m}\frac{d^2}{dx^2} + \frac{m\omega^2}{2}x^2\right)\psi_0 = \left(\frac{-\hbar^2}{2m}\left(-\frac{2m\omega}{2\hbar} + 4x^2\left(\frac{m\omega}{2\hbar}\right)^2\right) + \frac{m\omega^2}{2}x^2\right)\psi_0 = E_0\psi_0 \tag{6.34}$$

$$\left(\frac{\hbar\omega}{2} - \frac{m\omega^2}{2}x^2 + \frac{m\omega^2}{2}x^2\right)\psi_0 = \left(\frac{\hbar\omega}{2} - \frac{m\omega^2}{2}x^2 + \frac{m\omega^2}{2}x^2\right)\psi_0 = E_0\psi_0 \tag{6.35}$$

so that the value of the ground state energy, E_0, is

$$\boxed{E_0 = \frac{\hbar\omega}{2}} \tag{6.36}$$

6.2.1.1 *Uncertainty in position and momentum for the harmonic oscillator in the ground state*

The ground state wave function ψ_0 given by Eq. (6.32) is of even parity. This symmetry will be helpful when we evaluate integrals that give us the expectation values for position and momentum.

We start by considering uncertainty in position $\Delta x = (\langle x^2 \rangle - \langle x \rangle^2)^{1/2}$. To evaluate Δx, we will need to calculate the expectation value of the observable x associated with the position operator $\hat{x}$ and the expectation value of the observable x^2 associated with the operator $\hat{x}^2$. This is done by expressing the position operator and the position operator squared in terms of $\hat{b}^\dagger$ and $\hat{b}$:

$$\hat{x} = \left(\frac{\hbar}{2m\omega}\right)^{1/2} (\hat{b} + \hat{b}^\dagger) \tag{6.37}$$

$$\hat{x}^2 = \left(\frac{\hbar}{2m\omega}\right) (\hat{b} + \hat{b}^\dagger)^2 = \left(\frac{\hbar}{2m\omega}\right) (\hat{b}\hat{b} + \hat{b}^\dagger\hat{b}^\dagger + \hat{b}\hat{b}^\dagger + \hat{b}^\dagger\hat{b}) \tag{6.38}$$

The expectation values $\langle x \rangle$ and $\langle x^2 \rangle$ for the system in the ground state are now easy to evaluate.

$$\langle x \rangle = \int \psi_0^* x \psi_0 dx = 0 \tag{6.39}$$

The fact that $\langle x \rangle = 0$ follows directly from the observation that ψ_0 is an even function and x is an odd function, so the integral must, by symmetry, be zero.

The result for $\langle x^2 \rangle$ is almost as straightforward to evaluate. We start by writing down the expectation value in integral form:

$$\langle x^2 \rangle = \int \psi_0^* \hat{x}^2 \psi_0 dx = \frac{\hbar}{2m\omega} \int \psi_0^* (\hat{b}\hat{b} + \hat{b}^\dagger\hat{b}^\dagger + \hat{b}\hat{b}^\dagger + \hat{b}^\dagger\hat{b}) \psi_0 dx \tag{6.40}$$

The terms involving $\hat{b}\psi_0$ must, by definition of the ground state, be zero. The term $\hat{b}^\dagger\hat{b}^\dagger\psi_0$ creates a state ψ_2 that is orthogonal to ψ_0^* and so must contribute zero to the integral. This leaves the term $\hat{b}\hat{b}^\dagger\psi_0 = \psi_0$, which means that $\int \psi_0^* (\hat{b}\hat{b}^\dagger\psi_0) dx = \int \psi_0^* \psi_0 dx = 1$. Hence

$$\langle x^2 \rangle = \frac{\hbar}{2m\omega} \tag{6.41}$$

The same approach may be used to evaluate the uncertainty in momentum $\Delta p_x = (\langle p_x^2 \rangle - \langle p_x \rangle^2)^{1/2}$. As before, we express the momentum operator and the momentum operator squared in terms of $\hat{b}^\dagger$ and $\hat{b}$. The momentum operator can be written

$$\hat{p}_x = i\left(\frac{\hbar m\omega}{2}\right)^{1/2} (\hat{b}^\dagger - \hat{b}) \tag{6.42}$$

so that

$$\hat{p}_x^2 = \left(\frac{\hbar m\omega}{2}\right)(-\hat{b}\hat{b} - \hat{b}^\dagger\hat{b}^\dagger + \hat{b}\hat{b}^\dagger + \hat{b}^\dagger\hat{b}) \tag{6.43}$$

