7

The Harmonic Oscillator

7.1. Why Study the Harmonic Oscillator?

In this section I will put the harmonic oscillator in its place—on a pedestal. Not only is it a system that can be exactly solved (in classical and quantum theory) and a superb pedagogical tool (which will be repeatedly exploited in this text), but it is also a system of great physical relevance. As will be shown below, any system fluctuating by small amounts near a configuration of stable equilibrium may be described either by an oscillator or by a collection of decoupled harmonic oscillators. Since the dynamics of a collection of noninteracting oscillators is no more complicated than that of a single oscillator (apart from the obvious N-fold increase in degrees of freedom), in addressing the problem of the oscillator we are actually confronting the general problem of small oscillations near equilibrium of an arbitrary system.

A concrete example of a single harmonic oscillator is a mass m coupled to a spring of force constant k. For small deformations x, the spring will exert the force given by Hooke's law, $F=-kx$, (k being its force constant) and produce a potential $V=\frac{1}{2}kx^2$. The Hamiltonian for this system is

$$\mathscr{H}=T+V=\frac{p^2}{2m}+\frac{1}{2}m\omega^2x^2 \tag{7.1.1}$$

where $\omega=(k/m)^{1/2}$ is the classical frequency of oscillation. Any Hamiltonian of the above form, quadratic in the coordinate and momentum, will be called the *harmonic oscillator Hamiltonian*. Now, the mass-spring system is just one among the following family of systems described by the oscillator Hamiltonian. Consider a particle moving in a potential $V(x)$. If the particle is placed at one of its minima x_0, it will remain there in a state of stable, static equilibrium. (A maximum, which is a point of unstable static equilibrium, will not interest us here.) Consider now the dynamics of this particle as it fluctuates by small amounts near $x=x_0$. The potential it experiences may be expanded in a Taylor series:

$$V(x)=V(x_0)+\left.\frac{dV}{dx}\right|_{x_0}(x-x_0)+\frac{1}{2!}\left.\frac{d^2V}{dx^2}\right|_{x_0}(x-x_0)^2+\cdots \tag{7.1.2}$$

Now, the constant piece $V(x_0)$ is of no physical consequence and may be dropped. [In other words, we may choose $V(x_0)$ as the arbitrary reference point for measuring the potential.] The second term in the series also vanishes since x_0 is a minimum of $V(x)$, or equivalently, since at a point of static equilibrium, the force, $-dV/dx$, vanishes. If we now shift our origin of coordinates to x_0 Eq. (7.1.2) reads

$$V(x)=\frac{1}{2!}\left.\frac{d^2V}{dx^2}\right|_0 x^2+\frac{1}{3!}\left.\frac{d^3V}{dx^3}\right|_0 x^3+\cdots \tag{7.1.3}$$

For *small* oscillations, we may neglect all but the leading term and arrive at the potential (or Hamiltonian) in Eq. (7.1.1), d^2V/dx^2 being identified with $k=m\omega^2$. (By definition, x is small if the neglected terms in the Taylor series are small compared to the leading term, which alone is retained. In the case of the mass-spring system, x is small as long as Hooke's law is a good approximation.)

As an example of a system described by a collection of independent oscillators, consider the coupled-mass system from Example 1.8.6. (It might help to refresh your memory by going back and reviewing this problem.) The Hamiltonian for this system is

$$\begin{aligned}\mathscr{H}&=\frac{p_1^2}{2m}+\frac{p_2^2}{2m}+\frac{1}{2}m\omega^2[x_1^2+x_2^2+(x_1-x_2)^2]\\&=\mathscr{H}_1+\mathscr{H}_2+\tfrac{1}{2}m\omega^2(x_1-x_2)^2\end{aligned} \tag{7.1.4}$$

Now this $\mathscr{H}$ is not of the promised form, since the oscillators corresponding to $\mathscr{H}_1$ and $\mathscr{H}_2$ (associated with the coordinates x_1 and x_2) are coupled by the $(x_1-x_2)^2$ term. But we already know of an alternate description of this system in which it can be viewed as two *decoupled* oscillators. The trick is of course the introduction of normal coordinates. We exchange x_1 and x_2 for

$$x_{\mathrm{I}}=\frac{x_1+x_2}{2^{1/2}} \tag{7.1.5a}$$

and

$$x_{\mathrm{II}}=\frac{x_1-x_2}{2^{1/2}} \tag{7.1.5b}$$

By differentiating these equations with respect to time, we get similar ones for the velocities, and hence the momenta. In terms of the normal coordinates (and the corresponding momenta),

$$\mathscr{H}=\mathscr{H}_{\mathrm{I}}+\mathscr{H}_{\mathrm{II}}=\frac{p_{\mathrm{I}}^2}{2m}+\frac{1}{2}m\omega^2x_{\mathrm{I}}^2+\frac{p_{\mathrm{II}}^2}{2m}+\frac{3}{2}m\omega^2x_{\mathrm{II}}^2 \tag{7.1.6}$$

Thus the problem of the two coupled masses reduces to that of two uncoupled oscillators of frequencies $\omega_{\mathrm{I}}=\omega=(k/m)^{1/2}$ and $\omega_{\mathrm{II}}=3^{1/2}\omega=(3k/m)^{1/2}$.

Let us rewrite Eq. (7.1.4) as

$$\mathscr{H}=\frac{1}{2m}\sum_{i=1}^{2}\sum_{j=1}^{2}p_i\delta_{ij}p_j+\frac{1}{2}\sum_{i=1}^{2}\sum_{j=1}^{2}x_iV_{ij}x_j \tag{7.1.7}$$

where V_{ij} are elements of a real symmetric (Hermitian) matrix V with the following values:

$$V_{11}=V_{22}=2m\omega^2, \qquad V_{12}=V_{21}=-m\omega^2 \tag{7.1.8}$$

In switching to the normal coordinates $x_{\rm I}$ and $x_{\rm II}$ (and $p_{\rm I}$ and $p_{\rm II}$), we are going to a basis that diagonalizes V and reduces the potential energy to a sum of decoupled terms, one for each normal mode. The kinetic energy piece remains decoupled in both bases.

Now, just as the mass–spring system was just a representative element of a family of systems described by the oscillator Hamiltonian, the coupled-mass system is also a special case of a family that can be described by a collection of coupled harmonic oscillators. Consider a system with N Cartesian degrees of freedom $x_1 \ldots x_N$, with a potential energy function $V(x_1, \ldots, x_N)$. Near an equilibrium point (chosen as the origin), the expansion of V, in analogy with Eq. (7.1.3), is

$$V(x_1 \ldots x_N)=\frac{1}{2}\sum_{i=1}^{N}\sum_{j=1}^{N}\left.\frac{\partial^2 V}{\partial x_i\,\partial x_j}\right|_0 x_ix_j+\cdots \tag{7.1.9}$$

For small oscillations, the Hamiltonian is

$$\mathscr{H}=\sum_{i=1}^{N}\sum_{j=1}^{N}\frac{p_i\delta_{ij}p_j}{2m}+\frac{1}{2}\sum_{i=1}^{N}\sum_{j=1}^{N}x_iV_{ij}x_j \tag{7.1.10}$$

where

$$V_{ij}=\left.\frac{\partial^2 V}{\partial x_i\,\partial x_j}\right|_0=\left.\frac{\partial^2 V}{\partial x_j\,\partial x_i}\right|_0=V_{ji} \tag{7.1.11}$$

are the elements of a *Hermitian* matrix V. (We are assuming for simplicity that the masses associated with all N degrees of freedom are equal.) From the mathematical theory of Chapter 1, we know that there exists a new basis (i.e., a new set of coordinates $x_{\rm I}$, $x_{\rm II}, \ldots$) which will diagonalize V and reduce $\mathscr{H}$ to a sum of N decoupled oscillator Hamiltonians, one for each normal mode. Thus the general problem of small fluctuations near equilibrium of an arbitrary system reduces to the study of a single harmonic oscillator.

This section concludes with a brief description of two important systems which are described by a collection of independent oscillators. The first is a crystal (in three dimensions), the atoms in which jiggle about their mean positions on the lattice. The second is the electromagnetic field in free space. A crystal with N_0 atoms (assumed to be point particles) has $3N_0$ degrees of freedom, these being the displacements from equilibrium points on the lattice. For small oscillations, the Hamiltonian will be quadratic in the coordinates (and of course the momenta). Hence there will exist $3N_0$ normal coordinates and their conjugate momenta, in terms of which $\mathscr{H}$ will be a decoupled sum over oscillator Hamiltonians. What are the corresponding normal modes? Recall that in the case of two coupled masses, the normal modes corresponded to collective motions of the entire system, with the two masses in step in one case, and exactly out of step in the other. Likewise, in the present case, the motion is collective in the normal modes, and corresponds to plane waves traveling across the lattice. For a given wavevector **k**, the atoms can vibrate parallel to k (*longitudinal polarization*) or in any one of the two independent directions perpendicular to **k** (*transverse polarization*). Most books on solid state physics will tell you why there are only N_0 possible values for **k**. (This must of course be so, for with three polarizations at each **k**, we will have exactly $3N_0$ normal modes.) The modes, labeled $(\mathbf{k}, \lambda)$, where λ is the polarization index ($\lambda = 1, 2, 3$), form a complete basis for expanding any state of the system. The coefficients of the expansion, $a(\mathbf{k}, \lambda)$, are the normal coordinates. The normal frequencies are labeled $\omega(\mathbf{k}, \lambda)$.‡

In the case of the electromagnetic field, the coordinate is the potential $\mathbf{A}(\mathbf{r}, t)$ at each point in space. [$\dot{\mathbf{A}}(\mathbf{r}, t)$ is the "velocity" corresponding to the coordinate $\mathbf{A}(\mathbf{r}, t)$.] The normal modes are once again plane waves but with two differences: there is no restriction on **k**, but the polarization has to be transverse. The quantum theory of the field will be discussed at length in Chapter 18.

7.2. Review of the Classical Oscillator

The equations of motion for the oscillator are, from Eq. (7.1.1),

$$\dot{x} = \frac{\partial \mathscr{H}}{\partial p} = \frac{p}{m} \tag{7.2.1}$$

$$\dot{p} = -\frac{\partial \mathscr{H}}{\partial x} = -m\omega^2 x \tag{7.2.2}$$

By eliminating $\dot{p}$, we arrive at the familiar equation

$$\ddot{x} + \omega^2 x = 0$$

with the solution

$$x(t) = A\cos\omega t + B\sin\omega t = x_0\cos(\omega t + \phi) \tag{7.2.3}$$

where x_0 is the amplitude and ϕ the phase of oscillator. The conserved energy associated with the oscillator is

$$E = T + V = \tfrac{1}{2}m\dot{x}^2 + \tfrac{1}{2}m\omega^2 x^2 = \tfrac{1}{2}m\omega^2 x_0^2 \tag{7.2.4}$$

‡ To draw a parallel with the two-mass system, $(\mathbf{k}, \lambda)$ is like I or II, $a(\mathbf{k}, \lambda)$ is like x_{I} or x_{II} and $\omega(\mathbf{k}, \lambda)$ is like $(k/m)^{1/2}$ or $(3k/m)^{1/2}$.

