VI. The Harmonic Oscillator and Other Problems

A. The Time-Independent Schrödinger Equation

One of the postulates of quantum mechanics is that the state vector evolves according to

$$i\hbar \frac{\partial}{\partial t}\left|\Psi(t)\right\rangle = H(t)\left|\Psi(t)\right\rangle \tag{6.1}$$

where the Hamiltonian *H*(*t*) is a Hermitian operator whose eigenvectors can be used to make a basis set. When studying this equation in chapter 2, we noted that the problem could be simplified when the Hamiltonian was independent of time. Suppose we are trying to solve

$$i\hbar \frac{\partial}{\partial t}\left|\Psi(t)\right\rangle = H\left|\Psi(t)\right\rangle \tag{6.2}$$

We conjecture that there will be solutions of the form

$$\left|\Psi(t)\right\rangle = \left|\psi\right\rangle \phi(t) \tag{6.3}$$

Plugging this into (6.2), dividing by $\phi(t)$ and rearranging, we find

$$H\left|\psi\right\rangle = \left|\psi\right\rangle \left[i\hbar \frac{1}{\phi(t)} \frac{d}{dt}\phi(t) \right] \tag{6.4}$$

We therefore see that $\left|\psi\right\rangle$ is an eigenvector of *H*, and since *H* is Hermitian, it will have real eigenvalues. Calling the state $\left|\psi_n\right\rangle$ and the corresponding eigenvalue (energy) E_n, which we identify with the energy, we have

$$H\left|\psi_n\right\rangle = E_n\left|\psi_n\right\rangle \tag{6.5}$$

and

$$i\hbar \frac{1}{\phi(t)} \frac{d}{dt}\phi(t) = E_n \tag{6.6}$$

In a manner identical to what we did in chapter 2, we can solve (6.6). Up to a constant of integration, which ultimately becomes a multiplicative constant, we have $\phi(t) = e^{-iE_n t/\hbar}$. We substitute this into (6.3) and then take linear combinations of those solutions to find the most general solution of (6.2):

$$\left|\Psi(t)\right\rangle = \sum_n c_n \left|\psi_n\right\rangle \exp\left(-i E_n t/\hbar\right) \tag{6.7}$$

Because we can choose the eigenstates of *H* to form a complete, orthonormal basis, we choose to do so, so we have

$$\langle \psi_n | \psi_m \rangle = \delta_{nm} \tag{6.8}$$

Then if we know the wave function at a particular time, say at $t = 0$, then we can find the constants c_n by letting $\langle \psi_n |$ act on (6.7) which yields

$$c_n = \langle \psi_n | \Psi(t=0) \rangle \tag{6.9}$$

Formally, we now have a complete solution of any time-independent problem. We find the eigenstates and eigenvalues of H defined by (6.5), we choose them to be orthonormal as specified in (6.8), then for an arbitrary initial state we use (6.9) to get the constants c_n, and then we have the general solution (6.7).

Before proceeding, one small comment seems in order. In classical physics, the absolute energy of a system cannot be determined, only differences in energy. Does this rule apply in quantum physics as well? Suppose we have two Hamiltonians that differ by a constant, so

$$H' = H + \Delta E \tag{6.10}$$

The two Hamiltonians will have identical eigenvectors, but their eigenvalues will differ by the constant ΔE

$$E'_n = E_n + \Delta E \tag{6.11}$$

For an arbitrary initial state, the constants c_n as given by (6.9) will be identical, but the time evolution (6.7) will be slightly different:

$$\begin{aligned} |\Psi'(t)\rangle &= \sum_n c_n |\psi_n\rangle \exp(-i E'_n t/\hbar) = \sum_n c_n |\psi_n\rangle \exp(-i E_n t/\hbar) \exp(-it\Delta E/\hbar) \\ &= |\Psi(t)\rangle \exp(-it\Delta E/\hbar) \end{aligned} \tag{6.12}$$

Thus the wave functions of the two Hamiltonians will differ at any time only by a phase. As we have described before, such a phase difference makes no difference physically, so in fact a constant added to the Hamiltonian has no detectable effect. The two Hamiltonians in (6.10) should be treated as identical.

B. The Infinite Square Well

We now consider a specific example, which properly belongs in chapter 2, but we include it now. Consider a particle in one dimension trapped in an infinite square well, with Hamiltonian given by

$$H = \frac{P^2}{2m} + V(Q) \quad \text{where} \quad V(Q) = \begin{cases} 0 & \text{if } 0 < Q < a \\ \infty & \text{otherwise} \end{cases} \tag{6.13}$$

We start by trying to solve (6.5). We want to find eigenstates of the Hamiltonian, which must have finite energy. The infinite potential has the effect that the expectation value of the energy will be infinite for any wave function lying outside the allowed region, so certainly we want a wave function that vanishes outside this region. Furthermore, the derivative terms will cause problems if the wave function is not continuous. We therefore demand that the solutions of (6.5a) vanish at the two boundaries,

$$\psi_n(0) = 0 \tag{6.14a}$$

$$\psi_n(a) = 0 \tag{6.14b}$$

It remains to solve (6.5) in the allowed region, where the wave function will satisfy

$$E\psi(x) = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi(x) \tag{6.15}$$

Because (6.15) is a second-order linear differential equation, there will be two linearly independent solutions. The functions whose second derivative are proportional to their negatives are $\sin(kx)$ and $\cos(kx)$, so we write[1]

$$\psi(x) = A\sin(kx) + B\cos(kx) \tag{6.16}$$

Plugging (6.16) into (6.15), it is easy to see that

$$E = \frac{\hbar^2 k^2}{2m} \tag{6.17}$$

The first boundary condition (6.14a) will be satisfied only if we pick $B = 0$. Then the second boundary condition (6.14b) will demand that $\sin(ak) = 0$, which says that ak will be an integer multiple of π, so $k = \pi n/a$. Hence we can label our solutions by a single positive integer n, in terms of which

$$\psi_n(x) = A\sin\left(\frac{\pi n x}{a}\right) \tag{6.18}$$

We now demand that the wave function be normalized, that is

$$1 = \int_{-\infty}^{\infty} \left|\psi(x)\right| dx = |A|^2 \int_0^a \sin^2\left(\frac{\pi n x}{a}\right) dx = \tfrac{1}{2} a |A|^2 \tag{6.19}$$

