Chapter 14

Harmonic oscillator variables

We now build upon the machinery of the previous chapter, and consider the limit $j \gg 1$. The magnetic quantum number differs by an integer from this

$$m = j - n, \tag{14.1}$$

where we will consider the integer n as finite, so that it is also true that $m \gg 1$. Pictorially, this suggests that $\mathbf{J}$ points almost along the z axis. That is, we suppose $n \ll j$. Now the effect of the raising operator can be written in the form

$$\frac{1}{\hbar} J_+ |jm\rangle = \sqrt{(j-m)(j+m+1)}|jm+1\rangle = \sqrt{n(2j+1-n)}|jm+1\rangle, \tag{14.2}$$

and because j is large compared to n, we approximate this by

$$\frac{1}{\hbar} J_+ |jm\rangle \approx \sqrt{2j}\sqrt{n}|jm+1\rangle. \tag{14.3}$$

Similarly, because

$$\sqrt{(j+m)(j-m+1)} = \sqrt{(2j-n)(n+1)} \approx \sqrt{2j}\sqrt{n+1}, \tag{14.4}$$

we have for the lowering operator

$$\frac{1}{\hbar} J_- |jm\rangle \approx \sqrt{2j}\sqrt{n+1}|jm-1\rangle. \tag{14.5}$$

Now in the first case we recognize that increasing m by 1 decreases n by 1, and in the second case, decreasing m by 1 increases n by 1. Now redefine

$$\frac{1}{\hbar} J_+ = \sqrt{2j}y, \quad \frac{1}{\hbar} J_- = \sqrt{2j}y^\dagger, \tag{14.6}$$

so that Eqs. (14.3) and (14.5) become for very large j

$$y|n\rangle = \sqrt{n}|n-1\rangle, \quad y^\dagger|n\rangle = \sqrt{n+1}|n+1\rangle. \tag{14.7}$$

Further, because

$$\left[\frac{1}{\hbar}J_+, \frac{1}{\hbar}J_-\right] = 2\frac{1}{\hbar}J_z, \tag{14.8}$$

we learn that

$$2j[y, y^\dagger] \approx 2j, \tag{14.9}$$

since the eigenvalue of J_z is

$$\frac{1}{\hbar}J_z' = m = j - n \approx j \tag{14.10}$$

for all the states we are considering. Thus in this large j limit

$$[y, y^\dagger] = 1. \tag{14.11}$$

Look at the equation for $\mathbf{J}^2$, Eq. (13.64):

$$\mathbf{J}^2 = J_-J_+ + J_z^2 + \hbar J_z, \tag{14.12}$$

which for these states becomes, after removing the factor of $\hbar^2$,

$$j(j+1) = 2jy^\dagger y + (j-n)^2 + j - n \approx 2jy^\dagger y + j(j+1) - 2jn, \tag{14.13}$$

where in the last we dropped the terms independent of j. So we conclude that the eigenvalue of $y^\dagger y$ is n:

$$y^\dagger y|n\rangle = n|n\rangle, \tag{14.14}$$

so $|n\rangle$ is the eigenvector of $y^\dagger y$ with eigenvalue n. We can see this directly:

$$y^\dagger y|n\rangle = y^\dagger\sqrt{n}|n-1\rangle = \sqrt{n}y^\dagger|n-1\rangle = \sqrt{n}\sqrt{n}|n\rangle = n|n\rangle. \tag{14.15}$$

This connects to something we already know. Remember how the non-Hermitian operators are constructed:

$$\frac{1}{\hbar}J_+ = \sqrt{2j}y = \frac{1}{\hbar}(J_x + iJ_y), \tag{14.16a}$$

$$\frac{1}{\hbar}J_- = \sqrt{2j}y^\dagger = \frac{1}{\hbar}(J_x - iJ_y). \tag{14.16b}$$

Let us define Hermitian variables q and p by

$$\frac{1}{\hbar}J_x = \sqrt{j}q, \quad \frac{1}{\hbar}J_y = \sqrt{j}p, \tag{14.17}$$

so

$$y = \frac{q+ip}{\sqrt{2}}, \quad y^\dagger = \frac{q-ip}{\sqrt{2}}. \tag{14.18}$$

The commutation relation

$$[y, y^\dagger] = 1 \tag{14.19}$$

implies

$$[q, p] = i. \tag{14.20}$$

We recognize from this that q and p have continuous spectra. We saw the equivalent result at the end of last term, see Chapter 11.