Since x_0 is a continuous variable, so is the energy of the classical oscillator. The lowest value for E is zero, and corresponds to the particle remaining at rest at the origin.

By solving for $\dot{x}$ in terms of E and x from Eq. (7.2.4) we obtain

$$\dot{x}=(2E/m-\omega^2x^2)^{1/2}=\omega(x_0^2-x^2)^{1/2} \tag{7.2.5}$$

which says that the particle starts from rest at a turning point ($x=\pm x_0$), picks up speed till it reaches the origin, and slows down to rest by the time it reaches the other turning point.

You are reminded of these classical results, so that you may readily compare and contrast them with their quantum counterparts.

7.3. Quantization of the Oscillator (Coordinate Basis)

We now consider the quantum oscillator, that is to say, a particle whose state vector $|\psi\rangle$ obeys the Schrödinger equation

$$i\hbar\frac{d}{dt}|\psi\rangle=H|\psi\rangle$$

with

$$H=\mathscr{H}(x\to X, p\to P)=\frac{P^2}{2m}+\frac{1}{2}m\omega^2X^2$$

As observed repeatedly in the past, the complete dynamics is contained in the propagator $U(t)$, which in turn may be expressed in terms of the eigenvectors and eigenvalues of H. In this section and the next, we will solve the eigenvalue problem in the X basis and the H basis, respectively. In Section 7.5 the passage from the H basis to the X basis will be discussed. The solution in the P basis, trivially related to the solution in the X basis in this case, will be discussed in an exercise.

With an eye on what is to follow, let us first establish that the eigenvalues of H cannot be negative. For any $|\psi\rangle$,

$$\begin{aligned}\langle H\rangle&=\frac{1}{2m}\langle\psi|P^2|\psi\rangle+\frac{1}{2}m\omega^2\langle\psi|X^2|\psi\rangle\\&=\frac{1}{2m}\langle\psi|P^\dagger P|\psi\rangle+\frac{1}{2}m\omega^2\langle\psi|X^\dagger X|\psi\rangle\\&=\frac{1}{2m}\langle P\psi|P\psi\rangle+\frac{1}{2}m\omega^2\langle X\psi|X\psi\rangle\geq 0\end{aligned}$$

since the norms of the states $|P\psi\rangle$ and $|X\psi\rangle$ cannot be negative. If we now set $|\psi\rangle$ equal to any eigenstate of H, we get the desired result.

Armed with the above result, we are now ready to attack the problem in the X basis.

We begin by projecting the eigenvalue equation,

$$\left(\frac{P^2}{2m}+\frac{1}{2}m\omega^2X^2\right)|E\rangle=E|E\rangle \tag{7.3.1}$$

onto the X basis, using the usual substitutions

$$X\rightarrow x$$
$$P\rightarrow -i\hbar\frac{d}{dx}$$
$$|E\rangle\rightarrow \psi_E(x)$$

and obtain

$$\left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}+\frac{1}{2}m\omega^2x^2\right)\psi=E\psi \tag{7.3.2}$$

(The argument of ψ and the subscript E are implicit.)

We can rearrange this equation to the form

$$\frac{d^2\psi}{dx^2}+\frac{2m}{\hbar^2}\left(E-\frac{1}{2}m\omega^2x^2\right)\psi=0 \tag{7.3.3}$$

We wish to find all solutions to this equation that lie in the physical Hilbert space (of functions normalizable to unity or the Dirac delta function). Follow the approach closely—it will be invoked often in the future.

The first step is to write Eq. (7.3.3) in terms of dimensionless variables. We look for a new variable y which is dimensionless and related to x by

$$x=by \tag{7.3.4}$$

where b is a scale factor with units of length. Although any length b (say the radius of the solar system) will generate a dimensionless variable y, the idea is to choose the natural length scale generated by the equation itself. By feeding Eq. (7.3.4) into Eq. (7.3.3), we arrive at

$$\frac{d^2\psi}{dy^2}+\frac{2mEb^2}{\hbar^2}\psi-\frac{m^2\omega^2b^4}{\hbar^2}y^2\psi=0 \tag{7.3.5}$$

The last terms suggests that we choose

$$b=\left(\frac{\hbar}{m\omega}\right)^{1/2} \tag{7.3.6}$$

Let us also define a dimensionless variable ε corresponding to E:

$$\varepsilon=\frac{mEb^2}{\hbar^2}=\frac{E}{\hbar\omega} \tag{7.3.7}$$

(We may equally well choose $\varepsilon=2mEb^2/\hbar^2$. Constants of order unity are not uniquely suggested by the equation. In the present case, our choice of ε is in anticipation of the results.) In terms of the dimensionless variables, Eq. (7.3.5) becomes

$$\psi''+(2\varepsilon-y^2)\psi=0 \tag{7.3.8}$$

where the prime denotes differentiation with respect to y.

Not only do dimensionless variables lead to a more compact equation, they also provide the natural scales for the problem. By measuring x and E in units of $(\hbar/m\omega)^{1/2}$ and $\hbar\omega$, which are scales generated intrinsically by the parameters entering the problem, we develop a feeling for what the words "small" and "large" mean: for example the displacement of the oscillator is large if y is large. If we insist on using the same units for all problems ranging from the atomic physics to cosmology, we will not only be dealing with extremely large or extremely small numbers, we will also have no feeling for the size of quantities in the relevant scale. (A distance of 10^{-20} parsecs, small on the cosmic scale, is enormous if one is dealing with an atomic system.)

The next step is to examine Eq. (7.3.8) at limiting values of y to learn about the solution in these limits. In the limit $y\to\infty$, we may neglect the $2\varepsilon\psi$ term and obtain

$$\psi''-y^2\psi=0 \tag{7.3.9}$$

The solution to this equation *in the same limit* is

$$\psi=Ay^m\,e^{\pm y^2/2}$$

for

$$\psi''=Ay^{m+2}\cdot e^{\pm y^2/2}\left[1\pm\frac{2m+1}{y^2}+\frac{m(m-1)}{y^4}\right]$$

$$\xrightarrow[y\to\infty]{} Ay^{m+2}\,e^{\pm y^2/2}=y^2\psi$$

where we have dropped all but the leading power in y as $y\to\infty$. Of the two possibilities $y^m e^{\pm y^2/2}$, we pick $y^m e^{-y^2/2}$, for the other possibility is not a part of the physical Hilbert space since it grows exponentially as $y\to\infty$.

Consider next the $y\to 0$ limit. Equation (7.3.8) becomes, upon dropping the $y^2\psi$ term,

$$\psi''+2\varepsilon\psi=0$$

which has the solution

$$\psi=A\cos[\sqrt{2\varepsilon}y]+B\sin[\sqrt{2\varepsilon}y]$$

Since we have dropped the y^2 term in the equation as being too small, consistency demands that we expand the cosine and sine and drop terms of order y^2 and beyond. We then get

$$\psi \xrightarrow[y\to 0]{} A+cy+O(y^2)$$

where c is a new constant $[=B(2\varepsilon)^{1/2}]$.

We therefore infer that ψ is of the form

$$\psi(y)=u(y)\,e^{-y^2/2} \tag{7.3.10}$$

where u approaches $A+cy$ (plus higher powers) as $y\to 0$, and y^m (plus lower powers) as $y\to\infty$. To determine $u(y)$ completely, we feed the above *ansatz* into Eq. (7.3.8) and obtain

$$u''-2yu'+(2\varepsilon-1)u=0 \tag{7.3.11}$$

This equation has the desired features (to be discussed in Exercise 7.3.1) that indicate that a power-series solution is possible, i.e., if we assume

$$u(y)=\sum_{n=0}^{\infty} C_n y^n \tag{7.3.12}$$

the equation will determine the coefficients. [The series begins with $n=0$, and not some negative n, since we know that as $y\to 0$, $u\to A+cy+O(y^2)$.] Feeding this series into Eq. (7.3.11) we find

$$\sum_{n=0}^{\infty} C_n[n(n-1)y^{n-2}-2ny^n+(2\varepsilon-1)y^n]=0 \tag{7.3.13}$$

Consider the first of three pieces in the above series:

$$\sum_{n=0}^{\infty} C_n n(n-1)y^{n-2}$$

Due to the $n(n-1)$ factor, this series also equals

$$\sum_{n=2}^{\infty} C_n n(n-1)y^{n-2}$$

In terms of a new variable $m=n-2$ the series becomes

$$\sum_{m=0}^{\infty} C_{m+2}(m+2)(m+1)y^m \equiv \sum_{n=0}^{\infty} C_{n+2}(n+2)(n+1)y^n$$

since m is a dummy variable. Feeding this equivalent series back into Eq. (7.3.13) we get

$$\sum_{n=0}^{\infty} y^n[C_{n+2}(n+2)(n+1)+C_n(2\varepsilon-1-2n)]=0 \tag{7.3.14}$$

Since the functions y^n are linearly independent (you cannot express y^n as a linear combination of other powers of y) each coefficient in the linear relation above must vanish. We thus find

$$C_{n+2}=C_n\frac{(2n+1-2\varepsilon)}{(n+2)(n+1)} \tag{7.3.15}$$

Thus for any C_0 and C_1, the *recursion relation* above generates $C_2, C_4, C_6, \ldots$ and $C_3, C_5, C_7, \ldots$. The function $u(y)$ is given by

$$u(y)=C_0\left[1+\frac{(1-2\varepsilon)y^2}{(0+2)(0+1)}+\frac{(1-2\varepsilon)}{(0+2)(0+1)}\frac{(4+1-2\varepsilon)}{(2+2)(2+1)}y^4+\cdots\right]$$

$$+C_1\left[y+\frac{(2+1-2\varepsilon)y^3}{(1+2)(1+1)}+\frac{(2+1-2\varepsilon)}{(1+2)(1+1)}\frac{(6+1-2\varepsilon)}{(3+2)(3+1)}y^5+\cdots\right] \tag{7.3.16}$$

where C_0 and C_1 are arbitrary.

It appears as if the energy of the quantum oscillator is arbitrary, since ε has not been constrained in any way. But we know something is wrong, since we saw at the outset that the oscillator eigenvalues are nonnegative. The first sign of sickness in our solution, Eq. (7.3.16), is that $u(y)$ does not behave like y^m as $y\to\infty$ (as deduced at the outset) since it contains arbitrarily high powers of y. There is only one explanation. We have seen that as $y\to\infty$, there are just two possibilities

$$\psi(y) \xrightarrow[y\to\infty]{} y^m e^{\pm y^2/2}$$

If we write $\psi(y)=u(y)\,e^{-y^2/2}$, then the two possibilities for $u(y)$ are

$$u(y) \xrightarrow[y\to\infty]{} y^m \quad \text{or} \quad y^m e^{y^2}$$

Clearly $u(y)$ in Eq. (7.3.16), which is not bounded by any finite power of y as $y\to\infty$, corresponds to the latter case. We may explicitly verify this as follows.