It follows that

$$\langle p_x\rangle = 0 \tag{6.44}$$

and

$$\langle p_x^2\rangle = \frac{\hbar m\omega}{2} \tag{6.45}$$

We now have expressions for $\Delta x^2 = \langle x^2\rangle - \langle x\rangle^2$ and $\Delta p_x^2 = \langle p_x^2\rangle - \langle p_x\rangle^2$, which, because $\langle x\rangle^2 = 0$ and $\langle p_x\rangle^2 = 0$, give an uncertainty product:

$$\Delta x^2\Delta p_x^2 = \langle x^2\rangle\langle p_x^2\rangle = \frac{\hbar^2 m\omega}{4m\omega} = \frac{\hbar^2}{4} \tag{6.46}$$

Taking the square root of both sides gives the uncertainty product of position and momentum

$$\Delta x\Delta p_x = \frac{\hbar}{2} \tag{6.47}$$

which satisfies the Heisenberg uncertainty relation $\Delta p\Delta x \geq \hbar/2$. Thus, we may conclude that the ground state energy of the harmonic oscillator is just $E_0 = \hbar\omega/2$. The important physical interpretation of this result is that, according to the uncertainty relation, this ground state energy represents a minimum uncertainty in the product of position and momentum.

In contrast, the lowest energy of a *classical* harmonic oscillator is *zero*. In the classical case, the minimum energy of a particle in the harmonic potential $V(x) = \kappa x^2/2$ corresponds to both momentum and position simultaneously being zero. In quantum mechanics, this is impossible, since $\Delta x\Delta p_x \geq \hbar/2$. As we have seen, the uncertainty product between position and momentum that minimizes total energy gives the ground state energy $E_0 = \hbar\omega/2$.

6.2.2 Excited states of the harmonic oscillator and normalization of eigenstates

What we now need to know is how to use the operators $\hat{b}^\dagger$ and $\hat{b}$ to find the eigenstates and eigenenergies of all the other states of the system. These nonground states are called *excited states*.

Fortunately, it turns out that if we know ψ_0 we can generate all other ψ_n using the creation (or raising) operator $\hat{b}^\dagger$. To see that this is the case, we multiply the ground state of the harmonic oscillator by $\hat{b}^\dagger$ in the Schrödinger equation:

$$\hat{b}^\dagger\hbar\omega\left(\hat{b}^\dagger\hat{b} + \frac{1}{2}\right)\psi_n = \hat{b}^\dagger E_n\psi_n = \hat{b}^\dagger\hat{H}\psi_n \tag{6.48}$$

$$\hbar\omega\left(\hat{b}^\dagger\hat{b}^\dagger\hat{b} + \frac{\hat{b}^\dagger}{2}\right)\psi_n = E_n\hat{b}^\dagger\psi_n = \hat{b}^\dagger\hat{H}\psi_n \tag{6.49}$$

Now, using the commutation relation $\hat{b}\hat{b}^\dagger - \hat{b}^\dagger\hat{b} = 1$ and substituting for $\hat{b}^\dagger\hat{b} = \hat{b}\hat{b}^\dagger - 1$,

$$\hbar\omega\left(\hat{b}^\dagger(\hat{b}\hat{b}^\dagger - 1) + \frac{\hat{b}^\dagger}{2}\right)\psi_n = \hbar\omega\left((\hat{b}^\dagger\hat{b}\hat{b}^\dagger - \hat{b}^\dagger) + \frac{\hat{b}^\dagger}{2}\right)\psi_n = E_n\hat{b}^\dagger\psi_n \tag{6.50}$$

$$\hbar\omega\left((\hat{b}^\dagger\hat{b} - 1)\hat{b}^\dagger + \frac{\hat{b}^\dagger}{2}\right)\psi_n = \hbar\omega\left((\hat{b}^\dagger\hat{b} - 1) + \frac{1}{2}\right)\hat{b}^\dagger\psi_n = E_n\hat{b}^\dagger\psi_n \tag{6.51}$$

$$\hbar\omega\left(\hat{b}^\dagger\hat{b} + \frac{1}{2}\right)(\hat{b}^\dagger\psi_n) = (E_n + \hbar\omega)(\hat{b}^\dagger\psi_n) \tag{6.52}$$

This shows that the operator $\hat{b}^\dagger$, acting on the eigenstate ψ_n, generates a new eigenstate $(\hat{b}^\dagger\psi_n)$ with energy eigenvalue $(E_n + \hbar\omega)$.

It is now clear that $\hat{b}^\dagger$, operating on ψ_n, increases the eigenenergy by an amount $\hbar\omega$, so that the eigenenergy for the n-th state is

$$\boxed{E_n = \hbar\omega\left(n + \frac{1}{2}\right)} \tag{6.53}$$

where n is a positive integer $n = 0, 1, 2, \ldots$ Because the time independent Schrödinger equation for the harmonic oscillator is

$$\hat{H}\psi_n = \hbar\omega\left(\hat{b}^\dagger\hat{b} + \frac{1}{2}\right)\psi_n = \hbar\omega\left(n + \frac{1}{2}\right)\psi_n = E_n\psi_n \tag{6.54}$$

we may identify the number operator

$$\hat{n} = \hat{b}^\dagger\hat{b} \tag{6.55}$$

which, when operating on the eigenstate ψ_n has eigenvalue n. See Section 6.2.2.2.