Solving for A, and choosing it to be real and positive, we find $A = \sqrt{2/a}$. Putting everything together, we now have formulas for the eigenstates and energies.

$$\psi_n(x) = \langle x | \psi_n \rangle = \begin{cases} \sqrt{\dfrac{2}{a}}\sin\left(\dfrac{\pi n x}{a}\right) & \text{for } 0 < x < a \\ 0 & \text{otherwise} \end{cases} \tag{6.20}$$

$$E_n = \frac{\pi^2 \hbar^2 n^2}{2ma^2} \tag{6.21}$$

---

[1] There is an implicit assumption here that $E > 0$. If $E < 0$, then the solutions to (6.15) will take the form $e^{\alpha x}$ or $e^{-\alpha x}$; however, no linear combination of these two functions can satisfy (6.14)

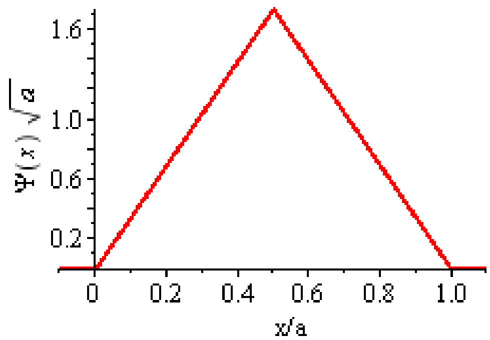

Figure 6-2: The initial wave function described by equation (6.22).

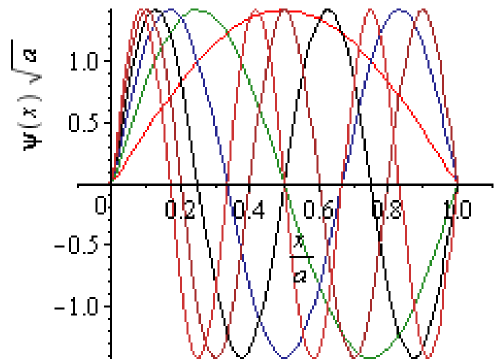

Figure 6-1: The first six wave functions of the infinite square well, for n = 1 through 6, in red, green, blue, black, brown, and orange respectively.

The first few wave functions (6.16a) are plotted in Fig. 6-1.

As an example, suppose we were told that the initial wave function is given by

$$\langle x|\Psi(t=0)\rangle = \begin{cases} \sqrt{12/a^3}\left(\tfrac{1}{2}a-\left|x-\tfrac{1}{2}a\right|\right) & \text{for } 0<x<a \\ 0 & \text{otherwise} \end{cases} \tag{6.22}$$

This function is illustrated in Fig. 6-2. It is straightforward to verify that this wave function is normalized. We now find the constants c_n with the help of (6.9), so we have

$$\begin{aligned} c_n &= \langle \Psi(t=0)|\psi_n\rangle = \int_0^a \Psi^*(x,0)\psi_n(x)\,dx \\ &= \frac{\sqrt{24}}{a^2}\int_0^a \left(\tfrac{1}{2}a-\left|\tfrac{1}{2}a-x\right|\right)\sin\left(\frac{n\pi x}{a}\right)dx \end{aligned} \tag{6.23}$$

For those who enjoy doing such integrals by hand, I will leave you to it, but this is a bit easier to do with the help of Maple.

```
> assume(n::integer,a>0);sqrt(24)/a^2*integrate((a/2-abs(
a/2-x))*sin(Pi*n*x/a),x=0..a);
```

$$c_n = \frac{4\sqrt{6}\sin\left(\tfrac{1}{2}\pi n\right)}{\pi^2 n^2} \tag{6.24}$$

It is easy to show that $\sin\left(\tfrac{1}{2}\pi n\right)$ vanishes for all the even n and alternates with values ± 1 for all odd n. We can then plug (6.24), (6.18) and (6.21) into (6.7) to get the wave function at all times in the allowed region.

$$\langle x|\Psi(t)\rangle = \sum_{n\text{ odd}} (-1)^{\frac{1}{2}(n-1)} \frac{8\sqrt{3}}{\pi^2 n^2\sqrt{a}} \sin\left(\frac{\pi n x}{a}\right)\exp\left(-i\frac{\pi^2\hbar n^2}{2ma^2}t\right) \tag{6.25}$$

It may be a bit disappointing that (6.25) is not in closed form (since it is an infinite sum), but as a practical matter, a computer numerically can sum (6.25) quite quickly. The sum would be faster still if we had picked a smoother function at t = 0.

C. The Harmonic Oscillator

It has been said that physics is a series of course on the harmonic oscillator, and quantum mechanics is no exception. Not only is it one of the few quantum mechanics problems we can solve exactly, it has great practical application. For example, consider *any* one-dimensional quantum mechanical system. In the neighborhood of any point x_0, the potential $V(x)$ can be expanded in a Taylor series:

$$V(x) \approx V(x_0) + V'(x_0)(x - x_0) + \tfrac{1}{2}V''(x_0)(x - x_0)^2 + \tfrac{1}{6}V'''(x_0)(x - x_0)^3 + \cdots \quad (6.26)$$

Often it is the case that a particle will classically be trapped in the neighborhood of the minimum of the potential, and if this is true quantum mechanically as well, we can choose x_0 to be this minimum point. In this case, the first derivative of V will vanish, and expanding to only the second derivative, we have

$$V(x) \approx V(x_0) + \tfrac{1}{2}V''(x_0)(x - x_0)^2 \quad (6.27)$$

As discussed in section A, the constant term plays no physical role, and hence the only relevant term is the quadratic one. We can redefine our origin to make $x_0 = 0$, as we will do below.