Consider the power series for $u(y)$ as $y\to\infty$. Just as the series is controlled by C_0 (the coefficient of the lowest power of y) as $y\to 0$, it is governed by its coefficients $C_{n\to\infty}$ as $y\to\infty$. The growth of the series is characterized by the ratio [see Eq. (7.3.15)]

$$\frac{C_{n+2}}{C_n}\xrightarrow[n\to\infty]{}\frac{2}{n} \tag{7.3.17}$$

Compare this to the growth of $y^m e^{y^2}$. Since

$$y^m e^{y^2}=\sum_{k=0}^{\infty}\frac{y^{2k+m}}{k!}$$

$C_n=$coefficient of $y^n=1/k!$; with $n=2k+m$ or $k=(n-m)/2$. Likewise

$$C_{n+2}=\frac{1}{[(n+2-m)/2]!}$$

so

$$\frac{C_{n+2}}{C_n}\xrightarrow[n\to\infty]{}\frac{[(n-m)/2]!}{[(n+2-m)/2]!}=\frac{1}{(n-m+2)/2}\sim\frac{2}{n}$$

In other words, $u(y)$ in Eq. (7.3.16) grows as $y^m e^{y^2}$, so that $\psi(y)\simeq y^m e^{y^2}e^{-y^2/2}\simeq y^m e^{+y^2/2}$, which is the rejected solution raising its ugly head! Our predicament is now reversed: from finding that every ε is allowed, we are now led to conclude that no ε is allowed. Fortunately there is a way out. If ε is one of the special values

$$\varepsilon_n=\frac{2n+1}{2},\qquad n=0,1,2,\ldots \tag{7.3.18}$$

the coefficient C_{n+2} (and others dependent on it) vanish. If we choose $C_1=0$ when n is even (or $C_0=0$ when n is odd) we have a finite polynomial of order n which satisfies the differential equation and behaves as y^n as $y\to\infty$:

$$\psi(y)=u(y)\,e^{-y^2/2}=\begin{Bmatrix}C_0+C_2y^2+C_4y^4+\cdots+C_ny^n\\ C_1y+C_3y^3+C_5y^5+\cdots+C_ny^n\end{Bmatrix}\cdot e^{-y^2/2} \tag{7.3.19}$$

Equation (7.3.18) tells us that energy is quantized: the only allowed values for $E=\varepsilon\hbar\omega$ (i.e., values that yield solutions in the physical Hilbert space) are

$$E_n=(n+\tfrac{1}{2})\hbar\omega,\qquad n=0,1,2,\ldots \tag{7.3.20}$$

For each value of n, Eq. (7.3.15) determines the corresponding polynomials of nth order, called *Hermite polynomials*, $H_n(y)$:

$$\begin{aligned} H_0(y) &= 1 \\ H_1(y) &= 2y \\ H_2(y) &= -2(1-2y^2) \\ H_3(y) &= -12(y-\tfrac{2}{3}y^3) \\ H_4(y) &= 12(1-4y^2+\tfrac{4}{3}y^4) \end{aligned} \tag{7.3.21}$$

The arbitrary initial coefficients C_0 and C_1 in H_n are chosen according to a standard convention. The normalized solutions are then

$$\begin{aligned} \psi_E(x) &\equiv \psi_{(n+1/2)\hbar\omega}(x) \equiv \psi_n(x) \\ &= \left(\frac{m\omega}{\pi\hbar 2^{2n}(n!)^2}\right)^{1/4} \exp\left(-\frac{m\omega x^2}{2\hbar}\right) H_n\left[\left(\frac{m\omega}{\hbar}\right)^{1/2} x\right] \end{aligned} \tag{7.3.22}$$

The derivation of the normalization constant

$$A_n = \left[\frac{m\omega}{\pi\hbar 2^{2n}(n!)^2}\right]^{1/4} \tag{7.3.23}$$

is rather tedious and will not be discussed here in view of a shortcut to be discussed in the next section.

The following recursion relations among Hermite polynomials are very useful:

$$H_n'(y) = 2nH_{n-1} \tag{7.3.24}$$

$$H_{n+1}(y) = 2yH_n - 2nH_{n-1} \tag{7.3.25}$$

as is the integral

$$\int_{-\infty}^{\infty} H_n(y)H_{n'}(y)\, e^{-y^2}\, dy = \delta_{nn'}(\pi^{1/2}2^n n!) \tag{7.3.26}$$

which is just the orthonormality condition of the eigenfunctions $\psi_n(x)$ and $\psi_{n'}(x)$ written in terms of $y = (m\omega/\hbar)^{1/2}x$.

We can now express the propagator as

$$\begin{aligned} U(x, t; x', t') = \sum_{n=0}^{\infty} A_n \exp\left(-\frac{m\omega}{2\hbar} x^2\right) H_n(x) A_n \exp\left(-\frac{m\omega}{2\hbar} x'^2\right) \\ \times H_n(x') \exp[-i(n+1/2)\omega(t-t')] \end{aligned} \tag{7.3.27}$$

Evaluation of this sum is a highly formidable task. We will not attempt it here since we will find an extremely simple way for calculating U in Chapter 8, devoted to the path integral formalism. The result happens to be

$$U(x, t; x', t') = \left(\frac{m\omega}{2\pi i\hbar \sin \omega T}\right)^{1/2} \exp\left[\frac{im\omega}{\hbar} \frac{(x^2+x'^2)\cos \omega T - 2xx'}{2 \sin \omega T}\right] \tag{7.3.28}$$

where $T = t - t'$.

This concludes the solution of the eigenvalue problem. Before analyzing our results let us recapitulate our strategy.

Step 1. Introduce dimensionless variables natural to the problem.
Step 2. Extract the asymptotic ($y \to \infty$, $y \to 0$) behavior of ψ.
Step 3. Write ψ as a product of the asymptotic form and an unknown function u. The function u will usually be easier to find than ψ.
Step 4. Try a power series to see if it will yield a recursion relation of the form Eq. (7.3.15).

*Exercise 7.3.1.** Consider the question why we tried a power-series solution for Eq. (7.3.11) but not Eq. (7.3.8). By feeding in a series into the latter, verify that a three-term recursion relation between C_{n+2}, C_n, and C_{n-2} obtains, from which the solution does not follow so readily. The problem is that ψ'' has two powers of y less than $2\varepsilon\psi$, while the $-y^2$ piece has two more powers of y. In Eq. (7.3.11) on the other hand, of the three pieces u'', $-2yu'$, and $(2\varepsilon-1)u$, the last two have the same powers of y.

Exercise 7.3.2. Verify that $H_3(y)$ and $H_4(y)$ obey the recursion relation, Eq. (7.3.15).

Exercise 7.3.3. If $\psi(x)$ is even and $\phi(x)$ is odd under $x \to -x$, show that

$$\int_{-\infty}^{\infty} \psi(x)\phi(x)\,dx = 0$$

Use this to show that $\psi_2(x)$ and $\psi_1(x)$ are orthogonal. Using the values of Gaussian integrals in Appendix A.2 verify that $\psi_2(x)$ and $\psi_0(x)$ are orthogonal.

Exercise 7.3.4. Using Eqs. (7.3.23)–(7.3.25), show that

$$\langle n'|X|n\rangle = \left(\frac{\hbar}{2m\omega}\right)^{1/2} [\delta_{n',n+1}(n+1)^{1/2} + \delta_{n',n-1}n^{1/2}]$$

$$\langle n'|P|n\rangle = \left(\frac{m\omega\hbar}{2}\right)^{1/2} i[\delta_{n',n+1}(n+1)^{1/2} - \delta_{n',n-1}n^{1/2}]$$

*Exercise 7.3.5.** Using the symmetry arguments from Exercise 7.3.3 show that $\langle n|X|n\rangle = \langle n|P|n\rangle = 0$ and thus that $\langle X^2\rangle = (\Delta X)^2$ and $\langle P^2\rangle = (\Delta P)^2$ in these states. Show that $\langle 1|X^2|1\rangle = 3\hbar/2m\omega$ and $\langle 1|P^2|1\rangle = \frac{3}{2}m\omega\hbar$. Show that $\psi_0(x)$ saturates the uncertainty bound $\Delta X \cdot \Delta P \geq \hbar/2$.

*Exercise 7.3.6.** Consider a particle in a potential

$$V(x) = \tfrac{1}{2}m\omega^2 x^2, \qquad x > 0$$
$$= \infty, \qquad x \le 0$$

What are the boundary conditions on the wave functions now? Find the eigenvalues and eigenfunctions.

We now discuss the eigenvalues and eigenfunctions of the oscillator. The following are the main features:

(1) The energy is quantized. In contrast to the classical oscillator whose energy is continuous, the quantum oscillator has a discrete set of levels given by Eq. (7.3.20). Note that the quantization emerges only after we supplement Schrödinger's equation with the requirement that ψ be an element of the physical Hilbert space. In this case it meant the imposition of the boundary condition $\psi(|x|\to\infty)\to 0$ [as opposed to $\psi(|x|\to\infty)\to\infty$, which is what obtained for all but the special values of E].

Why does the classical oscillator seem to have a continuum of energy values? The answer has to do with the relative sizes of the energy gap and the total energy of the classical oscillator. Consider, for example, a mass of 2 g, oscillating at a frequency of 1 rad/sec, with an amplitude of 1 cm. Its energy is

$$E = \tfrac{1}{2}m\omega^2 x_0^2 = 1 \text{ erg}$$

Compare this to the gap between allowed energies:

$$\Delta E = \hbar\omega \simeq 10^{-27} \text{ erg}$$

At the macroscopic level, it is practically impossible to distinguish between a system whose energy is continuous and one whose allowed energy levels are spaced 10^{-27} erg apart. Stated differently, the *quantum number* associated with this oscillator is

$$n = \frac{E}{\hbar\omega} - \frac{1}{2} \simeq 10^{27}$$

while the difference in n between adjacent levels is unity. We have here a special case of the *correspondence principle*, which states that as the quantum number tends to infinity, we regain the classical picture. (We know vaguely that when a system is big, it may be described classically. The correspondence principle tells us that the quantum number is a good measure of bigness.)

(2) The levels are spaced uniformly. The fact that the oscillator energy levels go up in steps of $\hbar\omega$ allows one to construct the following picture. We pretend that associated with an oscillator of classical frequency ω there exist fictitious particles called *quanta* each endowed with energy $\hbar\omega$. We view the $n\hbar\omega$ piece in the energy formula Eq. (7.3.20) as the energy of n such quanta. In other words, we forget about the mass and spring and think in terms of the quanta. When the quantum number n goes up (or down) by Δn, we say that Δn quanta have been created (or destroyed).

Although it seems like a matter of semantics, thinking of the oscillator in terms of these quanta has proven very useful.

In the case of the crystal, there are $3N_0$ oscillators, labeled by the $3N_0$ values of $(\mathbf{k}, \lambda)$, with frequencies $\omega(\mathbf{k}, \lambda)$. The quantum state of the crystal is specified by giving the number of quanta, called *phonons*, at each $(\mathbf{k}, \lambda)$. For a crystal whose Hamiltonian is exactly given by a sum of oscillator pieces, the introduction of the phonon concept is indeed a matter of semantics. If, however, we consider deviations from this, say to take into account nonleading terms in the Taylor expansion of the potential, or the interaction between the crystal and some external probe such as an electron shot at it, the phonon concept proves very useful. (The two effects mentioned above may be seen as phonon–phonon interactions and phonon–electron interactions, respectively.)

Similarly, the interaction of the electromagnetic field with matter may be viewed as the interaction between light quanta or *photons* and matter, which is discussed in Chapter 18.