Summarizing what we know so far, we may think of $\hat{b}^\dagger$ and $\hat{b}$ as creation (or raising) and annihilation (or lowering) operators, respectively, that act upon the state ψ_n in such a way that

$$\hat{b}^\dagger\psi_n = A_{n+1}\psi_{n+1} \tag{6.56}$$

and

$$\hat{b}\psi_n = A_{n-1}\psi_{n-1} \tag{6.57}$$

where A_{n+1} and A_{n-1} are normalization constants, which we will now find. The way we do this is to start by assuming that the n-th state is correctly normalized and then find the relationship between the normalization of the n-th state and the n-th-plus-one state. Rather than write ψ_n, we use the notation $|n\rangle$, and for ψ_n^* we use $\langle n|$. Since we have assumed that the n-th state is normalized, we may write

$$\int \psi_n^*\psi_n dx = \langle n|n\rangle = 1 \tag{6.58}$$

6.2.2.1 *Matrix elements*

The eigenstates $\psi_n = |n\rangle$ of the harmonic oscillator are orthonormal, so that

$$\langle n'|n\rangle = \delta_{n',n} \tag{6.68}$$

In our notation, $\langle n'|\hat{b}^\dagger|n\rangle = \int \psi_{n'}^* \hat{b}^\dagger \psi_n dx$ is a matrix element. It can be shown that the matrix elements involving $\hat{b}^\dagger$ and $\hat{b}$ only exist between adjacent states, so that

$$\langle n'|\hat{b}^\dagger|n\rangle = (n+1)^{1/2}\delta_{n'=n+1} \tag{6.69}$$

$$\langle n'|\hat{b}|n\rangle = n^{1/2}\delta_{n'=n-1} \tag{6.70}$$

6.2.2.2 *The number operator* $\hat{n}$

Sometimes it is convenient to define a *number* operator such that

$$\boxed{\hat{n} = \hat{b}^\dagger \hat{b}} \tag{6.71}$$

The eigenvalue of the operator $\hat{n}$ applied to an eigenstate labeled by quantum number n is just n:

$$\hat{b}^\dagger \hat{b}|n\rangle = \hat{b}^\dagger n^{1/2}|n-1\rangle = n^{1/2}\hat{b}^\dagger|n-1\rangle = n^{1/2}(n-1+1)^{1/2}|n\rangle = n|n\rangle \tag{6.72}$$

This operator commutes with $\hat{b}$ and $\hat{b}^\dagger$ in the following way

$$[\hat{n}, \hat{b}] = [\hat{b}^\dagger \hat{b}, b] = \hat{b}^\dagger[\hat{b}, \hat{b}] + [\hat{b}^\dagger, \hat{b}]\hat{b} \tag{6.73}$$

$$[\hat{n}, \hat{b}^\dagger] = [\hat{b}^\dagger \hat{b}, \hat{b}^\dagger] = \hat{b}^\dagger[\hat{b}, \hat{b}^\dagger] + [\hat{b}^\dagger, \hat{b}^\dagger]\hat{b} \tag{6.74}$$

However, we know from our previous work that $[\hat{b}, \hat{b}] = 0$, $[\hat{b}, \hat{b}^\dagger] = 1$, and $[\hat{b}^\dagger, b] = -1$, so that

$$[\hat{n}, \hat{b}] = -\hat{b} \tag{6.75}$$

and

$$[\hat{n}, \hat{b}^\dagger] = \hat{b}^\dagger \tag{6.76}$$

Obviously, since the Hamiltonian operator for the harmonic oscillator is $\hat{H} = \hbar\omega(\hat{n} + 1/2)$, the eigenfunctions of the Hamiltonian $\hat{H}$ are also eigenfunctions of the number operator $\hat{n}$.

We can summarize pictorially the results obtained so far in this chapter. In Fig. 6.2 the ground state energy level and excited-state energy levels near the n-th state of the one-dimensional harmonic oscillator are shown schematically. Transition between eigenstates of neighboring energy is achieved by applying the operators $\hat{b}^\dagger$ or $\hat{b}$ to a given eigenstate. The energy of an eigenstate is $\hbar\omega(n + 1/2)$, and the value of n is found by applying the operator $\hat{b}^\dagger \hat{b} = \hat{n}$ to the eigenstate. From Eqs. (6.17) and (6.71) it follows that $\hat{b}\hat{b}^\dagger = \hat{n} + 1$. The ground state ψ_0 is defined by $\hat{b}\psi_0 = 0$.