Now the eigenvalue equation

$$y^\dagger y|n\rangle = n|n\rangle, \tag{14.21}$$

implies, because

$$y^\dagger y = \frac{q - ip}{\sqrt{2}}\frac{q + ip}{\sqrt{2}} = \frac{q^2 + p^2}{2} + \frac{i}{2}[q, p] = \frac{q^2 + p^2}{2} - \frac{1}{2}, \tag{14.22}$$

that the eigenvalue of $(q^2 + p^2)/2$ is

$$\left(\frac{q^2 + p^2}{2}\right)' = n + \frac{1}{2}, \tag{14.23}$$

We can now construct the eigenstates, and the wavefunctions. Particularly easy is the $n = 0$ state, for which

$$y|0\rangle = 0, \quad \frac{q + ip}{\sqrt{2}}|0\rangle = 0. \tag{14.24}$$

Multiply this on the left by an eigenstate of q, having eigenvalue q':

$$0 = \langle q'|q + ip|0\rangle = \left(q' + \frac{\partial}{\partial q'}\right)\langle q'|0\rangle. \tag{14.25}$$

Here we used Eq. (11.93),

$$\langle q'|p = \frac{1}{i}\frac{\partial}{\partial q'}\langle q'|, \tag{14.26}$$

which is consistent with the commutation relation

$$[q, p] = i \to \left[q', \frac{1}{i}\frac{\partial}{\partial q'}\right] = i. \tag{14.27}$$

We can immediately solve the differential equation (14.25) for the wavefunction for the lowest state,

$$\langle q'|0\rangle = \psi_0(q') = \frac{1}{\pi^{1/4}}e^{-\frac{1}{2}q'^2}. \tag{14.28}$$

Here the normalization factor has been inserted, so that

$$\langle 0|0\rangle = \int_{-\infty}^{\infty}\langle 0|q'\rangle dq'\langle q'|0\rangle = \int_{-\infty}^{\infty} dq'\psi_0(q')^*\psi_0(q') = 1, \tag{14.29}$$

according to Eq. (11.107). That is,

$$\frac{1}{\sqrt{\pi}}\int_{-\infty}^{\infty} dq'\, e^{-q'^2} = 1. \tag{14.30}$$

See also Eq. (11.111). Equation (14.28) gives the ground-state wavefunction of the harmonic oscillator. We recall that $dq'|\psi_0(q')|^2$ is the probability of finding q' in the interval between q' and $q'+dq'$. So this normalization condition states that the total probability is unity. All other states of the harmonic oscillator can be constructed in terms of this ground-state wavefunction.

What is the wavefunction for the next highest state? Recalling Eq. (14.7), we have

$$|1\rangle = y^\dagger|0\rangle = \frac{q-ip}{\sqrt{2}}|0\rangle. \tag{14.31}$$

Take the q' component of this,

$$\langle q'|1\rangle = \langle q'|\frac{q-ip}{\sqrt{2}}|0\rangle = \frac{1}{\sqrt{2}}\left(q' - \frac{\partial}{\partial q'}\right)\langle q'|0\rangle. \tag{14.32}$$

We already know $\langle q'|0\rangle$ from Eq. (14.28). We can simply do the derivative, or simply remember

$$\left(q' + \frac{\partial}{\partial q'}\right) e^{-q'^2/2} = 0. \tag{14.33}$$

Then we have the wavefunction for the first excited state,

$$\psi_1(q') = \langle q'|1\rangle = \frac{\sqrt{2}}{\pi^{1/4}} q' e^{-\frac{1}{2}q'^2}. \tag{14.34}$$

Now the normalization has emerged automatically. Let us check this: Is

$$\int_{-\infty}^{\infty} dq'|\psi_1(q')|^2 = \frac{2}{\sqrt{\pi}}\int_{-\infty}^{\infty} dq'(q')^2 e^{-q'^2} = 1? \tag{14.35}$$

Indeed, we know

$$\int_{-\infty}^{\infty} dq' e^{-\lambda q'^2} = \sqrt{\frac{\pi}{\lambda}}, \tag{14.36}$$

and by differentiating with respect to λ and then setting $\lambda = 1$ we obtain

$$\int_{-\infty}^{\infty} dq' q'^2 e^{-q'^2} = \frac{\sqrt{\pi}}{2}, \tag{14.37}$$

which establishes Eq. (14.35).