Not only is the harmonic oscillator in one dimension, but the coupled harmonic oscillator can be used in three dimensions, or for multiple particles in three dimensions, or even for an infinite number of degrees of freedom in any number of dimensions, as we will ultimately discover when we quantize the electromagnetic field. Thus the harmonic oscillator is also the starting point for quantum field theory. But for now, let us start with the simplest case, a single particle in one dimension.

The harmonic oscillator Hamiltonian can be written in the form

$$H = \frac{P^2}{2m} + \tfrac{1}{2}kQ^2 \quad (6.28)$$

where m is the mass of the particle and k is the spring constant. In analogy with classical mechanics, or inspired by section 5I, it makes sense to define the classical angular frequency $\omega = \sqrt{k/m}$, in terms of which

$$H = \frac{P^2}{2m} + \tfrac{1}{2}m\omega^2 Q^2 \quad (6.29)$$

We now wish to find the eigenstates and eigenvalues of this Hamiltonian.

Examining (6.29), we immediately note that at large values of the eigenvalues of Q, the potential becomes infinite, and for any finite energy E, it follows that $E < V(\pm\infty)$. This guarantees that we will automatically be talking about bound states.

As a practical matter, when faced with a difficult problem, it is often helpful to "scale out" all the dimensionful variables in the problem. In this problem we have the constants m, ω, and once we start using quantum mechanics, $\hbar$. Since Q has units of distance, it is helpful to define a new operator q that is proportional to Q but has been divided by a constant with units of length. It is not hard to see that $\hbar/m\omega$ has units of length squared, so $Q\sqrt{m\omega/\hbar}$ will be dimensionless. Similarly, we can show that $\hbar m\omega$ has units of momentum squared, so $P/\sqrt{m\omega\hbar}$ will also be dimensionless. Ballinger defines these as q and p respectively. Beyond this a bit of inspiration is in order. We define the lowering and raising operations as

$$a = Q\sqrt{\frac{m\omega}{2\hbar}} + i\frac{P}{\sqrt{2m\omega\hbar}} \tag{6.30a}$$

$$a^\dagger = Q\sqrt{\frac{m\omega}{2\hbar}} - i\frac{P}{\sqrt{2m\omega\hbar}} \tag{6.30b}$$

We will often want the inverse versions of these relations, which are

$$Q = \sqrt{\frac{\hbar}{2m\omega}}\left(a + a^\dagger\right) \tag{6.31a}$$

$$P = i\sqrt{\frac{\hbar m\omega}{2}}\left(a^\dagger - a\right) \tag{6.31b}$$

These two new operators have commutation relations

$$\begin{aligned}\left[a, a^\dagger\right] &= \left[Q\sqrt{\frac{m\omega}{2\hbar}} + i\frac{P}{\sqrt{2m\omega\hbar}}, Q\sqrt{\frac{m\omega}{2\hbar}} - i\frac{P}{\sqrt{2m\omega\hbar}}\right] \\ &= \sqrt{\frac{m\omega}{2\hbar}}\frac{1}{\sqrt{2m\omega\hbar}}\left(\left[Q, -iP\right] + \left[iP, Q\right]\right) = \frac{(-i)(i\hbar) + i(-i\hbar)}{2\hbar} = 1\end{aligned} \tag{6.32}$$

or, summarizing

$$\begin{aligned}\left[a, a^\dagger\right] &= 1 \\ \left[a^\dagger, a^\dagger\right] &= \left[a, a\right] = 0\end{aligned} \tag{6.33}$$

Substituting (6.31a) and (6.31b) back into our Hamiltonian (6.29), we have

$$\begin{aligned}H &= \frac{1}{2m}\frac{\hbar m\omega}{2}\left[i\left(a^\dagger - a\right)\right]^2 + \tfrac{1}{2}m\omega^2\frac{\hbar}{2m\omega}\left(a + a^\dagger\right)^2 \\ &= \tfrac{1}{4}\hbar\omega\left[\left(a^\dagger + a\right)^2 - \left(a^\dagger - a\right)^2\right] = \tfrac{1}{4}\hbar\omega\left(a^\dagger a + aa^\dagger\right)\end{aligned} \tag{6.35}$$

We then rewrite $aa^\dagger = \left[a, a^\dagger\right] + a^\dagger a = 1 + a^\dagger a$ to find

$$H = \hbar\omega\left(a^\dagger a + \tfrac{1}{2}\right) \equiv \hbar\omega\left(N + \tfrac{1}{2}\right) \tag{6.36}$$

where we have defined the number operator

$$N \equiv a^\dagger a \tag{6.37}.$$

Finding the eigenstates and eigenvectors of H has been reduced to finding those of the Hermitian operator N.

Suppose we find a normalized eigenstate of *N*, which we name $|n\rangle$, so that

$$N|n\rangle = a^\dagger a|n\rangle = n|n\rangle \tag{6.38}$$

Now, consider the state $a|n\rangle$. It is an eigenstate of *N* also:

$$N\left(a|n\rangle\right) = a^\dagger aa|n\rangle = \left(\left[a^\dagger, a\right] + aa^\dagger\right)a|n\rangle = \left(-a + aN\right)|n\rangle = \left(n-1\right)\left(a|n\rangle\right) \tag{6.40}$$

Its eigenvalue is one less than that of $|n\rangle$, which is why *a* is called the lowering operator. It is not a *normalized* eigenstate, because

$$\left\|a|n\rangle\right\|^2 = \langle n|a^\dagger a|n\rangle = \langle n|N|n\rangle = n\langle n|n\rangle = n \tag{6.41}$$

We note immediately from (6.41) that we must have $n \geq 0$. For $n > 0$, we then identify a new eigenstate of *N* given by

$$|n-1\rangle = \frac{1}{\sqrt{n}}a|n\rangle \tag{6.42}$$

The procedure (6.42) can be repeated, yielding new states $|n-2\rangle$, $|n-3\rangle$, etc. However, it can not yield states with negative values of *n*, because of (6.41). It follows that the procedure must eventually stop, which can only happen when we get an eigenstate $n = 0$. This occurs only if we start with a non-negative integer.