Classical simple harmonic oscillation occurs in a single mode of frequency ω. The vibrational energy can be changed continuously by varying the oscillation amplitude.

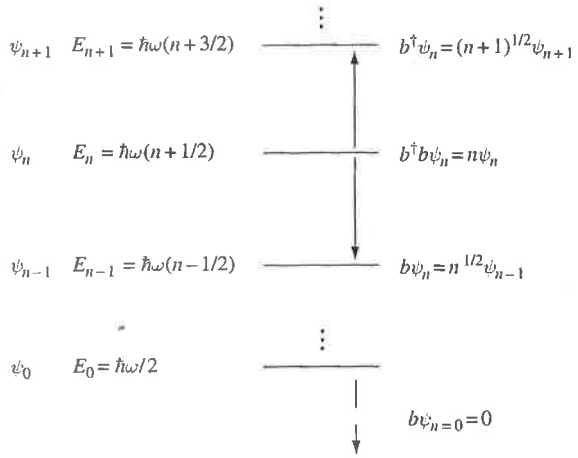

Fig. 6.2 Diagram showing the equally spaced energy levels of the one-dimensional harmonic oscillator. The raising or creation operator $\hat{b}^\dagger$ acts upon eigenstate ψ_n with eigenenergy E_n to form a new eigenstate ψ_{n+1} with eigenenergy E_{n+1}. In a similar way, the annihilation operator $\hat{b}$ acts upon eigenstate ψ_n with eigenenergy E_n to form a new eigenstate ψ_{n-1} with eigenenergy E_{n-1}. Energy levels are equally spaced in energy by $\hbar\omega$. The ground state ψ_0 of the harmonic oscillator is the single state for which $\hat{b}\psi_{n+1} = 0$. The ground state energy is $\hbar\omega/2$.

The quantum-mechanical oscillator also has a single oscillatory mode characterized by frequency ω but the vibrational energy is quantized in such a way that $E_n = \hbar\omega(n+1/2)$. If we associate a particle with each of the quanta $\hbar\omega$, then there can be n particles in a given mode. Each n-particle state of the system is associated with a different wave function ψ_n.

The manipulation of operators is similar to ordinary algebra, with the obvious exception that the order of operators must be accurately maintained. There is another important rule. One must not divide by an operator $\hat{b}$. To show this, consider the state formed by

$$\psi = \hat{b}\psi_0 \tag{6.77}$$

Now, if we divide both sides by $\hat{b}$, then

$$\frac{1}{\hat{b}}\psi = \psi_0 \tag{6.78}$$

To show that Eqs. (6.77) and (6.78) are inconsistent with each other, consider the situation in which ψ_0 is the ground state. In this case, $\psi = \hat{b}\psi_0 = 0$ by our definition of a ground state (Eq. (6.29)). However, Eq. (6.78) states $(1/\hat{b})\psi = \psi_0 \neq 0$. While one cannot multiply by $1/\hat{b}$, it is possible to multiply by an operator of the form $1/(\alpha + \hat{b})$ where α is a constant since this may be expanded as a power series in $\hat{b}$.

6.3 The harmonic oscillator wave functions

Previously, we derived expressions for the creation or raising operator $\hat{b}^\dagger$ and the ground state wave function ψ_0 for the one-dimensional harmonic oscillator so that

$$\hat{b}^\dagger = \left(\frac{m\omega}{2\hbar}\right)^{1/2}\left(x - \frac{\hbar}{m\omega}\frac{\partial}{\partial x}\right) \tag{6.79}$$

and

$$\psi_0(x) = A_0 \exp\left(-x^2 \frac{m\omega}{2\hbar}\right) \tag{6.80}$$

where the normalization constant for the Gaussian wave function is given by

$$A_0 = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} \tag{6.81}$$

To simplify the notation, it is convenient to introduce a new spatial variable

$$\xi = \left(\frac{m\omega}{\hbar}\right)^{1/2} x \tag{6.82}$$

Equation (6.79) may now be written as

$$\hat{b}^\dagger = \frac{1}{\sqrt{2}}\left(\left(\frac{m\omega}{\hbar}\right)^{1/2} x - \left(\frac{\hbar}{m\omega}\right)^{1/2} \frac{\partial}{\partial x}\right) = \frac{1}{\sqrt{2}}\left(\xi - \frac{\partial}{\partial \xi}\right) \tag{6.83}$$

and Eq. (6.80) for the ground state wave function becomes

$$\psi_0(\xi) = A_0 \exp(-\xi^2/2) \tag{6.84}$$

where the normalization constant is simply

$$A_0 = \left(\frac{1}{\pi}\right)^{1/4} \tag{6.85}$$

We can now generate the other higher-order states by using the operator $\hat{b}^\dagger$. Starting with the ground state and using Eq. (6.66) to ensure correct normalization, a natural sequence of wave functions is created:

