Lecture 12

The harmonic oscillator

12.1 Introduction

In this chapter, we are going to find explicitly the eigenfunctions and eigenvalues for the time-independent Schrödinger equation for the one-dimensional harmonic oscillator. We have already described the solutions in Chap. 3.

Recall that the TISE for the 1-dimensional quantum harmonic oscillator is

$$\left[\frac{\hat{P}^2}{2m} + \frac{1}{2}m\omega^2\hat{X}^2\right]u_n(x) = E_n u_n(x)\,,$$

which we write in Dirac notation as

$$\hat{H} \left| n \right\rangle = E_n \left| n \right\rangle$$

We have denoted by $|n\rangle$ the ket associated to the eigenfunctions $u_n(x)$.

12.2 Factorizing the Hamiltonian

The Hamiltonian for the harmonic oscillator is:

$$\hat{H} = \frac{\hat{P}^2}{2m} + \frac{1}{2}m\omega^2 \hat{X}^2.$$
(12.1)

Let us factor out $\hbar\omega$, and rewrite the Hamiltonian as:

$$\hat{H} = \hbar\omega \left[\frac{\hat{P}^2}{2m\hbar\omega} + \frac{m\omega}{2\hbar} \hat{X}^2 \right] \,. \tag{12.2}$$

Checking the dimensions of the constants, you can readily verify that:

$$[\hbar\omega] = \text{energy}, \quad [2m\omega\hbar] = \text{momentum}^2, \quad \left[\frac{2\hbar}{m\omega}\right] = \text{length}^2.$$
 (12.3)

Introducing the dimensionless quantities:

$$\hat{\xi} = \sqrt{\frac{m\omega}{2\hbar}} \hat{X}, \qquad (12.4)$$

$$\hat{\eta} = \frac{P}{\sqrt{2m\hbar\omega}}\,,\tag{12.5}$$

the Hamiltonian becomes:

$$\hat{H} = \hbar\omega \left[\hat{\eta}^2 + \hat{\xi}^2\right].$$
(12.6)

12.2. FACTORIZING THE HAMILTONIAN

The operators $\hat{\xi}$ and $\hat{\eta}$ are simply the position and the momentum operators rescaled by some real constants; therefore both of them are Hermitean. Their commutation relation can be easily computed using the canonical commutation relations:

$$\left[\hat{\xi},\hat{\eta}\right] = \frac{1}{2\hbar} \left[\hat{X},\hat{P}\right] = \frac{i}{2}.$$
(12.7)

If $\hat{\xi}$ and $\hat{\eta}$ were commuting variables, we would be tempted to factorize the Hamiltonian as:

$$\hat{H} = \hbar\omega \left(\hat{\xi} + i\hat{\eta}\right) \left(\hat{\xi} - i\hat{\eta}\right) \,. \tag{12.8}$$

We must be careful here, because the operators do not commute. So let us introduce:

$$\begin{cases} \hat{a} = \hat{\xi} + i\hat{\eta}, \\ \hat{a}^{\dagger} = \hat{\xi} - i\hat{\eta}; \end{cases}$$
(12.9)

the expressions for \hat{a} and \hat{a}^{\dagger} in terms of \hat{X} and \hat{P} are:

$$\hat{a} = \sqrt{\frac{m\omega}{2\hbar}} \hat{X} + \frac{i}{\sqrt{2m\omega\hbar}} \hat{P} \\ \hat{a}^{\dagger} = \sqrt{\frac{m\omega}{2\hbar}} \hat{X} - \frac{i}{\sqrt{2m\omega\hbar}} \hat{P}$$

We can then compute

$$\hat{a}\hat{a}^{\dagger} = \hat{\xi}^2 + i\left[\hat{\eta}, \hat{\xi}\right] + \hat{\eta}^2,$$
 (12.10)

$$\hat{a}^{\dagger}\hat{a} = \hat{\xi}^2 - i\left[\hat{\eta}, \hat{\xi}\right] + \hat{\eta}^2.$$
 (12.11)

Summing the two equations above:

$$\widehat{H} = \frac{\hbar\omega}{2} \left(\hat{a}\hat{a}^{\dagger} + \hat{a}^{\dagger}\hat{a} \right)$$
(12.12)

Subtracting the same two equations yields the commutation relation between \hat{a} and \hat{a}^{\dagger} :

$$\left[\hat{a}, \hat{a}^{\dagger}\right] = 1$$
(12.13)

This commutation relations plays an important role in the rest of this chapter.