As a second check of this we can use the lowering operator,

$$\frac{q+ip}{\sqrt{2}}|1\rangle = |0\rangle, \tag{14.38}$$

which is equivalent to the differential equation

$$\frac{1}{\sqrt{2}}\left(q'+\frac{\partial}{\partial q'}\right)\psi_1(q')=\psi_0(q'). \tag{14.39}$$

Indeed it is true that

$$\frac{1}{\pi^{1/4}}\left(q'+\frac{\partial}{\partial q'}\right)q'e^{-\frac{1}{2}q'^2}=\frac{1}{\pi^{1/4}}e^{-\frac{1}{2}q'^2}, \tag{14.40}$$

which uses Eq. (14.33).

Now we want to construct the general wavefunction, starting from

$$y^\dagger|n\rangle=\sqrt{n+1}|n+1\rangle, \tag{14.41}$$

or

$$y^\dagger|n-1\rangle=\sqrt{n}|n\rangle, \tag{14.42}$$

which gives the nth state in terms of the $n-1$st state, which in turn can be expressed in terms of the $n-2$nd state, etc. Thus

$$|n\rangle=\frac{1}{\sqrt{n}}\frac{1}{\sqrt{n-1}}y^\dagger y^\dagger|n-2\rangle=\ldots=\frac{1}{\sqrt{n!}}(y^\dagger)^n|0\rangle. \tag{14.43}$$

Alternatively, since

$$y^\dagger=\frac{q-ip}{\sqrt{2}}, \tag{14.44}$$

we have

$$|n\rangle=\frac{1}{\sqrt{2^n n!}}(q-ip)^n|0\rangle. \tag{14.45}$$

Now project this on the q' state:

$$\begin{aligned}\langle q'|n\rangle &= \frac{1}{\sqrt{2^n n!}}\langle q'|(q-ip)^n|0\rangle=\frac{1}{\sqrt{2^n n!}}\left(q'-\frac{\partial}{\partial q'}\right)\langle q'|(q-ip)^{n-1}|0\rangle\\ &= \frac{1}{\sqrt{2^n n!}}\left(q'-\frac{\partial}{\partial q'}\right)^n\langle q'|0\rangle.\end{aligned} \tag{14.46}$$

Since we know the ground-state wavefunction (14.28) we thus have a blueprint for how to construct all the wavefunctions,

$$\psi_n(q')=\frac{(-1)^n}{\sqrt{\pi^{1/2}2^n n!}}\left(\frac{d}{dq'}-q'\right)^n e^{-\frac{1}{2}q'^2}. \tag{14.47}$$

To work this out, think of

$$\frac{d}{dq'}\left[e^{-\frac{1}{2}q'^2}f(q')\right]=e^{-\frac{1}{2}q'^2}\left[\frac{d}{dq'}f(q')-q'f(q')\right], \tag{14.48}$$

so we recognize that

$$e^{-\frac{1}{2}q'^2}\left(\frac{d}{dq'}-q'\right)f(q')=\frac{d}{dq'}\left[e^{-\frac{1}{2}q'^2}f(q')\right]. \tag{14.49}$$

Continuing on, we see

$$\frac{d^2}{dq'^2}\left[e^{-\frac{1}{2}q'^2}f(q')\right] = \frac{d}{dq'}\left[e^{-\frac{1}{2}q'^2}\left(\frac{d}{dq'}-q'\right)f(q')\right] = e^{-\frac{1}{2}q'^2}\left(\frac{d}{dq'}-q'\right)^2 f(q'), \tag{14.50}$$

and in general,

$$\left(\frac{d}{dq'}\right)^n\left[e^{-\frac{1}{2}q'^2}f(q')\right] = e^{-\frac{1}{2}q'^2}\left(\frac{d}{dq'}-q'\right)^n f(q'). \tag{14.51}$$

Let $f(q') = e^{-q'^2/2}$; then we have

$$\left(\frac{d}{dq'}\right)^n e^{-q'^2} = e^{-\frac{1}{2}q'^2}\left(\frac{d}{dq'}-q'\right)^n e^{-\frac{1}{2}q'^2}, \tag{14.52}$$

and the wavefunction has the form

$$\psi_n(q') = \frac{(-1)^n}{\sqrt{\pi^{1/2}2^n n!}}e^{\frac{1}{2}q'^2}\left(\frac{d}{dq'}\right)^n e^{-q'^2}. \tag{14.53}$$