$$\psi_0 \tag{6.86}$$

$$\psi_1 = \hat{b}^\dagger \psi_0 \tag{6.87}$$

$$\psi_2 = \frac{1}{\sqrt{2}} \hat{b}^\dagger \psi_1 = \frac{1}{\sqrt{2}} (\hat{b}^\dagger)^2 \psi_0 \tag{6.88}$$

$$\psi_3 = \frac{1}{\sqrt{2}} \hat{b}^\dagger \psi_2 = \frac{1}{\sqrt{2}\sqrt{3}} (\hat{b}^\dagger)^2 \psi_1 = \frac{1}{\sqrt{3!}} (\hat{b}^\dagger)^3 \psi_0 \tag{6.89}$$

$$\psi_n = \frac{1}{\sqrt{n!}} (\hat{b}^\dagger)^n \psi_0 \tag{6.90}$$

Because we know the ground state wave function (Eq. (6.84)), it is now possible to generate all the other excited states of the system. The first few states are

$$\psi_0 = A_0 \exp(-\xi^2/2) \tag{6.91}$$

$$\psi_1 = \hat{b}^\dagger \psi_0 = \frac{1}{\sqrt{1!}} \frac{1}{\sqrt{2}} \left(\xi - \frac{\partial}{\partial \xi}\right) A_0 \exp(-\xi^2/2) = \frac{1}{\sqrt{2}} 2\xi A_0 \exp(-\xi^2/2) = \frac{1}{\sqrt{2}} 2\xi \psi_0 \tag{6.92}$$

$$\psi_2 = \hat{b}^\dagger \psi_1 = \frac{1}{\sqrt{2!}}(\hat{b}^\dagger)^2 \psi_0 = \frac{1}{\sqrt{2!}}\frac{1}{\sqrt{2}}\left(\xi - \frac{\partial}{\partial \xi}\right)\frac{1}{\sqrt{2}} 2\xi A_0 \exp(-\xi^2/2) \tag{6.93}$$

$$= \frac{1}{\sqrt{2}}\frac{1}{\sqrt{4}}(4\xi^2 - 2)\psi_0$$

$$\psi_3 = \hat{b}^\dagger \psi_2 = \frac{1}{\sqrt{3!}}(\hat{b}^\dagger)^3 \psi_0 = \frac{1}{\sqrt{3!}}\frac{1}{\sqrt{2}}\left(\xi - \frac{\partial}{\partial \xi}\right)\frac{1}{2}(4\xi^2 - 2)\psi_0 \tag{6.94}$$

$$= \frac{1}{\sqrt{6}}\frac{1}{\sqrt{8}}(8\xi^3 - 12\xi)\psi_0$$

$$\psi_4 = \hat{b}^\dagger \psi_3 = \frac{1}{\sqrt{4!}}(\hat{b}^\dagger)^4 \psi_0 = \frac{1}{\sqrt{24}}\frac{1}{\sqrt{16}}(16\xi^4 - 48\xi^2 + 12)\psi_0 \tag{6.95}$$

$$\psi_5 = \hat{b}^\dagger \psi_4 = \frac{1}{\sqrt{5!}}(\hat{b}^\dagger)^5 \psi_0 = \frac{1}{\sqrt{120}}\frac{1}{\sqrt{32}}(32\xi^5 - 160\xi^3 + 120\xi)\psi_0 \tag{6.96}$$

Notice that the wave functions are alternately even and odd functions.

It is clear from Eqs. (6.91) to (6.96) that there is a relationship between the wave functions that can be expressed as a Hermite polynomial $H_n(\xi)$ so that

$$\psi_n(\xi) = \hat{b}^\dagger \psi_{n-1}(\xi) = \frac{1}{\sqrt{2^n n!}} H_n(\xi)\psi_0(\xi) \tag{6.97}$$

Learning more about $H_n(\xi)$ one finds that the n-th polynomial is related to the $n-1$ and $n-2$ polynomial via

$$H_n(\xi) = 2\xi H_{n-1}(\xi) - 2(\xi - 1)H_{n-2}(\xi) \tag{6.98}$$

The Hermite polynomials themselves may be obtained from the generating function

$$\exp(-t^2 + 2t\xi) = \sum_{n=0}^{\infty} \frac{H_n(\xi)}{n!} t^n \tag{6.99}$$

or

$$H_n(\xi) = \left(\frac{d^n}{dt^n} \exp^{-t^2+2t\xi}\right)_{t=0} = (-1)^n \exp(\xi^2)\frac{d^n}{d\xi^n}\exp(\xi^{-2}) \tag{6.100}$$