With the help of (6.42), we can similarly show that

$$a^\dagger|n-1\rangle = \frac{1}{\sqrt{n}}a^\dagger a|n\rangle = \frac{1}{\sqrt{n}}N|n\rangle = \sqrt{n}|n\rangle \tag{6.43}$$

Summarizing (6.42) and (6.43), we have

$$\begin{aligned} a|n\rangle &= \sqrt{n}|n-1\rangle \\ a^\dagger|n\rangle &= \sqrt{n+1}|n+1\rangle \end{aligned} \tag{6.44}$$

Thus we can raise or lower from any eigenstate to any other using (6.44) repeatedly. For example, from the lowest energy state $n = 0$, we can find any other by using

$$|n\rangle = \frac{\left(a^\dagger\right)^n}{\sqrt{n!}}|0\rangle \tag{6.45}$$

The energy eigenvalues are given by (6.36), and we have

$$E_n = \hbar\omega\left(n + \tfrac{1}{2}\right) \tag{6.46}$$

The lowering operator must vanish when acting on the lowest energy $n= 0$ ground state, so

$$a|0\rangle = 0 \tag{6.47}$$

If we actually want a coordinate representation of the wave function, it is easiest to first find $\psi_0(x) \equiv \langle x|0\rangle$. Writing (6.45) out explicitly, we have

$$\left(Q\sqrt{\frac{m\omega}{2\hbar}} + i\frac{P}{\sqrt{2m\omega\hbar}}\right)|0\rangle = 0,$$

$$\left(x\sqrt{\frac{m\omega}{2\hbar}} + \frac{i}{\sqrt{2m\omega\hbar}}\frac{\hbar}{i}\frac{d}{dx}\right)\psi_0(x) = 0,$$

$$\frac{d}{dx}\psi_0(x) = -\frac{m\omega}{\hbar}x\psi_0(x),$$

$$\frac{d\psi_0(x)}{\psi_0(x)} = -\frac{m\omega}{\hbar}x\,dx \qquad (6.47)$$

Integrating both sides of (6.47) and then exponentiating both sides, we find

$$\psi_0(x) = C\exp\left(-\frac{m\omega x^2}{2\hbar}\right) \qquad (6.48)$$

The constant C came from the constant of integration. Since we want our eigenstates to be normalized, we have

$$1 = \int_{-\infty}^{\infty}|\psi_0(x)|^2\,dx = |C|^2\int_{-\infty}^{\infty}\exp\left(-\frac{m\omega x^2}{\hbar}\right)dx = |C|^2\sqrt{\frac{\pi\hbar}{m\omega}} \qquad (6.49)$$

If we choose $C > 0$, then

$$\psi_0(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4}\exp\left(-\frac{m\omega x^2}{2\hbar}\right) \qquad (6.50)$$

We can then use (6.45) to find any of the other wave functions explicitly.

$$\psi_n(x) = \frac{1}{\sqrt{n!}}\left(\frac{m\omega}{\pi\hbar}\right)^{1/4}\left(x\sqrt{\frac{m\omega}{2\hbar}} - \sqrt{\frac{\hbar}{2m\omega}}\frac{d}{dx}\right)^n\exp\left(-\frac{m\omega x^2}{2\hbar}\right) \qquad (6.51)$$

Explicit graphs of the first few wave functions given by (6.51) are shown in Fig. 6-3. The general trend is that as n increases, the wave functions spread out farther and farther from the origin. Notice also that the wave functions are even functions when n is even, and odd when n is odd.

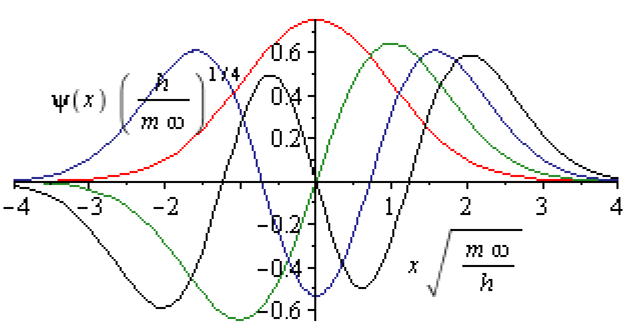

Figure 6-3: The first four harmonic oscillator wave functions, for n = 0, 1, 2, and 3 (red, green, black, blue respectively).

D. Working with the Harmonic Oscillator and Coherent States

Having found the eigenstates of the harmonic oscillator Hamiltonian, it is straightforward to find a general solution to Schrödinger's equation. Using (6.7) and (6.46), the general solution is

$$\left|\Psi(t)\right\rangle = \sum_n c_n \left|n\right\rangle \exp\left[-i\left(n+\tfrac{1}{2}\right)\omega t\right] \tag{6.52}$$

If we want expectation values of operators such as P or Q for such a state, we could, in principle, find explicit expressions for the wave functions using (6.51), and then compute them in a straightforward way. Though this will work, it is tedious and difficult. It is far easier to use the expressions such as (6.31) and (6.44) together with orthonormality to quickly evaluate the expectation values of operators. For example, suppose we are in an eigenstate of the Hamiltonian and we were asked to compute the expectation values of P and P^2. We would simply compute:

$$\begin{aligned}\left\langle n\right|P\left|n\right\rangle &= i\sqrt{\hbar m\omega/2}\left\langle n\right|\left(a^\dagger - a\right)\left|n\right\rangle = i\sqrt{\hbar m\omega/2}\left\langle n\right|\left(\sqrt{n+1}\left|n+1\right\rangle - \sqrt{n}\left|n-1\right\rangle\right) \\ &= i\sqrt{\hbar m\omega/2}\left(0-0\right) = 0 \\ \left\langle n\right|P^2\left|n\right\rangle &= \left\|P\left|n\right\rangle\right\|^2 = \left\|i\sqrt{\hbar m\omega/2}\left(a^\dagger - a\right)\left|n\right\rangle\right\|^2 \\ &= \tfrac{1}{2}\hbar m\omega\left\|\sqrt{n+1}\left|n+1\right\rangle - \sqrt{n}\left|n-1\right\rangle\right\|^2 = \tfrac{1}{2}\hbar m\omega\left(n+1+n\right) = \hbar m\omega\left(n+\tfrac{1}{2}\right)\end{aligned} \tag{6.53}$$