(3) The lowest possible energy is $\hbar\omega/2$ and not 0. Unlike the classical oscillator, which can be in a state of zero energy (with $x=p=0$) the quantum oscillator has a minimum energy of $\hbar\omega/2$. This energy, called the *zero-point energy*, is a reflection of the fact that the simultaneous eigenstate $|x=0, p=0\rangle$ is precluded by the canonical commutation relation $[X, P]=i\hbar$. This result is common to all oscillators, whether they describe a mechanical system or a normal mode of the electromagnetic field, since all these problems are mathematically identical and differ only in what the coordinate and its conjugate momentum represent. Thus, a crystal has an energy $\frac{1}{2}\hbar\omega(\mathbf{k}, \lambda)$ in each mode $(\mathbf{k}, \lambda)$ even when phonons are absent, and the electromagnetic field has an energy $\frac{1}{2}\hbar\omega(\mathbf{k}, \lambda)$ in each mode of frequency ω even when photons are absent. (The zero-point fluctuation of the field has measurable consequences, which will be discussed in Chapter 18.)

In the following discussion let us restrict ourselves to the mechanical oscillator and examine more closely the zero-point energy. We saw that it is the absence of the state $|x=0, p=0\rangle$ that is responsible for this energy. Such a state, with $\Delta X = \Delta P = 0$, is forbidden by the uncertainty principle. Let us therefore try to find a state that is quantum mechanically allowed and comes as close as possible (in terms of its energy) to the classical state $x=p=0$. If we choose a wave function $\psi(x)$ that is sharply peaked near $x=0$ to minimize the mean potential energy $\langle\frac{1}{2}m\omega^2X^2\rangle$, the wave function in P space spreads out and the mean kinetic energy $\langle P^2/2m\rangle$ grows. The converse happens if we pick a momentum space wave function sharply peaked near $p=0$. What we need then is a compromise $\psi_{\min}(x)$ that minimizes the *total* mean energy without violating the uncertainty principle. Let us now begin our quest for $\psi_{\min}(x)$. We start with a normalized trial state $|\psi\rangle$ and consider

$$\langle\psi|H|\psi\rangle = \langle H\rangle = \frac{\langle P^2\rangle}{2m} + \frac{1}{2}m\omega^2\langle X^2\rangle \tag{7.3.29}$$

Now

$$(\Delta P)^2 = \langle P^2\rangle - \langle P\rangle^2 \tag{7.3.30}$$

and

$$(\Delta X)^2 = \langle X^2\rangle - \langle X\rangle^2 \tag{7.3.31}$$

so that

$$\langle H\rangle=\frac{(\Delta P)^2+\langle P\rangle^2}{2m}+\frac{1}{2}m\omega^2[(\Delta X)^2+\langle X\rangle^2] \tag{7.3.32}$$

The first obvious step in minimizing $\langle H\rangle$ is to restrict ourselves to states with $\langle X\rangle=\langle P\rangle=0$. (Since $\langle X\rangle$ and $\langle P\rangle$ are independent of each other and of $(\Delta X)^2$ and $(\Delta P)^2$, such a choice is always possible.) For these states (from which we must pick the winner)

$$\langle H\rangle=\frac{(\Delta P)^2}{2m}+\frac{1}{2}m\omega^2(\Delta X)^2 \tag{7.3.33}$$

Now we use the uncertainty relation

$$\Delta X\cdot\Delta P\geq\hbar/2 \tag{7.3.34}$$

where the equality sign holds only for a Gaussian, as will be shown in Section 9.3. We get

$$\langle H\rangle\geq\frac{\hbar^2}{8m(\Delta X)^2}+\frac{1}{2}m\omega^2(\Delta X)^2 \tag{7.3.35}$$

We minimize $\langle H\rangle$ by choosing a Gaussian wave function, for which

$$\langle H\rangle_{\text{Gaussian}}=\frac{\hbar^2}{8m(\Delta X)^2}+\frac{1}{2}m\omega^2(\Delta X)^2 \tag{7.3.36}$$

What we have found is that the mean energy associated with the trial wave function is sensitive only to the corresponding ΔX and that, of all functions with the same ΔX, the Gaussian has the lowest energy. Finally we choose, from the family of Gaussians, the one with the ΔX that minimizes $\langle H\rangle_{\text{Gaussian}}$. By requiring

$$\frac{\partial\langle H\rangle_{\text{Gaussian}}}{\partial(\Delta X)^2}=0=\frac{-\hbar^2}{8m(\Delta X)^4}+\frac{1}{2}m\omega^2 \tag{7.3.37}$$

we obtain

$$(\Delta X)^2=\hbar/2m\omega \tag{7.3.38}$$

and

$$\langle H\rangle_{\text{min}}=\hbar\omega/2 \tag{7.3.39}$$

Thus, by systematically hunting in Hilbert space, we have found that the following normalized function has the lowest mean energy:

$$\psi_{\min}(x)=\left(\frac{m\omega}{\pi\hbar}\right)^{1/4}\exp\left(-\frac{m\omega x^2}{2\hbar}\right),\qquad \langle H\rangle_{\min}=\frac{\hbar\omega}{2} \tag{7.3.40}$$

If we apply the above result

$$\langle\psi_{\min}|H|\psi_{\min}\rangle\leq\langle\psi|H|\psi\rangle\quad(\text{for all }|\psi\rangle)$$

to $|\psi\rangle=|\psi_0\rangle=$ground-state vector, we get

$$\langle\psi_{\min}|H|\psi_{\min}\rangle\leq\langle\psi_0|H|\psi_0\rangle=E_0 \tag{7.3.41}$$

Now compare this with the result of Exercise 5.2.2:

$$E_0=\langle\psi_0|H|\psi_0\rangle\leq\langle\psi|H|\psi\rangle\quad\text{for all }|\psi\rangle$$

If we set $|\psi\rangle=|\psi_{\min}\rangle$ we get

$$E_0=\langle\psi_0|H|\psi_0\rangle\leq\langle\psi_{\min}|H|\psi_{\min}\rangle \tag{7.3.42}$$

It follows from Eq. (7.3.41) and (7.3.42) that

$$E_0=\langle\psi_0|H|\psi_0\rangle=\langle\psi_{\min}|H|\psi_{\min}\rangle=\frac{\hbar\omega}{2} \tag{7.3.43}$$

Also, since there was only one state, $|\psi_{\min}\rangle$, with energy $\hbar\omega/2$, it follows that

$$|\psi_0\rangle=|\psi_{\min}\rangle \tag{7.3.44}$$

We have thus managed to find the oscillator ground-state energy and state vector without solving the Schrödinger equation.

It would be a serious pedagogical omission if it were not emphasized at this juncture that the uncertainty relation has been unusually successful in the above context. Our ability here to obtain all the information about the ground state using the uncertainty relation is a consequence of the special form of the oscillator Hamiltonian [which allowed us to write $\langle H\rangle$ in terms of $(\Delta X)^2$ and $(\Delta P)^2$] and the fact that its ground-state wave function is a Gaussian (which has a privileged role with respect to the uncertainty relation). In more typical instances, the use of the uncertainty relation will have to be accompanied by some hand-waving [before $\langle H\rangle$ can be approximated by a function of $(\Delta X)^2$ and $(\Delta P)^2$] and then too will yield only an *estimate* for the ground-state energy. As for the wave function, we can only get an estimate for ΔX, the spread associated with it.

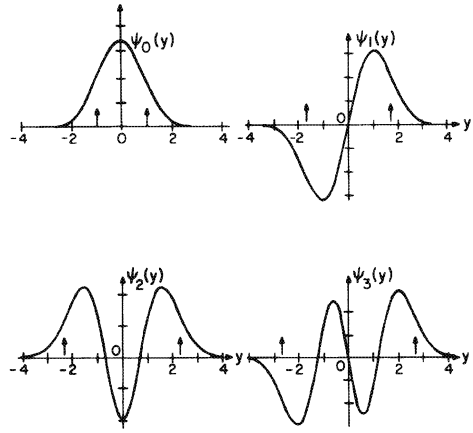

Figure 7.1. Normalized eigenfunctions for $n=0, 1, 2,$ and 3. The small arrows at $|y|=(2n+1)^{1/2}$ stand for the classical turning points. Recall that $y=(m\omega/\hbar)^{1/2}x$.

(4) The solutions (Fig. 7.1) $\psi_n(x)$ contain only even or odd powers of x, depending on whether n is even or odd. Consequently the eigenfunctions are even or odd:

$$\begin{aligned} \psi_n(-x) &= \psi_n(x), \qquad n \text{ even} \\ &= -\psi_n(x), \qquad n \text{ odd} \end{aligned}$$

In Chapter 11 on symmetries it will be shown that the eigenfunctions had to have this property.

(5) The wave function does not vanish beyond the classical turning points, but dies out exponentially as $x \to \infty$. [Verify that the classical turning points are given by $y_0 = \pm(2n+1)^{1/2}$.] Notice, however, that when n is large (Fig. 7.2) the excursions outside the turning points are small compared to the classical amplitude. This exponentially damped amplitude in the classically forbidden region was previously encountered in Chapter 5 when we studied tunneling.

(6) The probability distribution $P(x)$ is very different from the classical case. The position of a given classical oscillator is of course exactly known. But we could ask the following probabilistic question: if I suddenly walk into a room containing the oscillator, where am I likely to catch it? If the velocity of the oscillator at a point x is $v(x)$, the time it spends near the x, and hence the probability of our catching it there during a random spot check, varies inversely with $v(x)$:

$$P_{\text{cl}}(x) \propto \frac{1}{v(x)} = \frac{1}{\omega(x_0^2 - x^2)^{1/2}} \qquad (7.3.45)$$

which is peaked near $\pm x_0$ and has a minimum at the origin. In the quantum case, for the ground state in particular, $|\psi(x)|^2$ seems to go just the other way (Fig. 7.1). There is no contradiction here, for quantum mechanics *is* expected to differ from classical mechanics. The correspondence principle, however, tells us that for large n

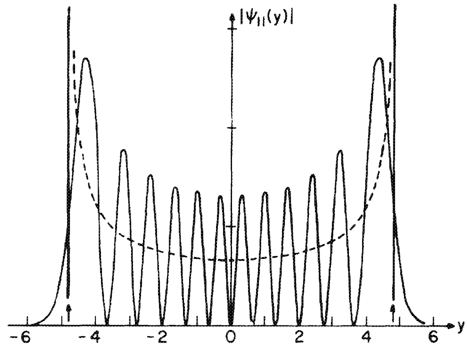

Figure 7.2. Probability density in the state $n=11$. The broken curve gives the classical probability distribution in a state with the same energy.

the two must become indistinguishable. From Fig. 7.2, which shows the situations at $n=11$, we can see how the classical limit is reached: the quantum distribution $P(x)=|\psi(x)|^2$ wiggles so rapidly (in a scale set by the classical amplitude) that only its mean can be detected at these scales, and this agrees with $P_{\mathrm{cl}}(x)$. We are reminded here of the double-slit experiment performed with macroscopic particles: there is a dense interference pattern, whose mean is measured in practice and agrees with the classical probability curve.