The first few Hermite polynomials are

$$H_0(\xi) = 1 \tag{6.101}$$

$$H_1(\xi) = 2\xi \tag{6.102}$$

$$H_2(\xi) = 4\xi^2 - 2 \tag{6.103}$$

$$H_3(\xi) = 8\xi^3 - 12\xi \tag{6.104}$$

$$H_4(\xi) = 16\xi^4 - 48\xi^2 + 12 \tag{6.105}$$

$$H_5(\xi) = 32\xi^5 - 160\xi^3 + 120\xi \tag{6.106}$$

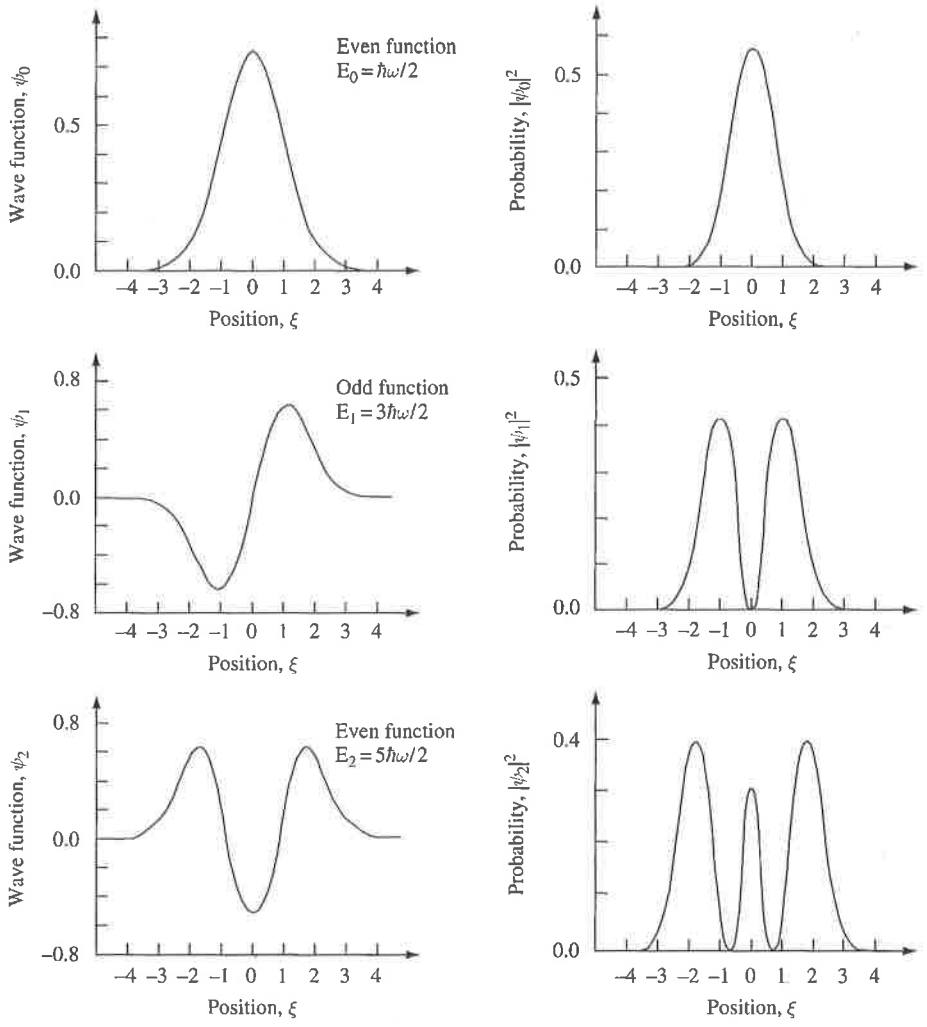

Fig. 6.3 Plot of wave function and probability function for the three lowest-energy states of the one-dimensional harmonic oscillator. Position is measured in normalized units of $\xi = x(m\omega/\hbar)^{1/2}$.

The Schrödinger equation for the one-dimensional harmonic oscillator can be written in terms of the variable ξ to give

$$\left(\frac{d^2}{d\xi^2} + \left(\frac{2E}{\hbar\omega} - \xi^2\right)\right)\psi_n(\xi) = 0 \tag{6.107}$$

The solutions are the Hermite–Gaussian functions

$$\psi_n(\xi) = \left(\frac{1}{\sqrt{\pi}2^n n!}\right)^{1/2} H_n(\xi)\exp(-\xi^2/2) = \frac{1}{\sqrt{2^n n!}} H_n(\xi)\psi_0(\xi) \tag{6.108}$$

where $H_n(\xi)$ are Hermite polynomials. These satisfy the differential equation

$$\left(\frac{d^2}{d\xi^2} - 2\xi\frac{d}{d\xi} + 2n\right) H_n(\xi) = 0 \tag{6.109}$$

and n is related to the energy E_n by

$$E_n = \left(n + \frac{1}{2}\right)\hbar\omega \tag{6.110}$$

where $n = 0, 1, 2, \ldots$ Alternately, if we know the two starting functions ψ_0 and ψ_1 then the n-th wave function can be generated by using

$$\psi_n(\xi) = \sqrt{\frac{2}{n}}\left(\xi\psi_{n-1}(\xi) - \sqrt{\frac{n-1}{2}}\psi_{n-2}(\xi)\right) \tag{6.111}$$

In Fig. 6.3, the wave function and probability function for the three lowest-energy states of the one-dimensional harmonic oscillator are plotted. The wave functions $\psi_n(\xi)$ form a complete orthogonal set. So we may conclude that the eigenvalues given by Eq. (6.53) and the eigenfunctions $\psi_n(\xi)$ are the only solutions of the Hamiltonian describing the harmonic oscillator.