Now let us make contact with some 19th century mathematics. We recall that

$$\left(\frac{d}{dq'}\right)^n e^{-q'^2} = e^{-q'^2} \times \text{polynomial of order } n \text{ in } q'. \tag{14.54}$$

The standard definition for the Hermite polynomial $H_n(q')$ is

$$(-1)^n\left(\frac{d}{dq'}\right)^n e^{-q'^2} = e^{-q'^2}H_n(q'). \tag{14.55}$$

Thus our nth wavefunction is

$$\psi_n(q') = \frac{1}{\sqrt{\pi^{1/2}2^n n!}}H_n(q')e^{-\frac{1}{2}q'^2}. \tag{14.56}$$

We already know the first two H_n's, from ψ_0 and ψ_1 we find

$$H_0(q') = 1, \quad H_1(q') = 2q'. \tag{14.57}$$

And from the definition,

$$\left(\frac{d}{dq'}\right)^2 e^{-q'^2} = \frac{d}{dq'}\left(-2q'e^{-q'^2}\right) = (4q'^2-2)e^{-q'^2}, \tag{14.58}$$

so

$$H_2(q') = 4q'^2 - 2. \tag{14.59}$$

Figure 14.1 shows how these wavefunctions look. Notice that the $n = 0$ wavefunction is even, and has no zeros. The $n = 1$ wavefunction is odd, and vanishes once at $q' = 0$. The $n = 2$ wavefunction is again even, but has zeros

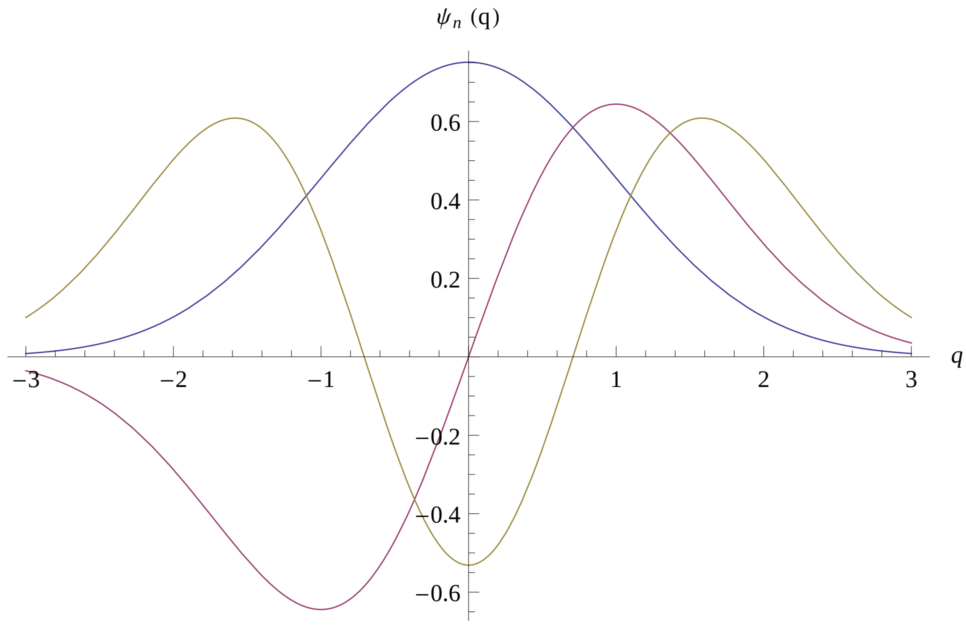

Figure 14.1: The lowest three wavefunctions of the harmonic oscillator, corresponding to the energies $E_0 = \hbar\omega/2$, $E_1 = 3\hbar\omega/2$, and $5\hbar\omega/2$.

at $q' = \pm 1/\sqrt{2}$. In general, ψ_n has n zeroes. These wavefunctions have to be mutually orthonormal:

$$\langle n|n'\rangle = \int_{-\infty}^{\infty} dq' \psi_n(q')^* \psi_{n'}(q') = \delta_{nn'}. \tag{14.60}$$

Since ψ_0 is positive everywhere, it follows that ψ_1 must change sign; since ψ_2 must be orthogonal to both ψ_0 and ψ_1, it must have a more complicated structure.