An alternative, and more useful, expression for \hat{H} is

$$\hat{H} = \left(\hat{a}^{\dagger}\hat{a} + \frac{1}{2}\right)\hbar\omega \qquad (12.14)$$

12.3 Creation and annihilation

We are now going to find the eigenvalues of \hat{H} using the operators \hat{a} and \hat{a}^{\dagger} . First let us compute the commutators $[\hat{H}, \hat{a}]$ and $[\hat{H}, \hat{a}^{\dagger}]$:

$$[\hat{H}, \hat{a}] = \left[\left(\hat{a}^{\dagger}\hat{a} + \frac{1}{2}\right)\hbar\omega, \hat{a}\right] = \hbar\omega[\hat{a}^{\dagger}\hat{a}, \hat{a}] \quad \text{since} \quad \left[\frac{1}{2}, \hat{a}\right] = 0.$$

Now

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

so that we obtain

$$\left[\hat{H},\hat{a}\right] = -\hbar\omega\hat{a} \qquad (12.15)$$

Similarly

$$[\hat{H}, \hat{a}^{\dagger}] = \left[\left(\hat{a}^{\dagger} \hat{a} + \frac{1}{2} \right) \hbar \omega, \hat{a}^{\dagger} \right] = \hbar \omega [\hat{a}^{\dagger} \hat{a}, \hat{a}^{\dagger}] \quad \text{since} \quad \left[\frac{1}{2}, \hat{a}^{\dagger} \right] = 0$$

and

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

so that we obtain

$$\left[\hat{H}, \hat{a}^{\dagger}\right] = \hbar \omega \hat{a}^{\dagger}.$$
(12.16)

Let us now compute:

$$\hat{H}(\hat{a}|n\rangle) = \hat{\hat{a}}\hat{H}|n\rangle + \left[\hat{H},\hat{a}\right]|n\rangle, \qquad (12.17)$$

$$= E_n \hat{a} |n\rangle - \hbar \omega \hat{a} |n\rangle, \qquad (12.18)$$

$$= (E_n - \hbar\omega) \left(\hat{a} | n \right) \right). \tag{12.19}$$

We have found an eigenvalue equation: it states that $\hat{a} |n\rangle$ is an eigenfunction of \hat{H} belonging to the eigenvalue $(E_n - \hbar \omega)$, unless $\hat{a} |n\rangle \equiv 0$. We say that the operator \hat{a} is a *lowering operator*; its action on an energy eigenstate is to turn it into another energy eigenstate of lower energy. It is also called an *annihilation operator*, because it removes one quantum of energy $\hbar \omega$ from the system.

Similarly it is straightforward to show that

$$\hat{H}\hat{a}^{\dagger} \left| n \right\rangle = (E_n + \hbar \omega) \hat{a}^{\dagger} \left| n \right\rangle \,,$$

which says that $\hat{a}^{\dagger} |n\rangle$ is an eigenfunction of \hat{H} belonging to the eigenvalue $(E_n + \hbar\omega)$, unless $\hat{a}^{\dagger} |n\rangle \equiv 0$. We say that the operator \hat{a}^{\dagger} is a *raising operator*; its action on an energy eigenstate is to turn it into another energy eigenstate of higher energy. It is also called an *creation operator*, because it adds one quantum of energy $\hbar\omega$ to the system.

110

12.4. EIGENSYSTEM

We can summarise these results by denoting the states of energy $E_n\pm\hbar\omega$ by $|n\pm1\rangle$ and writing

$$\hat{a} |n\rangle = c_n |n-1\rangle$$
 and $\hat{a}^{\dagger} |n\rangle = d_n |n+1\rangle$,

where c_n and d_n are constants of proportionality (NOT eigenvalues!) and

$$\begin{split} \dot{H} & |n-1\rangle &= E_{n-1} & |n-1\rangle = (E_n - \hbar\omega) & |n-1\rangle \\ \dot{H} & |n+1\rangle &= E_{n+1} & |n+1\rangle = (E_n + \hbar\omega) & |n+1\rangle \,. \end{split}$$

12.4 Eigensystem

12.4.1 Eigenvalues

It should be clear that repeated application of the lowering operator, \hat{a} , generates states of successively lower energy ad infinitum *unless there is a state of lowest energy*; application of the operator to such a state must yield zero identically (because otherwise we would be able to generate another state of lower energy still, a contradiction).

Is there such a state? The answer is yes because the Hamiltonian can only have positive eigenvalues. Consider the expectation value of \hat{H} in an arbitrary state $|\Psi\rangle$:

$$\langle \hat{H} \rangle = \langle \frac{\hat{p}^2}{2m} \rangle + \langle \frac{1}{2}m\omega^2 x^2 \rangle \,,$$

and both terms on the right hand side are non-negative. Thus there cannot be any states of negative energy.

We denote the state of lowest energy, or ground state, by $|0\rangle$. Then since there cannot be a state of lower energy,

$$\hat{a} \left| 0 \right\rangle = 0$$
.