Interestingly, note that the expectation value for the momentum vanishes, no matter which eigenstate it is in. Also note that the kinetic energy term in the Hamiltonian, $P^2/2m$, will have an expectation value of $\tfrac{1}{2}\hbar\omega\left(n+\tfrac{1}{2}\right)$, exactly half of the energy E_n of this state. The other half of the energy is in the potential term, as you might expect.

One surprise is that $\left\langle P\right\rangle$ vanishes for all these states; it is easily demonstrated that $\left\langle Q\right\rangle$ vanishes as well. This is true for energy eigenstates (also called *stationary states*) even when you include the time-dependence (6.52). This is surprising because we might expect that when we put a lot of energy into the system, we might expect it to behave more or less like a classical harmonic oscillator. Furthermore, for the energy eigenstates, it is easy to show that the uncertainty in the position and momentum grow as n grows, so the wave is in no sense located at a particular place or a particular momentum.

The key, of course, is to *not* use stationary states, but instead include states that have mixtures of different eigenvectors. The simplest example would be

$$\left|\Psi(t)\right\rangle = \tfrac{1}{\sqrt{2}}\left\{\left|n-1\right\rangle \exp\left[-i\left(n-\tfrac{1}{2}\right)\omega t\right] + \left|n\right\rangle \exp\left[-i\left(n+\tfrac{1}{2}\right)\omega t\right]\right\} \tag{6.54}$$

This is an exact solution of Schrödinger's time-dependent equation. The expectation value of P, for example, will be

$$\begin{aligned}\left\langle\Psi(t)\right|P\left|\Psi(t)\right\rangle = \tfrac{1}{2}&\left\{\left\langle n-1\right|\exp\left[i\left(n-\tfrac{1}{2}\right)\omega t\right] + \left\langle n\right|\exp\left[i\left(n+\tfrac{1}{2}\right)\omega t\right]\right\} \\ &\cdot P\left\{\left|n-1\right\rangle \exp\left[-i\left(n-\tfrac{1}{2}\right)\omega t\right] + \left|n\right\rangle \exp\left[-i\left(n+\tfrac{1}{2}\right)\omega t\right]\right\}\end{aligned}$$

$$= \tfrac{1}{2} i\sqrt{\hbar m\omega/2}\left(\langle n-1| e^{-i\omega t/2} + \langle n| e^{i\omega t/2}\right)\begin{bmatrix}\left(\sqrt{n}\,|n\rangle - \sqrt{n-1}\,|n-2\rangle\right)e^{i\omega t/2} \\ +\left(\sqrt{n+1}\,|n+1\rangle - \sqrt{n}\,|n-1\rangle\right)e^{-i\omega t/2}\end{bmatrix}$$

$$= \tfrac{1}{2} i\sqrt{\hbar m\omega/2}\left(\sqrt{n}e^{i\omega t} - \sqrt{n}e^{-i\omega t}\right) = \tfrac{1}{2} i\sqrt{\hbar m\omega n/2}\left(2i\sin(\omega t)\right)$$

$$\langle \Psi(t)|P|\Psi(t)\rangle = -\sqrt{\hbar m\omega n/2}\sin(\omega t) \tag{6.55}$$

It can be shown that $\langle Q\rangle$ oscillates as well. This, then, bears a greater resemblance to a classical harmonic oscillator, though if you calculate the uncertainty of the two operators *P* and *Q*, you will find they are still unacceptably large.

You can do far better, if instead of working with just one or two eigenstates of the Hamiltonian, you work with many, even an infinite number. Perhaps most interesting is to work with *coherent states*, quantum states $|z\rangle$ for any complex number *z* defined by

$$|z\rangle = e^{-|z|^2/2}\sum_{n=0}^{\infty}\frac{z^n}{\sqrt{n!}}|n\rangle \tag{6.56}$$

These states are defined to make them eigenstates of the annihilation operator *a*:

$$a|z\rangle = e^{-|z|^2/2}\sum_{n=0}^{\infty}\frac{z^n}{\sqrt{n!}}a|n\rangle = e^{-|z|^2/2}\sum_{n=0}^{\infty}\frac{z^n}{\sqrt{n!}}\sqrt{n}\,|n-1\rangle = e^{-|z|^2/2}\sum_{n=1}^{\infty}\frac{z^n}{\sqrt{(n-1)!}}|n-1\rangle$$

$$= e^{-|z|^2/2}\sum_{n=0}^{\infty}\frac{z^{n+1}}{\sqrt{n!}}|n\rangle = z\left[e^{-|z|^2/2}\sum_{n=0}^{\infty}\frac{z^n}{\sqrt{n!}}a|n\rangle\right],$$

$$a|z\rangle = z|z\rangle \tag{6.57}$$

Since *a* is *not* a Hermitian operator, the eigenstates $|z\rangle$ will not generally have real eigenvalues, nor will they be orthogonal. It is not hard to show they are normal $\langle z|z\rangle = 1$. We will also find useful the Hermitian conjugate of (6.57), which is

$$\langle z|a = \langle z|z^* \tag{6.58}$$

Let's suppose that at $t = 0$ we are in a coherent state, so

$$|\Psi(t=0)\rangle = |z_0\rangle = e^{-|z_0|^2/2}\sum_{n=0}^{\infty}\frac{z_0^n}{\sqrt{n!}}|n\rangle \tag{6.59}$$