14.1 Physical variables; Uncertainty principle

The physical harmonic oscillator is described by the Hamiltonian

$$\hat{H} = \frac{\hat{p}^2}{2m} + \frac{1}{2} m\omega^2 \hat{q}^2. \tag{14.61}$$

Here m is the mass and ω is the frequency of the oscillator. We want to relate this to what we did above, where

$$H = \frac{1}{2}p^2 + \frac{1}{2}q^2. \tag{14.62}$$

Since the latter has eigenvalues $n+1/2$, which has no energy scale, the energies should be related by

$$\hat{H} = H\hbar\omega, \tag{14.63}$$

since the energy scale of the oscillator is $\hbar\omega$. Thus,

$$\hat{p} = (m\hbar\omega)^{1/2} p, \quad \hat{q} = \left(\frac{\hbar}{m\omega}\right)^{1/2} q. \tag{14.64}$$

Thus the energies of the physical harmonic oscillator are

$$E_n = \left(n + \frac{1}{2}\right)\hbar\omega, \tag{14.65}$$

and the canonical commutation relations for the physical position and momentum operators are

$$[\hat{q}, \hat{p}] = i\hbar. \tag{14.66}$$

Note that this means, on an eigenstate of position,

$$\langle \hat{q}'|\hat{q} = \frac{\hbar}{i}\frac{\partial}{\partial \hat{q}'}\langle \hat{q}'|. \tag{14.67}$$

From Eq. (14.66) we can derive Heisenberg's uncertainty principle. (This derivation appeared on the Final Exam for Physics 3803; for convenience we repeat it here.) Recall that in homework last term we proved the Cauchy-Schwartz inequality, for any two vectors:

$$|\langle 1|2\rangle|^2 \le \langle 1|1\rangle\langle 2|2\rangle. \tag{14.68}$$

Suppose we have two Hermitian operators, q and p that satisfy the Heisenberg commutation relation

$$[q, p] = i\hbar. \tag{14.69}$$

Suppose $|\ \rangle$ is some state in which the average values of q and p are $\bar{q}$ and $\bar{p}$,

$$\bar{q} = \langle\ |q|\ \rangle, \quad \bar{p} = \langle\ |p|\ \rangle. \tag{14.70}$$

Since these average values are numbers, it is also true that

$$[q - \bar{q}, p - \bar{p}] = i\hbar. \tag{14.71}$$

Then

$$\begin{aligned} i\hbar &= \langle [q-\bar{q}, p-\bar{p}]\rangle = \langle\ |(q-\bar{q})(p-\bar{p})|\ \rangle - \langle\ |(p-\bar{p})(q-\bar{q})|\ \rangle \\ &= \langle\ |(q-\bar{q})(p-\bar{p})|\ \rangle - \langle\ |(q-\bar{q})(p-\bar{p})|\ \rangle^* \\ &= 2i\mathrm{Im}\langle\ |(q-\bar{q})(p-\bar{p})|\ \rangle. \end{aligned} \tag{14.72}$$

Now use Cauchy-Schwartz (14.68) for the states

$$|1\rangle = (q-\bar{q})|\ \rangle, \quad |2\rangle = (p-\bar{p})|\ \rangle, \tag{14.73}$$

$$\begin{aligned}\langle 1|1\rangle\langle 2|2\rangle &= \langle\ |(q-\bar{q})^2|\ \rangle\langle\ |(p-\bar{p})^2|\ \rangle \\ &\geq |\langle 1|2\rangle|^2 = |\langle\ |(q-\bar{q})(p-\bar{p})|\ \rangle|^2 \\ &= (\mathrm{Re}\langle\ |(q-\bar{q})(p-\bar{p})|\ \rangle)^2 + (\mathrm{Im}\langle\ |(q-\bar{q})(p-\bar{p})|\ \rangle)^2 \\ &\geq (\mathrm{Im}\langle\ |(q-\bar{q})(p-\bar{p})|\ \rangle)^2 = \left(\frac{\hbar}{2}\right)^2,\end{aligned} \tag{14.74}$$

which proves

$$\Delta q \Delta p \geq \frac{\hbar}{2}, \tag{14.75}$$

where the rms fluctuations in position and momentum are defined by

$$(\Delta q)^2 = \langle\ |(q-\bar{q})^2|\ \rangle = \langle\ |q^2|\ \rangle - \langle\ |q|\ \rangle^2, \tag{14.76a}$$

$$(\Delta p)^2 = \langle\ |(p-\bar{p})^2|\ \rangle = \langle\ |p^2|\ \rangle - \langle\ |p|\ \rangle^2. \tag{14.76b}$$