A remark that was made in more general terms in Chapter 6: the classical oscillator that we often refer to, is a figment lodged in our imagination and doesn't exist. In other words, all oscillators, including the 2-g mass and spring system, are ultimately governed by the laws of quantum mechanics, and thus have discrete energies, can shoot past the "classical" turning points, and have a zero-point energy of $\frac{1}{2}\hbar\omega$ even while they play dead. Note however that what I am calling nonexistent is an oscillator that *actually* has the properties attributed to it in classical mechanics, and not one that *seems* to have them when examined at the macroscopic level.

Exercise 7.3.7. The Oscillator in Momentum Space.* By setting up an eigenvalue equation for the oscillator in the P basis and comparing it to Eq. (7.3.2), show that the momentum space eigenfunctions may be obtained from the ones in coordinate space through the substitution $x\to p$, $m\omega\to 1/m\omega$. Thus, for example,

$$\psi_0(p)=\left(\frac{1}{m\pi\hbar\omega}\right)^{1/4} e^{-p^2/2m\hbar\omega}$$

There are several other pairs, such as ΔX and ΔP in the state $|n\rangle$, which are related by the substitution $m\omega\to 1/m\omega$. You may wish to watch out for them. (Refer back to Exercise 7.3.5.)

7.4. The Oscillator in the Energy Basis

Let us orient ourselves by recalling how the eigenvalue equation

$$\left(\frac{P^2}{2m}+\frac{1}{2}m\omega^2X^2\right)|E\rangle=E|E\rangle \tag{7.4.1}$$

was solved in the coordinate basis: (1) We made the assignments $X \to x$, $P \to -i\hbar\, d/dx$. (2) We solved for the components $\langle x | E \rangle = \psi_E(x)$ and the eigenvalues.

To solve the problem in the momentum basis, we first compute the X and P operators in this basis, given their form in the coordinate basis. For instance,

$$\langle p'|X|p\rangle = \iint \underbrace{\langle p'|x\rangle}_{\frac{e^{-ip'x/\hbar}}{(2\pi\hbar)^{1/2}}} \underbrace{\langle x|X|x'\rangle}_{\substack{x\delta(x-x') \\ \text{(given)}}} \underbrace{\langle x'|p\rangle}_{\frac{e^{ipx'/\hbar}}{(2\pi\hbar)^{1/2}}} dx\, dx'$$

$$= -i\hbar\delta'(p-p')$$

We then find P and $H(X, P)$ in this basis. The eigenvalue equation, (7.4.1), will then become a differential equation that we will proceed to solve.

Now suppose that we want to work in the energy basis. We must first find the eigenfunctions of H, i.e., $\langle x|E\rangle$, so that we can carry out the change of basis. But finding $\langle x|E\rangle = \psi_E(x)$ amounts to solving the full eigenvalue problem in the coordinate basis. Once we have done this, there is not much point in setting up the problem in the E basis.

But there is a clever way due to Dirac, which allows us to work in the energy basis without having to know ahead of time the operators X and P in this basis. All we will need is the commutation relation

$$[X, P] = i\hbar I = i\hbar \tag{7.4.2}$$

which follows from $X \to x$, $P \to -i\hbar\, d/dx$, *but is basis independent*. The next few steps will seem rather mysterious and will not fit into any of the familiar schemes discussed so far. You must be patient till they begin to pay off.

Let us first introduce the operator

$$a = \left(\frac{m\omega}{2\hbar}\right)^{1/2} X + i\left(\frac{1}{2m\omega\hbar}\right)^{1/2} P \tag{7.4.3}$$

and its adjoint

$$a^\dagger = \left(\frac{m\omega}{2\hbar}\right)^{1/2} X - i\left(\frac{1}{2m\omega\hbar}\right)^{1/2} P \tag{7.4.4}$$

(Note that $m\omega \to 1/m\omega$ as $X \leftrightarrow P$.) They satisfy the commutation relation (which you should verify)

$$[a, a^\dagger] = 1 \tag{7.4.5}$$

Note next that the Hermitian operator $a^\dagger a$ is simply related to H:

$$a^\dagger a = \frac{m\omega}{2\hbar} X^2 + \frac{1}{2m\omega\hbar} P^2 + \frac{i}{2\hbar}[X, P]$$

$$= \frac{H}{\hbar\omega} - \frac{1}{2}$$

so that

$$H = (a^\dagger a + 1/2)\hbar\omega \tag{7.4.6}$$

[This method is often called the "method of factorization" since we are expressing $H = P^2 + X^2$ (ignoring constants) as a product of $(X + iP) = a$ and $(X - iP) = a^\dagger$. The extra $\hbar\omega/2$ in Eq. (7.4.6) comes from the non-commutative nature of X and P.]

Let us next define an operator $\hat{H}$,

$$\hat{H} = \frac{H}{\hbar\omega} = (a^\dagger a + 1/2) \tag{7.4.7}$$

whose eigenvalues ε measure energy in units of $\hbar\omega$. We wish to solve the eigenvalue equation for $\hat{H}$:

$$\hat{H}|\varepsilon\rangle = \varepsilon|\varepsilon\rangle \tag{7.4.8}$$

where ε is the energy measured in units of $\hbar\omega$. Two relations we will use shortly are

$$[a, \hat{H}] = [a, a^\dagger a + 1/2] = [a, a^\dagger a] = a \tag{7.4.9}$$

and

$$[a^\dagger, \hat{H}] = -a^\dagger \tag{7.4.10}$$

The utility of a and $a^\dagger$ stems from the fact that given an eigenstate of $\hat{H}$, they generate others. Consider

$$\begin{aligned}\hat{H}a|\varepsilon\rangle &= (a\hat{H} - [a, \hat{H}])|\varepsilon\rangle \\ &= (a\hat{H} - a)|\varepsilon\rangle \\ &= (\varepsilon - 1)a|\varepsilon\rangle\end{aligned} \tag{7.4.11}$$

We infer from Eq. (7.4.11) that $a|\varepsilon\rangle$ is an eigenstate with eigenvalue $\varepsilon-1$, i.e.,

$$a|\varepsilon\rangle=C_\varepsilon|\varepsilon-1\rangle \tag{7.4.12}$$

where C_ε is a constant, and $|\varepsilon-1\rangle$ and $|\varepsilon\rangle$ are normalized eigenkets.‡

Similarly we see that

$$\begin{aligned}\hat{H}a^\dagger|\varepsilon\rangle&=(a^\dagger\hat{H}-[a^\dagger, H])|\varepsilon\rangle\\&=(a^\dagger\hat{H}+a^\dagger)|\varepsilon\rangle\\&=(\varepsilon+1)a^\dagger|\varepsilon\rangle\end{aligned} \tag{7.4.13}$$

so that

$$a^\dagger|\varepsilon\rangle=C_{\varepsilon+1}|\varepsilon+1\rangle \tag{7.4.14}$$

One refers to a and $a^\dagger$ as *lowering and raising operators* for obvious reasons. They are also called *destruction and creation operators* since they destroy or create quanta of energy $\hbar\omega$.

We are thus led to conclude that if ε is an eigenvalue of $\hat{H}$, so are $\varepsilon+1, \varepsilon+2, \varepsilon+3, \ldots, \varepsilon+\infty$; and $\varepsilon-1, \ldots, \varepsilon-\infty$. The latter conclusion is in conflict with the result that the eigenvalues of H are nonnegative. So, it must be that the downward chain breaks at some point: there must be a state $|\varepsilon_0\rangle$ that cannot be lowered further:

$$a|\varepsilon_0\rangle=0 \tag{7.4.15}$$

Operating with $a^\dagger$, we get

$$a^\dagger a|\varepsilon_0\rangle=0$$

or

$$(\hat{H}-1/2)|\varepsilon_0\rangle=0 \quad \text{[from Eq. (7.4.7)]}$$

or

$$\hat{H}|\varepsilon_0\rangle=\tfrac{1}{2}|\varepsilon_0\rangle$$

or

$$\varepsilon_0=\tfrac{1}{2} \tag{7.4.16}$$

‡ We are using the fact that there is no degeneracy in one dimension.

We may, however, raise the state $|\varepsilon_0\rangle$ indefinitely by the repeated application of $a^\dagger$. We thus find that the oscillator has a sequence of levels given by

$$\varepsilon_n = (n + 1/2), \qquad n = 0, 1, 2, \ldots$$

or

$$E_n = (n + 1/2)\hbar\omega, \qquad n = 0, 1, 2, \ldots \tag{7.4.17}$$

Are these the only levels? If there were another family, it too would have to have a ground state $|\varepsilon_0'\rangle$ such that

$$a|\varepsilon_0'\rangle = 0$$

or

$$a^\dagger a|\varepsilon_0'\rangle = 0$$

or

$$\hat{H}|\varepsilon_0'\rangle = \tfrac{1}{2}|\varepsilon_0'\rangle \tag{7.4.18}$$

But we know that there is no degeneracy in one dimension (Theorem 15). Consequently it follows from Eqs. (7.4.16) and (7.4.18) that $|\varepsilon_0\rangle$ and $|\varepsilon_0'\rangle$ represent the same state. The same goes for the families built from $|\varepsilon_0\rangle$ and $|\varepsilon_0'\rangle$ by the repeated action of $a^\dagger$.

We now calculate the constants C_ε and $C_{\varepsilon+1}$ appearing in Eqs. (7.4.12) and (7.4.14). Since $\varepsilon = n + 1/2$, let us label the kets by the integer n. We want to determine the constant C_n appearing in the equation

$$a|n\rangle = C_n|n-1\rangle \tag{7.4.19a}$$

Consider the adjoint of this equation

$$\langle n|a^\dagger = \langle n-1|C_n^* \tag{7.4.19b}$$

By combining these equations we arrive at

$$\begin{aligned}
\langle n|a^\dagger a|n\rangle &= \langle n-1|n-1\rangle C_n^* C_n \\
\langle n|\hat{H} - \tfrac{1}{2}|n\rangle &= C_n^* C_n \quad (\text{since } |n-1\rangle \text{ is normalized}) \\
\langle n|n|n\rangle &= |C_n|^2 \quad (\text{since } \hat{H}|n\rangle = (n+1/2)|n\rangle) \\
|C_n|^2 &= n \\
C_n &= (n)^{1/2}\, e^{i\phi} \quad (\phi \text{ is arbitrary})
\end{aligned} \tag{7.4.20}$$

It is conventional to choose ϕ as zero. So we have

$$a|n\rangle = n^{1/2}|n-1\rangle \tag{7.4.21}$$

It can similarly be shown (by you) that

$$a^\dagger|n\rangle = (n+1)^{1/2}|n+1\rangle \tag{7.4.22}$$

[Note that in Eqs. (7.4.21) and (7.4.22) the larger of the n's labeling the two kets appears under the square root.] By combining these two equations we find

$$a^\dagger a|n\rangle = a^\dagger n^{1/2}|n-1\rangle = n^{1/2}n^{1/2}|n\rangle = n|n\rangle \tag{7.4.23}$$