We know that (6.52) gives the general solution of Schrödinger's equation, so

$$|\Psi(t)\rangle = e^{-|z_0|^2/2}\sum_{n=0}^{\infty}\frac{z_0^n}{\sqrt{n!}}|n\rangle\exp\left(-i\omega\left(n+\tfrac{1}{2}\right)t\right) = e^{-i\omega t/2}e^{-|z_0|^2/2}\sum_{n=0}^{\infty}\frac{1}{\sqrt{n!}}\left(z_0e^{-i\omega t}\right)^n|n\rangle \tag{6.60}$$

Since $\left|z_0e^{-i\omega t}\right| = |z_0|$, this state is also a coherent state, apart from the phase factor out front, so we have

$$|\Psi(t)\rangle = e^{-i\omega t/2}\left|z_0e^{-i\omega t}\right\rangle \tag{6.61}$$

It can be shown that this wave function has a much smaller uncertainty in its position or momentum than previous wave functions we have considered, such as (6.54). It is also easy to see using (6.57) and (6.58) that expectation values such as the momentum and position oscillate as we would expect. For example,

$$\begin{aligned}\left\langle \Psi(t)\middle|P\middle|\Psi(t)\right\rangle &= e^{i\omega t/2}\left\langle z_0 e^{-i\omega t}\middle|P\middle|z_0 e^{-i\omega t}\right\rangle e^{-i\omega t/2} \\ &= i\sqrt{\hbar m\omega/2}\left\langle z_0 e^{-i\omega t}\middle|\left(a^\dagger - a\right)\middle|z_0 e^{-i\omega t}\right\rangle \\ &= i\sqrt{\hbar m\omega/2}\left\langle z_0 e^{-i\omega t}\middle|\left[\left(z_0 e^{-i\omega t}\right)^* - \left(z_0 e^{-i\omega t}\right)\right]\middle|z_0 e^{-i\omega t}\right\rangle \\ &= i\sqrt{\hbar m\omega/2}\,(-2i)\,\mathrm{Im}\left(z_0 e^{-i\omega t}\right) = \sqrt{2\hbar m\omega}\,\mathrm{Im}\left(z_0 e^{-i\omega t}\right).\end{aligned} \tag{6.62}$$

We cannot simplify this further since z_0 might have real and imaginary parts.

E. Multiple Particles and Harmonic Oscillators

We now wish to consider more complicated systems of multiple harmonic oscillators, but first we must consider what our vector space will look like with multiple particles. A fuller discussion of this topic will come in a later chapter, but for now, suppose we have multiple particles in one dimension. According to our postulates, the state of the quantum system at fixed time must be described by a single vector in our vector space. Instead of describing such a system as a function of a single position $\psi(x)$, it must be a function of all the particle's positions, $\psi(x_1, x_2, \ldots, x_N)$, where N is the number of particles. The classical description of the energy of the particles,

$$E = \sum_{i=1}^{N} \frac{p_i^2}{2m_i} + V(x_1, x_2, \ldots, x_N) \tag{6.63}$$

will then become the quantum Hamiltonian

$$H = \sum_{i=1}^{N} \frac{P_i^2}{2m_i} + V(Q_1, Q_2, \ldots, Q_N) \tag{6.64}$$

The position and momentum operators are most easily defined by their action on a wave function

$$\begin{aligned} Q_i\psi(x_1, x_2, \ldots, x_N) &= x_i\psi(x_1, x_2, \ldots, x_N) \\ P_i\psi(x_1, x_2, \ldots, x_N) &= \frac{\hbar}{i}\frac{\partial}{\partial x_i}\psi(x_1, x_2, \ldots, x_N) \end{aligned} \tag{6.65}$$

These will have commutation relations

$$\begin{aligned} \left[Q_i, P_j\right] &= i\hbar\delta_{ij} \\ \left[Q_i, Q_j\right] &= \left[P_i, P_j\right] = 0 \end{aligned} \tag{6.66}$$

We are now prepared to write down the problem of multiple uncoupled harmonic oscillators. To simplify, assume all the particles have the same mass, so then we have

$$H = \sum_{i=1}^{N} \frac{1}{2m} P_i^2 + \frac{1}{2}\sum_{i=1}^{N} k_i Q_i^2 \tag{6.67}$$

We will attempt to solve this by the same techniques we did the single harmonic oscillator. First we define $\omega_i = \sqrt{k_i/m}$, and then define a set of raising and lowering operators by

$$a_i = Q_i\sqrt{\frac{m\omega_i}{2\hbar}} + i\frac{P_i}{\sqrt{2m\omega_i\hbar}} \tag{6.68a}$$

$$a_i^\dagger = Q_i\sqrt{\frac{m\omega_i}{2\hbar}} - i\frac{P_i}{\sqrt{2m\omega_i\hbar}} \tag{6.68b}$$

These have commutation relations

$$\begin{gathered}\left[a_i, a_j^\dagger\right] = \delta_{ij} \\ \left[a_i^\dagger, a_j^\dagger\right] = \left[a_i, a_j\right] = 0\end{gathered} \tag{6.69}$$

The Hamiltonian in terms of these is given by

$$H = \sum_{i=1}^{N} \hbar\omega_i \left(a_i^\dagger a_i + \tfrac{1}{2}\right) \tag{6.70}$$

If we define the number operators $N_i = a_i^\dagger a_i$, then it is clear that all the N_i's will commute with each other, and hence they can all be diagonalized simultaneously. Hence we can choose our basis states to be simultaneously eigenstates of all of the N_i's, and we write a general basis state as

$$\left|n_1, n_2, \ldots, n_N\right\rangle \tag{6.71}$$

We can now go through the exact same arguments as before to prove that each of the n_i's will be non-negative integers. We can also show that as before, the action of a single raising or lowering operator on (6.68) is to increase or decrease one of the eigenvalues by one, so we have

$$\begin{aligned}a_i\left|n_1, n_2, \ldots, n_i, \ldots, n_N\right\rangle &= \sqrt{n_i}\left|n_1, n_2, \ldots, n_i - 1, \ldots, n_N\right\rangle \\ a_i^\dagger\left|n_1, n_2, \ldots, n_i, \ldots, n_N\right\rangle &= \sqrt{n_i + 1}\left|n_1, n_2, \ldots, n_i + 1, \ldots, n_N\right\rangle\end{aligned} \tag{6.72}$$