6.3.1 The classical turning point of the harmonic oscillator

Consider a one-dimensional classical harmonic oscillator consisting of a particle of mass m subject to a restoring force $-\kappa x$. The frequency of oscillation is $\omega = \sqrt{\kappa/m}$, and the total energy is $E_{\text{total}} = m\omega^2 A^2/2 = \kappa A^2/2$, where A is the classical amplitude of oscillation. If we equate the total energy of the classical harmonic oscillator with the energy of a one-dimensional quantum mechanical oscillator in the n-th state, we have

$$E_{\text{total}} = \kappa A_n^2/2 = \hbar\omega\left(n + \frac{1}{2}\right) \tag{6.112}$$

The classical turning point for the harmonic oscillator occurs at position x_n, corresponding to the classical amplitude A_n. This value is just

$$x_n = (\hbar\omega/\kappa)^{1/2}(2n+1)^{1/2} = \left(\frac{\hbar}{m\omega}\right)^{1/2}(2n+1)^{1/2} \tag{6.113}$$

The eigenfunctions of the quantum-mechanical harmonic oscillator extend beyond the classical turning point. A portion of each wave function tunnels into a region of the potential which is not accessible classically. This means that there is a finite probability of finding the particle outside the region bounded by the potential.

Using Eq. (6.113) we see that the classical turning point for the ground state and the first two excited states of the harmonic oscillator are

$$x_0 = \left(\frac{\hbar}{m\omega}\right)^{1/2} \tag{6.114}$$

$$x_1 = \sqrt{3}\left(\frac{\hbar}{m\omega}\right)^{1/2} \tag{6.115}$$

$$x_2 = \sqrt{5}\left(\frac{\hbar}{m\omega}\right)^{1/2} \tag{6.116}$$

or, in terms of the parameter $\xi = x(m\omega/\hbar)^{1/2}$,

$$\xi_0 = 1 \tag{6.117}$$

$$\xi_1 = \sqrt{3} \tag{6.118}$$

$$\xi_2 = \sqrt{5} \tag{6.119}$$

$$\xi_n = (2n+1)^{1/2} \tag{6.120}$$

Figure 6.4 illustrates the classical turning point $\pm x_n$ for the ground state ψ_0 and the first two excited states ψ_1 and ψ_2 of the one-dimensional harmonic oscillator. In the figure the potential $V(x) = \kappa x^2/2$, the energy levels E_n and the position of x_n are indicated.

The portion of an eigenstate that is outside the classically allowed region can be used to obtain the probability of finding a particle in that region. If the particle is in a particular eigenstate, then all that needs to be done is integrate the square of the wave function in the classically inaccessible region.

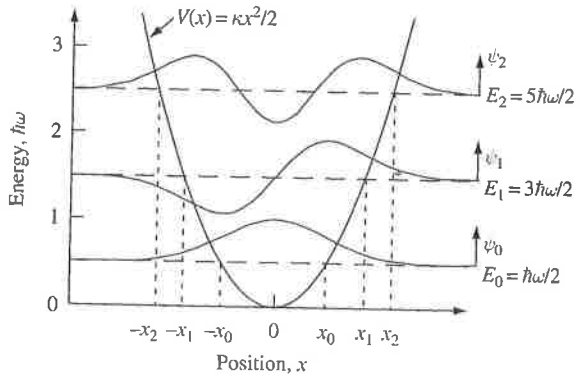

Fig. 6.4 Diagram showing the first three lowest-energy eigenfunctions of the one-dimensional harmonic oscillator. The wave functions penetrate into the regions of the potential that are not accessible according to classical mechanics. The classical turning points are x_0, x_1, and x_2 for the ground state and first two excited states of the harmonic oscillator respectively.