In terms of

$$N = a^\dagger a \tag{7.4.24}$$

called the *number operator* (since it counts the quanta)

$$\hat{H} = N + \tfrac{1}{2} \tag{7.4.25}$$

Equations (7.4.21) and (7.4.22) are very important. They allow us to compute the matrix elements of all operators in the $|n\rangle$ basis. First consider a and $a^\dagger$ themselves:

$$\langle n'|a|n\rangle = n^{1/2}\langle n'|n-1\rangle = n^{1/2}\delta_{n',n-1} \tag{7.4.26}$$

$$\langle n'|a^\dagger|n\rangle = (n+1)^{1/2}\langle n'|n+1\rangle = (n+1)^{1/2}\delta_{n',n+1} \tag{7.4.27}$$

To find the matrix elements of X and P, we invert Eqs. (7.4.3) and (7.4.4) to obtain

$$X = \left(\frac{\hbar}{2m\omega}\right)^{1/2}(a+a^\dagger) \tag{7.4.28}$$

$$P = i\left(\frac{m\omega\hbar}{2}\right)^{1/2}(a^\dagger - a) \tag{7.4.29}$$

and then use Eqs. (7.4.26) and (7.4.27). The details are left as an exercise. The two basic matrices in this energy basis are

$$a^\dagger \leftrightarrow \begin{array}{c} \\ n=0 \\ n=1 \\ n=2 \\ \cdot \\ \cdot \end{array} \begin{array}{c} \begin{array}{cccc} n=0 & n=1 & n=2 & \ldots \end{array} \\ \begin{bmatrix} 0 & 0 & 0 & \ldots \\ 1^{1/2} & 0 & 0 & \\ 0 & 2^{1/2} & 0 & \\ 0 & 0 & 3^{1/2} & \\ \vdots & & & \end{bmatrix} \end{array} \tag{7.4.30}$$

and its adjoint

$$a \leftrightarrow \begin{bmatrix} 0 & 1^{1/2} & 0 & 0 & \cdots \\ 0 & 0 & 2^{1/2} & 0 & \\ 0 & 0 & 0 & 3^{1/2} & \\ \vdots & & & & \end{bmatrix} \tag{7.4.31}$$

Both matrices can be constructed either from Eqs. (7.4.26) and (7.4.27) or Eqs. (7.4.21) and (7.4.22) combined with our mnemonic involving images of the transformed vectors $a^\dagger|n\rangle$ and $a|n\rangle$. We get the matrices representing X and P by turning to Eqs. (7.4.28) and (7.4.29):

$$X \leftrightarrow \left(\frac{\hbar}{2m\omega}\right)^{1/2} \begin{bmatrix} 0 & 1^{1/2} & 0 & 0 & \cdots \\ 1^{1/2} & 0 & 2^{1/2} & 0 & \\ 0 & 2^{1/2} & 0 & 3^{1/2} & \\ 0 & 0 & 3^{1/2} & 0 & \\ \vdots & & & & \end{bmatrix} \tag{7.4.32}$$

$$P \leftrightarrow i\left(\frac{m\omega\hbar}{2}\right)^{1/2} \begin{bmatrix} 0 & -1^{1/2} & 0 & 0 & \cdots \\ 1^{1/2} & 0 & -2^{1/2} & 0 & \\ 0 & 2^{1/2} & 0 & -3^{1/2} & \\ 0 & 0 & 3^{1/2} & 0 & \\ \vdots & & & & \end{bmatrix} \tag{7.4.33}$$

The Hamiltonian is of course diagonal in its own basis:

$$H \leftrightarrow \hbar\omega \begin{bmatrix} 1/2 & 0 & 0 & 0 & \cdots \\ 0 & 3/2 & 0 & 0 & \\ 0 & 0 & 5/2 & & \\ \vdots & & & & \end{bmatrix} \tag{7.4.34}$$

Equation (7.4.22) also allows us to express all normalized eigenvectors $|n\rangle$ in terms of the ground state $|0\rangle$:

$$|n\rangle = \frac{a^\dagger}{n^{1/2}}|n-1\rangle = \frac{a^\dagger}{n^{1/2}}\frac{a^\dagger}{(n-1)^{1/2}}|n-2\rangle \cdots = \frac{(a^\dagger)^n}{(n!)^{1/2}}|0\rangle \tag{7.4.35}$$

The a and $a^\dagger$ operators greatly facilitate the calculation of the matrix of elements of other operators between oscillator eigenstates. Consider, for example, $\langle 3|X^3|2\rangle$. In the X basis one would have to carry out the following integral:

$$\langle 3|X^3|2\rangle=\left(\frac{m\omega}{\pi\hbar}\right)^{1/2}\left(\frac{1}{2^3 3!}\cdot\frac{1}{2^2 2!}\right)^{1/2}\int_{-\infty}^{\infty}\left\{\exp\left(-\frac{m\omega x^2}{2\hbar}\right)\right.$$
$$\left.\times H_3\left[\left(\frac{m\omega}{\hbar}\right)^{1/2}x\right]x^3\exp\left(-\frac{m\omega x^2}{2\hbar}\right)H_2\left[\left(\frac{m\omega}{\hbar}\right)^{1/2}x\right]\right\}dx$$

whereas in the $|n\rangle$ basis

$$\langle 3|X^3|2\rangle=\left(\frac{\hbar}{2m\omega}\right)^{3/2}\langle 3|(a+a^\dagger)^3|2\rangle$$
$$=\left(\frac{\hbar}{2m\omega}\right)^{3/2}\langle 3|(a^3+a^2a^\dagger+aa^\dagger a+aa^\dagger a^\dagger$$
$$+a^\dagger aa+a^\dagger aa^\dagger+a^\dagger a^\dagger a+a^\dagger a^\dagger a^\dagger)|2\rangle$$

Since a lowers n by one unit and $a^\dagger$ raises it by one unit and we want to go up by one unit from $n=2$ to $n=3$, the only nonzero contribution comes from $a^\dagger a^\dagger a$, $aa^\dagger a^\dagger$, and $a^\dagger aa^\dagger$. Now

$$a^\dagger a^\dagger a|2\rangle=2^{1/2}a^\dagger a^\dagger|1\rangle=2^{1/2}2^{1/2}a^\dagger|2\rangle=2^{1/2}2^{1/2}3^{1/2}|3\rangle$$

$$aa^\dagger a^\dagger|2\rangle=3^{1/2}aa^\dagger|3\rangle=3^{1/2}4^{1/2}a|4\rangle=3^{1/2}4^{1/2}4^{1/2}|3\rangle$$

$$a^\dagger aa^\dagger|2\rangle=3^{1/2}a^\dagger a|3\rangle=3^{1/2}N|3\rangle=3^{1/2}3|3\rangle$$

so that

$$\langle 3|X^3|2\rangle=\left(\frac{\hbar}{2m\omega}\right)^{3/2}[2(3^{1/2})+4(3^{1/2})+3(3^{1/2})]$$

What if we want not some matrix element of X, but the probability of finding the particle in $|n\rangle$ at position x? We can of course fall back on Postulate III, which tells us to find the eigenvectors $|x\rangle$ of the matrix X [Eq. (7.4.32)] and evaluate the inner product $\langle x|n\rangle$. A more practical way will be developed in the next section.

Consider a remarkable feature of the above solution to the eigenvalue problem of H. Usually we work in the X basis and set up the eigenvalue problem (as a differential equation) by invoking Postulate II, which gives the action of X and P in the X basis ($X\to x$, $P\to -i\hbar\, d/dx$). In some cases (the linear potential problem), the P basis recommends itself, and then we use the Fourier-transformed version of Postulate II, namely, $X\to i\hbar\, d/dp$, $P\to p$. In the present case we could not transform this operator assignment to the energy eigenbasis, for to do so we first had to solve for the energy eigenfunctions in the X basis, which was begging the question. Instead we used just the commutation relation $[X, P]=i\hbar$, which follows from Postulate II, but is true in all bases, in particular the energy basis. Since we obtained the complete solution given just this information, it would appear that the essence of Postulate II is just the commutator. This in fact is the case. In other words, we may trade our present Postulate II for a more general version:

> *Postulate II.* The independent variables x and p of classical mechanics now become Hermitian operators X and P defined by the canonical commutator $[X, P]=i\hbar$. Dependent variables $\omega(x, p)$ are given by operators $\Omega=\omega(x\to X, p\to P)$.

To regain our old version, we go to the X basis. Clearly in its own basis $X\to x$. We must then pick P such that $[X, P]=i\hbar$. If we make the conventional choice $P=-i\hbar\, d/dx$, we meet this requirement and arrive at Postulate II as stated earlier. But the present version of Postulate II allows us some latitude in the choice of P, for we can add to $-i\hbar\, d/dx$ any function of x without altering the commutator: the assignment

$$X \xrightarrow[X \text{ basis}]{} x \tag{7.4.36a}$$

$$P \xrightarrow[X \text{ basis}]{} -i\hbar\frac{d}{dx}+f(x) \tag{7.4.36b}$$

is equally satisfactory. Now, it is not at all obvious that in every problem (and not just the harmonic oscillator) the same physics will obtain if we make this our starting point. For example if we project the eigenvalue equation

$$P|p\rangle=p|p\rangle \tag{7.4.37a}$$

onto the X basis, we now get

$$\left[-i\hbar\frac{d}{dx}+f(x)\right]\psi_p(x)=p\psi_p(x) \tag{7.4.37b}$$

from which it follows that $\psi_p(x)$ is no longer a plane wave $\propto e^{ipx/\hbar}$. How can the physics be the same as before? The answer is that the wave function is never measured directly. What we do measure are probabilities $|\langle\omega|\psi\rangle|^2$ for obtaining some result ω when Ω is measured, squares of matrix elements $|\langle\psi_1|\Omega|\psi_2\rangle|^2$, or the eigenvalue spectrum of operators such as the Hamiltonian. In one of the exercises that follows, you will be guided toward the proof that these measurable quantities are in fact left invariant under the change to the nontraditional operator assignment Eq. (7.4.36).

Dirac emphasized the close connection between the commutation rule

$$[X, P]=i\hbar$$

of the quantum operators and the Poisson brackets (PB) of their classical counterparts

$$\{x, p\}=1$$

which allows us to write the defining relation of the quantum operators as

$$[X, P] = i\hbar\{x, p\} = i\hbar \tag{7.4.38}$$

The virtue of this viewpoint is that its generalization to the "quantization" of a system of N degrees of freedom is apparent:

Postulate II (For N Degrees of Freedom). The Cartesian coordinates $x_1, \ldots, x_N$ and momenta $p_1, \ldots, p_N$ of the classical description of a system with N degrees of freedom now become Hermitian operators $X_1, \ldots, X_N$; $P_1, \ldots, P_N$ obeying the commutation rules

$$\begin{aligned}
[X_i, P_j] &= i\hbar\{x_i, p_j\} = i\hbar\delta_{ij} \\
[X_i, X_j] &= i\hbar\{x_i, x_j\} = 0 \\
[P_i, P_j] &= i\hbar\{p_i, p_j\} = 0
\end{aligned} \tag{7.4.39}$$

Similarly $\omega(x, p) \to \omega(x \to X, p \to P) = \Omega$.

[We restrict ourselves to Cartesian coordinates to avoid certain subtleties associated with the quantization of non-Cartesian but canonical coordinates; see Exercise (7.4.10). Once the differential equations are obtained, we may abandon Cartesian coordinates in looking for the solutions.]