Applying the Hamiltonian to this state we see that

$$\hat{H} \left| 0 \right\rangle = \hbar \omega \left(\hat{a}^{\dagger} \hat{a} + \frac{1}{2} \right) \left| 0 \right\rangle = \frac{1}{2} \hbar \omega \left| 0 \right\rangle \equiv E_0 \left| 0 \right\rangle.$$

Thus we have found the ground state energy: $E_0 = \frac{1}{2}\hbar\omega$. Application of the raising operator to the ground state generates the state $|1\rangle$ with energy $E_1 = \frac{3}{2}\hbar\omega$, whilst *n* applications of the raising operator generates the state $|n\rangle$ with energy $(n + \frac{1}{2})\hbar\omega$, so that

$$E_n = (n + \frac{1}{2})\hbar\omega$$
 $n = 0, 1, 2, 3, \dots$

which is the previously quoted result for the energy eigenvalues of the 1-dimensional oscillator!

12.4.2 Normalisation of Eigenstates

Requiring that both $|n\rangle$ and $|n-1\rangle$ be normalised enables us to determine the constant of proportionality c_n . Consider

$$\langle n|\hat{a}^{\dagger}\hat{a}|n\rangle = c_n \langle n|\hat{a}^{\dagger}|n-1\rangle \quad \text{from property of } \hat{a} = c_n \langle n-1|\hat{a}|n\rangle^* \quad \text{from definition of } \dagger = c_n c_n^* \langle n-1|n-1\rangle^* \quad \text{from property of } \hat{a} = |c_n|^2 \quad \text{since } \langle n-1|n-1\rangle^* = 1 \,.$$

We can evaluate the left-hand side if we note that $\hat{a}^{\dagger}\hat{a} = \left(\hat{H}/\hbar\omega\right) - \frac{1}{2}$, giving

$$\langle n|\hat{a}^{\dagger}\hat{a}|n\rangle = n \langle n|n\rangle = n$$
.

Thus $|c_n|^2 = n$ and if we choose the phase so that c_n is real we can write

$$c_n = \sqrt{n}$$
.

A similar calculation shows that

$$\langle n|\hat{a}\hat{a}^{\dagger}|n\rangle = |d_n|^2 = (n+1),$$

so that if we again choose the phase so that d_n is real we obtain

$$d_n = \sqrt{n+1} \, .$$

In summary then we have

$$\hat{a} \left| n \right\rangle = \sqrt{n} \left| n - 1 \right\rangle$$
 and $\hat{a}^{\dagger} \left| n \right\rangle = \sqrt{n+1} \left| n + 1 \right\rangle$

12.4.3 Wave functions

Finally let us show that we can reproduce the analytic expression for the eigenfunctions of the energy.

The ground state is defined by the relation:

$$\hat{a}|0\rangle = 0. \tag{12.20}$$

We can rewrite the equation above as a differential operator acting on the wave function of the ground state $u_0(x)$:

$$\hat{a}u_0(x) = \left[\sqrt{\frac{m\omega}{2\hbar}}\,\hat{X} + \frac{i}{\sqrt{2m\omega\hbar}}\,\hat{P}\right]u_0(x) \tag{12.21}$$

$$= \left[\sqrt{\frac{m\omega}{2\hbar}} x + \frac{\hbar}{\sqrt{2m\omega}} \frac{d}{dx}\right] u_0(x) \tag{12.22}$$

$$= 0.$$
 (12.23)

12.5. SUMMARY

Hence:

$$\frac{d}{dx}u_0(x) = -\sqrt{\frac{2m\omega}{\hbar}}\sqrt{\frac{m\omega}{2\hbar}}xu_0(x)$$
(12.24)

$$= -\frac{m\omega}{\hbar} x u_0(x) \tag{12.25}$$

$$= -\alpha^2 x u_0(x) , \qquad (12.26)$$

where $\alpha^2 = m\omega/\hbar$. The solution of the equation above is the Gaussian that we have already seen in Chap. 3:

$$u_0(x) = C_0 \exp[-\alpha^2 x^2/2]. \qquad (12.27)$$

Every other eigenfunctions is obtained by repeatedly applying the creation operator \hat{a}^{\dagger} to ground state:

$$u_n(x) = \frac{1}{\sqrt{n!}} \left(\hat{a}^{\dagger} \right)^n u_0(x) \,. \tag{12.28}$$

Remember that \hat{a}^{\dagger} is just a differential operator acting on wave functions. Check that you can reproduce the wave functions for the first and second excited states of the harmonic oscillator.

12.5 Summary

As usual, we summarize the main concepts introduced in this lecture.

- Raising and lowering operators; factorization of the Hamitonian.
- Commutation relations and interpretation of the raising and lowering operators.
- Existence of the ground states, construction and normalization of the excited states. Eigenvalues of the Hamiltonian.
- Construction of the wave functions.