As an example, consider a particle that is in the ground state ψ_0 with eigenenergy $E_0 = \hbar\omega/2$. The region where $V(x) > \hbar\omega/2$ is not accessible classically. Rewriting this condition,

$$\frac{1}{2}m\omega^2 x^2 > \frac{1}{2}\hbar\omega \tag{6.121}$$

$$\left| x\sqrt{\frac{m\omega}{\hbar}} \right| > 1 \tag{6.122}$$

$$|\xi| > 1 \tag{6.123}$$

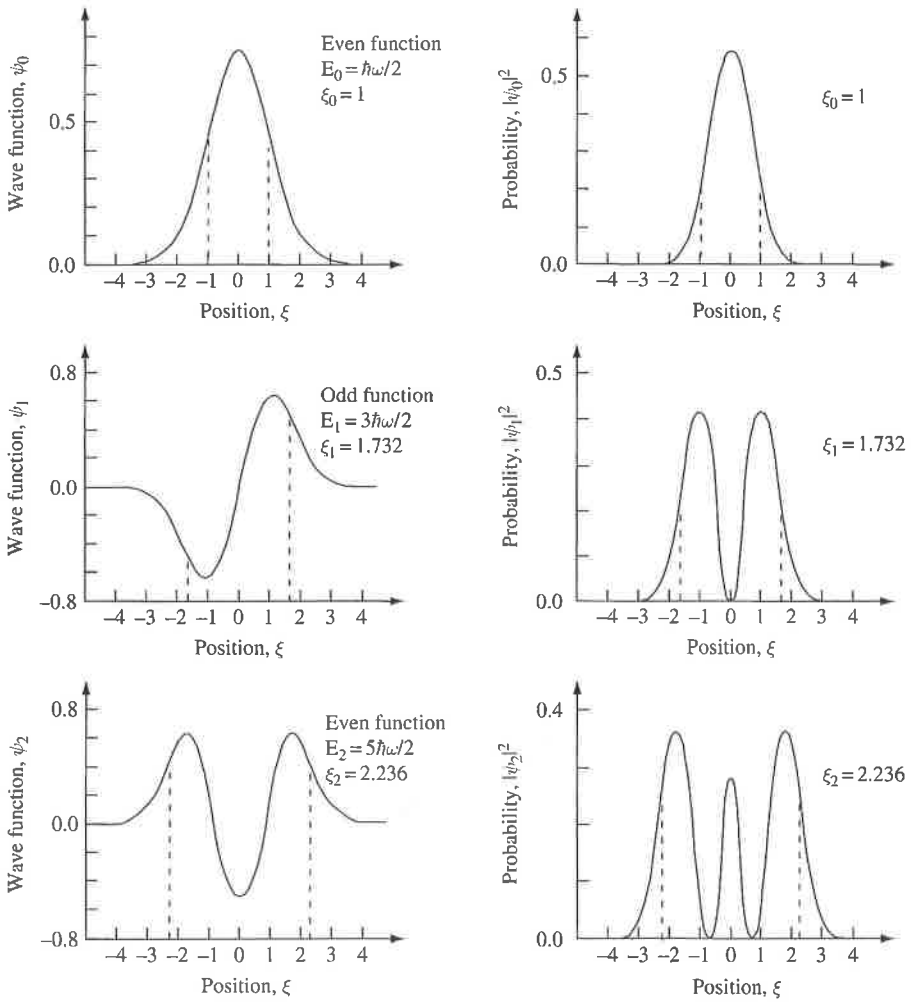

Fig. 6.5 Plot of wave function and probability function for the three lowest-energy states of the one-dimensional harmonic oscillator. Position is measured in normalized units of $\xi = x(m\omega/\hbar)^{1/2}$. The classical turning points are ξ_0, ξ_1, and ξ_2 for the ground state and first two excited-states of the harmonic oscillator, respectively.

The probability of finding the particle in this nonclassical region is given by

$$\int_{\left|x\sqrt{\frac{m\omega}{\hbar}}\right|>1} \psi_0^*(x)\psi_0(x)dx = \int_{|\xi|>1} \psi_0^*(\xi)\psi_0(\xi)d\xi = \frac{1}{\sqrt{\pi}} \int_{|\xi|>1} \exp^{(-\xi^2)}\, d\xi = 0.157 \tag{6.124}$$

where we have used the fact that the ground state wave function written as a function of the variable ξ (Eq. (6.82)) is (Eq. (6.84)):

$$\psi_0(\xi) = \left(\frac{1}{\pi}\right)^{1/4} \exp^{(-\xi^2/2)} \tag{6.125}$$

The numerical value of the integral in Eq. (6.124) is found from tables of values for the error function.

The excited states of the harmonic oscillator have a reduced probability of finding the particle in this nonclassical region. This probability decreases slowly as the energy eigenstate increases.

Figure 6.5 illustrates the classical turning point for the wave function and probability function of the one-dimensional harmonic oscillator. Position is measured in normalized units of $\xi = x(m\omega/\hbar)^{1/2}$, so that the classical turning points $\xi_n = (2n+1)^{1/2}$ for the ground state and first two excited states are $\xi_0 = 1$, $\xi_1 = \sqrt{3}$, and $\xi_2 = \sqrt{5}$, respectively.