The eigenvalues of the Hamiltonian are simply given by

$$E_{n_1, n_2, \ldots, n_N} = \sum_{i=1}^{N} \hbar\omega_i \left(n_i + \tfrac{1}{2}\right) \tag{6.73}$$

With considerable effort, you can write down explicit wave functions, starting from the demand that $a_i\left|0, \ldots, 0\right\rangle = 0$. We find for the ground state

$$\psi_{0,\ldots,0}(x) = \prod_{i=1}^{N} \left(\frac{m\omega_i}{\pi\hbar} \right)^{1/4} \exp\left(-\frac{m\omega_i x_i^2}{2\hbar} \right) \tag{6.74}$$

Other explicit wave functions can be found by acting on (6.74) with the various raising operators. In fact, such wave functions are so unwieldy to work with that we will avoid them whenever possible, simply writing our quantum states in the form $|n_1, n_2, \ldots, n_N\rangle$.

We have succeeded in solving the uncoupled harmonic oscillator. What do we do if our harmonic oscillator is coupled? Consider the Hamiltonian

$$H = \sum_{i=1}^{N} \frac{1}{2m} P_i^2 + \frac{1}{2} \sum_{i=1}^{N} \sum_{j=1}^{N} k_{ij} Q_i Q_j \tag{6.75}$$

We can always write the coupling terms k_{ij} in such a way that it is symmetric, so $k_{ij} = k_{ji}$. How would we solve this problem if we were doing the problem classically? The answer is to change coordinates to new coordinates such that the interactions *become* diagonal.

Think of the spring constants k_{ij} as a $N \times N$ matrix k, defined by

$$k = \begin{pmatrix} k_{11} & k_{12} & \cdots & k_{1N} \\ k_{21} & k_{22} & \cdots & k_{2N} \\ \vdots & \vdots & \ddots & \vdots \\ k_{N1} & k_{N2} & \cdots & k_{NN} \end{pmatrix} \tag{6.76}$$

Since it is real and symmetric, it is Hermitian. As discussed in chapter 4, section I, any such matrix can be diagonalized by multiplying by an appropriate unitary matrix V on the right and its Hermitian conjugate $V^\dagger$ on the left. In this case, however, since our matrix is real, the eigenvectors of K can be chosen real, so that V will be a real matrix, so we have $V^\dagger = V^T$, and with the appropriate choice of V,

$$k' = V^T k V = \begin{pmatrix} k_1' & 0 & \cdots & 0 \\ 0 & k_2' & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & k_N' \end{pmatrix} \tag{6.77}$$

where the numbers $k_1', k_2', \ldots k_N'$ are the eigenvalues of k. The matrix V is unitary, or, since it is real, orthogonal, which means

$$V^T V = V V^T = 1 \tag{6.78}$$

Now, define new operators Q_i' and P_i' related to the old ones by

$$\begin{aligned} Q_i &= \sum_{j=1}^{N} V_{ij} Q_j' \\ P_i &= \sum_{j=1}^{N} V_{ij} P_j' \end{aligned} \tag{6.79}$$

We will need the inverse relations as well, which we can quickly find, since the inverse of V is V^T.

$$Q_i' = \sum_{j=1}^{N} V_{ji} Q_j$$
$$P_i' = \sum_{j=1}^{N} V_{ji} P_j \tag{6.80}$$

Using (6.80), we can easily work out the commutators of the new operators

$$\left[Q_i', P_j'\right] = \left[\sum_{k=1}^{N} V_{ki} Q_k, \sum_{l=1}^{N} V_{lj} P_l\right] = \sum_{k=1}^{N} V_{ki} \sum_{l=1}^{N} V_{lj} \left[P_l, Q_k\right] = i\hbar \sum_{k=1}^{N} V_{ki} \sum_{l=1}^{N} V_{lj} \delta_{lk}$$
$$= i\hbar \sum_{k=1}^{N} V_{ki} V_{kj} = i\hbar \left(V^T V\right)_{ij} = i\hbar \delta_{ij} \tag{6.81}$$
$$\left[Q_i', Q_j'\right] = \left[P_i', P_j'\right] = 0$$

So the new operators have the same commutation relations as the old ones. We now rewrite the Hamiltonian (6.75) in terms of these operators:

$$H = \frac{1}{2m} \sum_{i=1}^{N} \sum_{k=1}^{N} \sum_{l=1}^{N} V_{ik} V_{il} P_k' P_l' + \frac{1}{2} \sum_{i=1}^{N} \sum_{j=1}^{N} \sum_{k=1}^{N} \sum_{l=1}^{N} k_{ij} V_{ik} V_{jl} Q_k' Q_l'$$
$$= \frac{1}{2m} \sum_{k=1}^{N} \sum_{l=1}^{N} P_k' P_l' \sum_{i=1}^{N} \left(V_{ki}^T V_{il}\right) + \frac{1}{2} \sum_{k=1}^{N} \sum_{l=1}^{N} Q_k' Q_l' \sum_{i=1}^{N} \sum_{j=1}^{N} \left(V_{ki}^T k_{ij} V_{jl}\right) \tag{6.82}$$
$$= \frac{1}{2m} \sum_{k=1}^{N} \sum_{l=1}^{N} P_k' P_l' \delta_{kl} + \frac{1}{2} \sum_{k=1}^{N} \sum_{l=1}^{N} Q_k' Q_l' k_{kl}' = \frac{1}{2m} \sum_{i=1}^{N} P_i'^2 + \frac{1}{2} \sum_{i=1}^{N} k_i' Q_i'^2$$

This reduces the Hamiltonian to the uncoupled one, (6.67), which we already know how to solve. For example, the Hamiltonian ultimately takes the form (6.70), and the energy values (6.73), where

$$\omega_i = \sqrt{k_i'/m} \tag{6.83}$$

Note that to find expressions for the frequencies, and hence the Hamiltonian or the energies, all we need is the eigenvalues k_i' of the matrix k. It is not necessary to actually work out the matrices V.