It is evident that the generalization provided towards the end of Section 4.2, namely,

$$X_i \xrightarrow[X\text{ basis}]{} x_i$$

$$P_i \xrightarrow[X\text{ basis}]{} -i\hbar\frac{\partial}{\partial x_i}$$

is *a* choice but not *the* choice satisfying the canonical commutation rules, Eq. (7.4.39), for the same reason as in the $N=1$ case.

Given the commutation relations between X and P, the ones among dependent operators follow from the repeated use of the relations

$$[\Omega, \Lambda\Gamma] = \Lambda[\Omega, \Gamma] + [\Omega, \Lambda]\Gamma$$

and

$$[\Omega\Lambda, \Gamma] = \Omega[\Lambda, \Gamma] + [\Omega, \Gamma]\Lambda$$

Since PB obey similar rules (Exercise 2.7.1) except for the lack of emphasis on ordering of the classical variables, it turns out that if

$$\{\omega(x, p), \lambda(x, p)\} = \gamma(x, p)$$

then

$$[\Omega(X, P), \Lambda(X, P)] = i\hbar\Gamma(X, P) \tag{7.4.40}$$

except for differences arising from ordering ambiguities; hence the formal similarity between classical and quantum mechanics, first encountered in Chapter 6.

Although the new form of postulate II provides a general, basis-independent specification of the quantum operators corresponding to classical variables, that is to say for "quantizing," in practice one typically works in the X basis and also ignores the latitude in the choice of P_i and sticks to the traditional one, $P_i = -i\hbar\, \partial/\partial x_i$, which leads to the simplest differential equations. The solution to the oscillator problem, given just the commutation relations (and a little help from Dirac) is atypical.

*Exercise 7.4.1.** Compute the matrix elements of X and P in the $|n\rangle$ basis and compare with the result from Exercise 7.3.4.

*Exercise 7.4.2.** Find $\langle X\rangle$, $\langle P\rangle$, $\langle X^2\rangle$, $\langle P^2\rangle$, $\Delta X \cdot \Delta P$ in the state $|n\rangle$.

*Exercise 7.4.3.** (*Virial Theorem*). The virial theorem in classical mechanics states that for a particle bound by a potential $V(r) = ar^k$, the average (over the orbit) kinetic and potential energies are related by

$$\bar{T} = c(k)\bar{V}$$

when $c(k)$ depends only on k. Show that $c(k) = k/2$ by considering a circular orbit. Using the results from the previous exercise show that for the oscillator ($k = 2$)

$$\langle T\rangle = \langle V\rangle$$

in the quantum state $|n\rangle$.

Exercise 7.4.4. Show that $\langle n|X^4|n\rangle = (\hbar/2m\omega)^2[3 + 6n(n+1)]$.

*Exercise 7.4.5.** At $t = 0$ a particle starts out in $|\psi(0)\rangle = 1/2^{1/2}(|0\rangle + |1\rangle)$. (1) Find $|\psi(t)\rangle$; (2) find $\langle X(0)\rangle = \langle\psi(0)|X|\psi(0)\rangle$, $\langle P(0)\rangle$, $\langle X(t)\rangle$, $\langle P(t)\rangle$; (3) find $\langle\dot{X}(t)\rangle$ and $\langle\dot{P}(t)\rangle$ using Ehrenfest's theorem and solve for $\langle X(t)\rangle$ and $\langle P(t)\rangle$ and compare with part (2).

*Exercise 7.4.6.** Show that $\langle a(t)\rangle = e^{-i\omega t}\langle a(0)\rangle$ and that $\langle a^\dagger(t)\rangle = e^{i\omega t}\langle a^\dagger(0)\rangle$.

Exercise 7.4.7. Verify Eq. (7.4.40) for the case

(1) $\Omega = X, \quad \Lambda = X^2 + P^2$
(2) $\Omega = X^2, \quad \Lambda = P^2$

The second case illustrates the ordering ambiguity.

*Exercise 7.4.8.** Consider the three angular momentum variables in classical mechanics:

$$l_x = yp_z - zp_y$$

$$l_y = zp_x - xp_z$$

$$l_z = xp_y - yp_x$$

(1) Construct L_x, L_y, and L_z, the quantum counterparts, and note that there are no ordering ambiguities.
(2) Verify that $\{l_x, l_y\} = l_z$ [see Eq. (2.7.3) for the definition of the PB].
(3) Verify that $[L_x, L_y] = i\hbar L_z$.

Exercise 7.4.9 (Important). Consider the unconventional (but fully acceptable) operator choice

$$X \to x$$

$$P \to -i\hbar \frac{d}{dx} + f(x)$$

in the X basis.

(1) Verify that the canonical commutation relation is satisfied.
(2) It is possible to interpret the change in the operator assignment as a result of a unitary change of the X basis:

$$|x\rangle \to |\tilde{x}\rangle = e^{ig(X)/\hbar}|x\rangle = e^{ig(x)/\hbar}|x\rangle$$

where

$$g(x) = \int^x f(x')\, dx'$$

First verify that

$$\langle \tilde{x}|X|\tilde{x}'\rangle = x\delta(x - x')$$

i.e.,

$$X \xrightarrow[\text{new } X \text{ basis}]{} x$$

Next verify that

$$\langle \tilde{x}|P|\tilde{x}'\rangle = \left[-i\hbar \frac{d}{dx} + f(x)\right]\delta(x - x')$$

i.e.,

$$P \xrightarrow[\text{new } X \text{ basis}]{} -i\hbar \frac{d}{dx} + f(x)$$

This exercise teaches us that the "X basis" is not unique; given a basis $|x\rangle$, we can get another $|\tilde{x}\rangle$, by multiplying by a phase factor which changes neither the norm nor the orthogonality. The matrix elements of P change with f, the standard choice corresponding to $f=0$. Since the presence of f is related to a change of basis, the invariance of the physics under a change in f (from zero to nonzero) follows. What is novel here is that we are changing from one X basis to another X basis rather than to some other Ω basis. Another lesson to remember is that two different differential operators $\omega(x, -i\hbar\, d/dx)$ and $\omega(x, -i\hbar\, d/dx + f)$ can have the same eigenvalues and a one-to-one correspondence between their eigenfunctions, since they both represent the same abstract operator $\Omega(X, P)$. □

*Exercise 7.4.10.** Recall that we always quantize a system by promoting the Cartesian coordinates $x_1, \ldots, x_N$; and momenta $p_1, \ldots, p_N$ to operators obeying the canonical commutation rules. If non-Cartesian coordinates seem more natural in some cases, such as the eigenvalue problem of a Hamiltonian with spherical symmetry, we first set up the differential equation in Cartesian coordinates and *then* change to spherical coordinates (Section 4.2). In Section 4.2 it was pointed out that if $\mathscr{H}$ is written in terms of non-Cartesian but canonical coordinates $q_1 \ldots q_N$; $p_1 \ldots p_N$; $\mathscr{H}(q_i \to q_i, p_i \to -i\hbar\, \partial/\partial q_i)$ does not generate the correct Hamiltonian H, even though the operator assignment satisfies the canonical commutation rules. In this section we revisit this problem in order to explain some of the subtleties arising in the direct quantization of non-Cartesian coordinates without the use of Cartesian coordinates in intermediate stages.

(1) Consider a particle in two dimensions with

$$\mathscr{H} = \frac{p_x^2 + p_y^2}{2m} + a(x^2 + y^2)^{1/2}$$

which leads to

$$H \to \frac{-\hbar^2}{2m}\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}\right) + a(x^2 + y^2)^{1/2}$$

in the coordinate basis. Since the problem has rotational symmetry we use polar coordinates

$$\rho = (x^2 + y^2)^{1/2}, \qquad \phi = \tan^{-1}(y/x)$$

in terms of which

$$H \xrightarrow[\text{basis}]{\text{coordinate}} \frac{-\hbar^2}{2m}\left(\frac{\partial^2}{\partial \rho^2} + \frac{1}{\rho}\frac{\partial}{\partial \rho} + \frac{1}{\rho^2}\frac{\partial^2}{\partial \phi^2}\right) + a\rho \qquad (7.4.41)$$

Since ρ and ϕ are not mixed up as x and y are [in the $(x^2 + y^2)^{1/2}$ term] the polar version can be more readily solved.

The question we address is the following: why not *start* with $\mathscr{H}$ expressed in terms of polar coordinates and the conjugate momenta

$$p_\rho = \mathbf{e}_\rho \cdot \mathbf{p} = \frac{xp_x + yp_y}{(x^2+y^2)^{1/2}}$$

(where $\mathbf{e}_\rho$ is the unit vector in the radial direction), and

$$p_\phi = xp_y - yp_x \quad \text{(the angular momentum, also called } l_z\text{)}$$

i.e.,

$$\mathscr{H} = \frac{p_\rho^2}{2m} + \frac{p_\phi^2}{2m\rho^2} + a\rho \quad \text{(verify this)}$$

and directly promote all classical variables ρ, p_ρ, ϕ, and p_ϕ to quantum operators obeying the canonical commutations rules? Let's do it and see what happens. If we choose operators

$$P_\rho \to -i\hbar \frac{\partial}{\partial \rho}$$

$$P_\phi \to -i\hbar \frac{\partial}{\partial \phi}$$

that obey the commutation rules, we end up with

$$H \xrightarrow[\text{basis}]{\text{coordinate}} \frac{-\hbar^2}{2m}\left(\frac{\partial^2}{\partial \rho^2} + \frac{1}{\rho^2}\frac{\partial^2}{\partial \phi^2}\right) + a\rho \tag{7.4.42}$$

which disagrees with Eq. (7.4.41). Now this in itself is not serious, for as seen in the last exercise the same physics may be hidden in two different equations. In the present case this isn't true: as we will see, the Hamiltonians in Eqs. (7.4.41) and (7.4.42) do not have the same eigenvalues.‡ We know Eq. (7.4.41) is the correct one, since the quantization procedure in terms of Cartesian coordinates has empirical support. What do we do now?

(2) A way out is suggested by the fact that although the choice $P_\rho \to -i\hbar\, \partial/\partial\rho$ leads to the correct commutation rule, it is not Hermitian! Verify that

$$\begin{aligned}\langle \psi_1 | P_\rho | \psi_2 \rangle &= \int_0^\infty \int_0^{2\pi} \psi_1^* \left(-i\hbar \frac{\partial \psi_2}{\partial \rho}\right) \rho \, d\rho \, d\phi \\ &\neq \int_0^\infty \int_0^{2\pi} \left(-i\hbar \frac{\partial \psi_1}{\partial \rho}\right)^* \psi_2 \rho \, d\rho \, d\phi \\ &= \langle \mathbf{P}_\rho \psi_1 | \psi_2 \rangle\end{aligned}$$

(You may assume $\rho\psi_1^*\psi_2 \to 0$ as $\rho \to 0$ or ∞. The problem comes from the fact that $\rho\, d\rho\, d\phi$ and not $d\rho\, d\phi$ is the measure for integration.)

‡ What we will see is that $P_\rho = -i\hbar\, d/d\rho$, and hence the H constructed with it, are non-Hermitian.

Show, however, that

$$P_\rho \to -i\hbar\left(\frac{\partial}{\partial\rho}+\frac{1}{2\rho}\right) \tag{7.4.43}$$

is indeed Hermitian and also satisfies the canonical commutation rule. The angular momentum $P_\phi \to -i\hbar\,\partial/\partial\phi$ is Hermitian, as it stands, on single-valued functions: $\psi(\rho, \phi) = \psi(\rho, \phi+2\pi)$.