F. The Complex Harmonic Oscillator

It is sometimes helpful to adopt a complex notation when describing two (or more) harmonic oscillators. Let's back up and explain this in classical terms. Suppose we had a classical energy for a complex position *z* given by

$$E = m\left(\dot{z}^*\dot{z} + \omega^2 z^* z\right) \tag{6.84}$$

where $\dot{z}$ just denotes the time derivative of *z*. There is nothing particularly unusual about this formula, you just need to think of *z* as a way of combining two real variables, *x* and *y*, into a single complex variable according to

$$z = \tfrac{1}{\sqrt{2}}\left(x + iy\right) \tag{6.85}$$

Substituting this into (6.84), we see that the energy can be written in terms of the real positions as

$$\begin{aligned} E &= \tfrac{1}{2}m\left(\dot{x}^2 + \dot{y}^2\right) + \tfrac{1}{2}m\omega^2\left(x^2 + y^2\right) \\ &= \frac{p_x^2 + p_y^2}{2m} + \tfrac{1}{2}m\omega^2\left(x^2 + y^2\right) \end{aligned} \tag{6.86}$$

We then replace *E* by the Hamiltonian and the four quantities p_x, p_y, *x* and *y* by their corresponding operators to obtain

$$H = \frac{P_x^2 + P_y^2}{2m} + \tfrac{1}{2}m\omega^2\left(Q_x^2 + Q_y^2\right) \tag{6.87}$$

We have, of course, already solved this equation, as (6.67). We define two lowering operators a_x and a_y, with commutation relations

$$\left[a_x, a_x^\dagger\right] = \left[a_y, a_y^\dagger\right] = 1, \quad \text{all others vanish} \tag{6.88}$$

We then write the Hamiltonian using (6.70).

$$H = \hbar\omega\left(a_x^\dagger a_x + a_y^\dagger a_y + 1\right) \tag{6.89}$$

We now define two new creation and annihilation operators as

$$\begin{aligned} a_\pm &\equiv \tfrac{1}{\sqrt{2}}\left(a_x \pm i a_y\right) \\ a_\pm^\dagger &\equiv \tfrac{1}{\sqrt{2}}\left(a_x^\dagger \mp i a_y^\dagger\right) \end{aligned} \tag{6.90}$$

These operators can be shown to have commutation relations

$$\left[a_+, a_+^\dagger\right] = \left[a_-, a_-^\dagger\right] = 1, \quad \text{all others vanish} \tag{6.91}$$

The Hamiltonian (6.81) can, with a bit of work, be rewritten in terms of these operators

$$\begin{aligned} H &= \hbar\omega\left[\tfrac{1}{2}\left(a_+^\dagger + a_-^\dagger\right)\left(a_+ + a_-\right) - \tfrac{1}{2}\left(a_+^\dagger - a_-^\dagger\right)\left(a_- - a_+\right) + 1\right] \\ H &= \hbar\omega\left(a_+^\dagger a_+ + a_-^\dagger a_- + 1\right) \end{aligned} \tag{6.92}$$

We will later need to reinterpret z and $\dot{z}$ as operators, and we will want to do so in terms of our new raising and lowering operators $a_\pm$ and $a_\pm^\dagger$. We make the quantum identification

$$z = \tfrac{1}{\sqrt{2}}\left(x + iy\right) \quad \to \quad \tfrac{1}{\sqrt{2}}\left(Q_x + iQ_y\right) = \sqrt{\frac{\hbar}{2m\omega}}\tfrac{1}{\sqrt{2}}\left(a_x + a_x^\dagger + ia_y - ia_y^\dagger\right) = \sqrt{\frac{\hbar}{2m\omega}}\left(a_+ + a_-^\dagger\right)$$

$$z \quad \to \quad \sqrt{\frac{\hbar}{2m\omega}}\left(a_+ + a_-^\dagger\right) \tag{6.93}$$

A similar computation will show

$$\dot{z} = \tfrac{1}{\sqrt{2}}\left(\dot{x} + i\dot{y}\right) = \tfrac{1}{\sqrt{2}}\frac{p_x + ip_y}{m} \quad \to \quad \tfrac{1}{\sqrt{2}} i \frac{1}{m}\sqrt{\frac{\hbar\omega}{2m}}\left(a_x^\dagger - a_x + ia_y^\dagger - ia_y\right) = i\sqrt{\frac{\hbar\omega}{2m}}\left(a_-^\dagger - a_+\right)$$

$$\dot{z} \quad \to \quad i\sqrt{\frac{\hbar\omega}{2m}}\left(a_-^\dagger - a_+\right) \tag{6.94}$$

Not surprisingly, if you take the complex conjugate of a classical quantity, it gets mapped to the Hermitian conjugate when you make the quantum identification, so we have

$$\begin{aligned} z \quad &\to \quad \sqrt{\frac{\hbar}{2m\omega}}\left(a_+ + a_-^\dagger\right) \\ z^* \quad &\to \quad \sqrt{\frac{\hbar}{2m\omega}}\left(a_- + a_+^\dagger\right) \\ \dot{z} \quad &\to \quad i\sqrt{\frac{\hbar\omega}{2m}}\left(a_-^\dagger - a_+\right) \\ \dot{z}^* \quad &\to \quad i\sqrt{\frac{\hbar\omega}{2m}}\left(a_+^\dagger - a_-\right) \end{aligned} \tag{6.95}$$

Thus, if we are faced with an energy expression of the form (6.84), we will immediately convert it to the form (6.91), assume the commutation relations (6.90) apply, and for any quantities where we need to make quantum operators out of classical quantities, we will use the conversion formulas (6.95). This will prove very handy when we quantize the electromagnetic field in a later chapter.