(3) In the Cartesian case we saw that adding an arbitrary $f(x)$ to $-i\hbar\,\partial/\partial x$ didn't have any physical effect, whereas here the addition of a function of ρ to $-i\hbar\,\partial/\partial\rho$ seems important. Why? [Is $f(x)$ completely arbitrary? Mustn't it be real? Why? Is the same true for the $-i\hbar/2\rho$ piece?]

(4) Feed in the new momentum operator P_ρ and show that

$$H \xrightarrow[\text{basis}]{\text{coordinate}} \frac{-\hbar^2}{2m}\left(\frac{\partial^2}{\partial\rho^2}+\frac{1}{\rho}\frac{\partial}{\partial\rho}-\frac{1}{4\rho^2}+\frac{1}{\rho^2}\frac{\partial^2}{\partial\phi^2}\right)+a\rho$$

which still disagrees with Eq. (7.4.41). We have satisfied the commutation rules, chosen Hermitian operators, and yet do not get the right quantum Hamiltonian. The key to the mystery lies in the fact that $\mathscr{H}$ doesn't determine H uniquely since terms of order $\hbar$ (or higher) may be present in H but absent in $\mathscr{H}$. While this ambiguity is present even in the Cartesian case, it is resolved by symmetrization in all interesting cases. With non-Cartesian coordinates the ambiguity is more severe. There *are* ways of constructing H given $\mathscr{H}$ (the path integral formulation suggests one) such that the substitution $P_\rho \to -i\hbar(\partial/\partial\rho + 1/2\rho)$ leads to Eq. (7.4.41). In the present case the quantum Hamiltonian corresponding to

$$\mathscr{H} = \frac{p_\rho^2}{2m}+\frac{p_\phi^2}{2m\rho^2}+a\rho$$

is given by

$$H \xrightarrow[\text{basis}]{\text{coordinate}} \mathscr{H}\left(\rho\to\rho,\ p_\rho\to -i\hbar\left[\frac{\partial}{\partial\rho}+\frac{1}{2\rho}\right];\ \phi\to\phi,\ p_\phi\to -i\hbar\frac{\partial}{\partial\phi}\right)-\frac{\hbar^2}{8m\rho^2} \tag{7.4.44}$$

Notice that the additional term is indeed of nonzero order in $\hbar$.

We will not get into a discussion of these prescriptions for generating H since they finally reproduce results more readily available in the approach we are adopting. □

7.5. Passage from the Energy Basis to the X Basis

It was remarked in the last section that although the $|n\rangle$ basis was ideally suited for evaluating the matrix elements of operators between oscillator eigenstates, the amplitude for finding the particle in a state $|n\rangle$ at the point x could not be readily computed: it seemed as if one had to find the eigenkets $|x\rangle$ of the operators X [Eq. (7.4.32)] and then take the inner product $\langle x|n\rangle$. But there is a more direct way to get $\psi_n(x) = \langle x|n\rangle$.

We start by projecting the equation defining the ground state of the oscillator

$$a|0\rangle = 0 \tag{7.5.1}$$

on the X basis:

$$|0\rangle \to \langle x|0\rangle = \psi_0(x)$$

$$a = \left(\frac{m\omega}{2\hbar}\right)^{1/2} X + i\left(\frac{1}{2m\omega\hbar}\right)^{1/2} P$$

$$\to \left(\frac{m\omega}{2\hbar}\right)^{1/2} x + \left(\frac{\hbar}{2m\omega}\right)^{1/2} \frac{d}{dx} \tag{7.5.2}$$

In terms of $y = (m\omega/\hbar)^{1/2}x$,

$$a = \frac{1}{2^{1/2}}\left(y + \frac{d}{dy}\right) \tag{7.5.3}$$

For later use we also note that (since d/dy is *anti*-Hermitian),

$$a^\dagger = \frac{1}{2^{1/2}}\left(y - \frac{d}{dy}\right) \tag{7.5.4}$$

In the X basis Eq. (7.5.1) then becomes

$$\left(y + \frac{d}{dy}\right)\psi_0(y) = 0 \tag{7.5.5}$$

or

$$\frac{d\psi_0(y)}{\psi_0(y)} = -y\,dy$$

or

$$\psi_0(y) = A_0\,e^{-y^2/2}$$

or

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

or (upon normalizing)

$$=\left(\frac{m\omega}{\pi\hbar}\right)^{1/4}\exp\left(-\frac{m\omega x^2}{2\hbar}\right) \tag{7.5.6}$$

By projecting the equation

$$|n\rangle=\frac{(a^\dagger)^n}{(n!)^{1/2}}|0\rangle$$

onto the X basis, we get the *normalized* eigenfunctions

$$\langle x|n\rangle=\psi_n\left[x=\left(\frac{\hbar}{m\omega}\right)^{1/2}y\right]=\frac{1}{(n!)^{1/2}}\left[\frac{1}{2^{1/2}}\left(y-\frac{d}{dy}\right)\right]^n\left(\frac{m\omega}{\pi\hbar}\right)^{1/4}e^{-y^2/2} \tag{7.5.7}$$

A comparison of the above result with Eq. (7.3.22) shows that

$$H_n(y)=e^{y^2/2}\left(y-\frac{d}{dy}\right)^n e^{-y^2/2} \tag{7.5.8}$$

We now conclude our rather lengthy discussion of the oscillator. If you understand this chapter thoroughly, you should have a good grasp of how quantum mechanics works.

Exercise 7.5.1. Project Eq. (7.5.1) on the P basis and obtain $\psi_0(p)$.

Exercise 7.5.2. Project the relation

$$a|n\rangle=n^{1/2}|n-1\rangle$$

on the X basis and derive the recursion relation

$$H_n'(y)=2nH_{n-1}(y)$$

using Eq. (7.3.22).

Exercise 7.5.3. Starting with

$$a+a^\dagger=2^{1/2}y$$

and

$$(a+a^\dagger)|n\rangle=n^{1/2}|n-1\rangle+(n+1)^{1/2}|n+1\rangle$$

and Eq. (7.3.22), derive the relation

$$H_{n+1}(y) = 2yH_n(y) - 2nH_{n-1}(y)$$

Exercise 7.5.4. Thermodynamics of Oscillators.* The Boltzman formula

$$P(i) = e^{-\beta E(i)}/Z$$

where

$$Z = \sum_i e^{-\beta E(i)}$$

gives the probability of finding a system in a state i with energy $E(i)$, when it is in thermal equilibrium with a reservoir of absolute temperature $T = 1/\beta k$, $k = 1.4 \times 10^{-16}$ ergs/° K; being Boltzman's constant. (The "probability" referred to above is in relation to a classical ensemble of similar systems and has nothing to do with quantum mechanics.)

(1) Show that the thermal average of the system's energy is

$$\bar{E} = \sum_i E(i)P(i) = \frac{-\partial}{\partial\beta} \ln Z$$

(2) Let the system be a classical oscillator. The index i is now continuous and corresponds to the variables x and p describing the state of the oscillator, i.e.,

$$i \to x, p$$

and

$$\sum_i \to \iint dx\, dp$$

and

$$E(i) \to E(x, p) = \frac{p^2}{2m} + \frac{1}{2} m\omega^2 x^2$$

Show that

$$Z_{\text{cl}} = \left(\frac{2\pi}{\beta m\omega^2}\right)^{1/2} \left(\frac{2\pi m}{\beta}\right)^{1/2} = \frac{2\pi}{\omega\beta}$$

and that

$$\bar{E}_{\text{cl}} = \frac{1}{\beta} = kT$$

Note that $\bar{E}_{\text{cl}}$ is independent of m and ω.

(3) For the quantum oscillator the quantum number n plays the role of the index i. Show that

$$Z_{\text{qu}} = e^{-\beta\hbar\omega/2}(1 - e^{-\beta\hbar\omega})^{-1}$$

and

$$\bar{E}_{\text{qu}} = \hbar\omega\left(\frac{1}{2} + \frac{1}{e^{\beta\hbar\omega} - 1}\right)$$

(4) It is intuitively clear that as the temperature T increases (and $\beta = 1/kT$ decreases) the oscillator will get more and more excited and eventually (from the correspondence principle)

$$\bar{E}_{\text{qu}} \xrightarrow[T\to\infty]{} \bar{E}_{\text{cl}}$$

Verify that this is indeed true and show that "large T" means $T \gg \hbar\omega/k$.

(5) Consider a crystal with N_0 atoms, which, for small oscillations, is equivalent to $3N_0$ decoupled oscillators. The mean thermal energy of the crystal $\bar{E}_{\text{crystal}}$ is $\bar{E}_{\text{cl}}$ or $\bar{E}_{\text{qu}}$ summed over all the normal modes. Show that if the oscillators are treated classicaly, the specific heat per atom is

$$C_{\text{cl}}(T) = \frac{1}{N_0}\frac{\partial \bar{E}_{\text{crystal}}}{\partial T} = 3k$$

which is independent of T and the parameters of the oscillators and hence the same for all crystals.‡ This agrees with experiment at high temperatures but not as $T \to 0$. Empirically,

$$\begin{aligned} C(T) &\to 3k \quad (T \text{ large}) \\ &\to 0 \quad (T \to 0) \end{aligned}$$

Following Einstein, treat the oscillators quantum mechanically, asuming for simplicity that they all have the same frequency ω. Show that

$$C_{\text{qu}}(T) = 3k\left(\frac{\theta_E}{T}\right)^2 \frac{e^{\theta_E/T}}{(e^{\theta_E/T} - 1)^2}$$

where $\theta_E = \hbar\omega/k$ is called the *Einstein temperature* and varies from crystal to crystal. Show that

$$C_{\text{qu}}(T) \xrightarrow[T\gg\theta_E]{} 3k$$

$$C_{\text{qu}}(T) \xrightarrow[T\ll\theta_E]{} 3k\left(\frac{\theta_E}{T}\right)^2 e^{-\theta_E/T}$$

Although $C_{\text{qu}}(T) \to 0$ as $T \to 0$, the exponential falloff disagrees with the observed $C(T) \to_{T\to 0} T^3$ behavior. This discrepancy arises from assuming that the frequencies of all

‡ More precisely, for crystals whose atoms behave as point particles with no internal degrees of freedom.

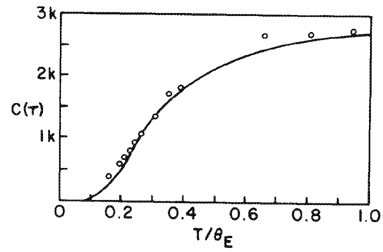

Figure 7.3. Comparison of experiment with Einstein's theory for the specific heat in the case of diamond. (θ_E is chosen to be 1320 K.)

normal modes are equal, which is of course not generally true. [Recall that in the case of two coupled masses we get $\omega_{\mathrm{I}} = (k/m)^{1/2}$ and $\omega_{\mathrm{II}} = (3k/m)^{1/2}$.] This discrepancy was eliminated by Debye.

But Einstein's simple picture by itself is remarkably successful (see Fig. 7.3).