A Matrix Representation of the Harmonic Oscillator

Having derived a lot of formalism of quantum mechanics, it is useful to go back and apply it to some of the problems we have solved previously. The harmonic oscillator, because of its algebraic method of solution, is a particularly neat case (Griffiths Problem 3.33.)

The stationary states of the harmonic oscillator (i.e. the eigenstates of $\hat{H} = \dfrac{\hat{p}^2}{2M} + \frac{1}{2}M\omega^2 x^2$) are

$$|n\rangle = \psi_n(x) = \left(\frac{M\omega}{\pi\hbar}\right)^{1/2} \frac{1}{\sqrt{2^n n!}} H_n(\xi) e^{-\xi^2/2} \text{ where } \xi = \sqrt{\frac{M\omega}{\hbar}}\,x. \qquad (n=0,1,2,...) \qquad (1)$$

(I am using M for the particle mass, since I will later use m as an index.) The eigenfunctions can be generated using the “ladder operators”

$$a_\pm = \frac{1}{\sqrt{2M\hbar\omega}}(\mp i\hat{p} + M\omega\hat{x}), \qquad \text{Griffiths [2.47]} \qquad (2)$$

which have the following effects on the normalized eigenfunctions:

$$a_+|n\rangle = \sqrt{n+1}\,|n+1\rangle, \qquad a_-|n\rangle = \sqrt{n}\,|n-1\rangle \qquad [2.66] \qquad (3)$$

The matrix representing an operator can be calculated either by determining its effects on the column matrix of components (Eq. [A.33]), or – for an orthonormal basis – applying Eq. [A.35]: $T_{ij} = \langle i|\hat{T}|j\rangle$. In the basis $|n\rangle$, the operators a_+ and a_- have the following matrix representations:

$$\boldsymbol{a}_+ = \begin{pmatrix} 0 & 0 & 0 & 0 & \cdots \\ 1 & 0 & 0 & 0 & \cdots \\ 0 & \sqrt{2} & 0 & 0 & \cdots \\ \vdots & & & & \end{pmatrix} \qquad \boldsymbol{a}_- = \begin{pmatrix} 0 & 1 & 0 & 0 & \cdots \\ 0 & 0 & \sqrt{2} & 0 & \cdots \\ 0 & 0 & 0 & \sqrt{3} & \cdots \\ \vdots & & & & \end{pmatrix} \qquad (4)$$

Note that the matrices representing a_+ and a_- are not hermitian matrices, but they are hermitian conjugates of each other. It is also easy to show (using (3)) that the operators themselves form a hermitian conjugate pair, i.e. $\langle n|a_+m\rangle = \langle a_-n|m\rangle$ for any basis vectors and hence for any vectors in the solution space.

The matrix representing the Hamiltonian operator is (of course) diagonal in the basis of its eigenvectors:

$$\boldsymbol{H} = \hbar\omega \begin{pmatrix} 1/2 & 0 & 0 & \cdots \\ 0 & 3/2 & 0 & \cdots \\ 0 & 0 & 5/2 & \cdots \\ \vdots & & & \end{pmatrix} . \qquad (5)$$

What about the matrices representing the operators $\hat{x}$ and $\hat{p}$? Since the basis is orthonormal, we can apply Eq. [A.35]: $T_{ij} = \langle i|\hat{T}|j\rangle$. Calculating these matrix elements directly from the basis functions would involve evaluating a lot of unpleasant integrals, but there is a much simpler method. Taking the sum and difference of the equations [2.47], we find [2.69]

$$\hat{x} = \sqrt{\frac{\hbar}{2M\omega}}(a_+ + a_-) \quad \text{and} \quad \hat{p} = i\sqrt{\frac{M\hbar\omega}{2}}(a_+ - a_-). \qquad (6)$$

Consider the matrix $\boldsymbol{X}$ which represents the operator $\hat{x}$. The matrix element (row n, column m) is given by

$$\boldsymbol{X}_{nm} = \langle n\,|\,x\,|\,m\rangle = \sqrt{\tfrac{\hbar}{2M\omega}}\left\{\langle n\,|\,a_+\,|\,m\rangle + \langle n\,|\,a_-\,|\,m\rangle\right\} = \sqrt{\tfrac{\hbar}{2M\omega}}\left\{\sqrt{m+1}\langle n\,|\,m+1\rangle + \sqrt{m}\langle n\,|\,m-1\rangle\right\}. \quad (7)$$

Note that the numbering of rows and columns begins with 0, not 1. The first term vanishes unless the column number m is equal to the row number (n) minus 1, in which case the constant $\sqrt{m+1}$ is equal to the square root of the row number. The second term vanishes unless the column number m is equal to the row number (n) plus 1, in which case the constant $\sqrt{m}$ is equal to the square root of the column number. Thus,

$$\boldsymbol{X} = \sqrt{\tfrac{\hbar}{2M\omega}}\begin{pmatrix} 0 & 1 & 0 & 0 & 0 & \cdots \\ 1 & 0 & \sqrt{2} & 0 & 0 & \cdots \\ 0 & \sqrt{2} & 0 & \sqrt{3} & 0 & \cdots \\ 0 & 0 & \sqrt{3} & 0 & \sqrt{4} & \cdots \\ \vdots & & & & & \end{pmatrix}. \quad (8)$$

Alternately, this matrix can be constructed directly from the matrices of (4) using relation (6). The matrix $\boldsymbol{X}$ is clearly Hermitian ($\boldsymbol{X}^\dagger = \boldsymbol{X}$), as it must be because the operator $\hat{x}$ represents an observable.

The matrix representing the observable x^2 can be constructed by applying Eq. (6) twice:

$$(x^2)_{op} = \hat{x}\hat{x} = \tfrac{\hbar}{2M\omega}(a_+^2 + a_-^2 + a_+a_- + a_-a_+) = \tfrac{\hbar}{2M\omega}(a_+^2 + a_-^2 + \tfrac{2\hat{H}}{\hbar\omega}), \quad (9)$$

where the second relationship follows from Griffiths [2.53] and [2.56]. Applying relations (3) twice, we obtain

$$\begin{aligned}\langle n\,|\,x^2\,|\,m\rangle &= \tfrac{\hbar}{2M\omega}\left\{\langle n\,|\,a_+a_+\,|\,m\rangle + \langle n\,|\,a_-a_-\,|\,m\rangle + \tfrac{2}{\hbar\omega}\langle n\,|\,\hat{H}\,|\,m\rangle\right\} \\ &= \tfrac{\hbar}{2M\omega}\left\{\sqrt{(m+1)(m+2)}\,\langle n\,|\,m+2\rangle + \sqrt{m(m-1)}\,\langle n\,|\,m-2\rangle + \tfrac{2E_m}{\hbar\omega}\langle n\,|\,m\rangle\right\}.\end{aligned} \quad (10)$$

Using the fact that $E_n = (n+½)\hbar\omega$, the matrix representing x^2 becomes

$$\boldsymbol{X}^2 = \tfrac{\hbar}{2M\omega}\begin{pmatrix} 1 & 0 & \sqrt{2} & 0 & 0 & \cdots \\ 0 & 3 & 0 & \sqrt{6} & 0 & \cdots \\ \sqrt{2} & 0 & 5 & 0 & \sqrt{12} & \cdots \\ 0 & \sqrt{6} & 0 & 7 & 0 & \cdots \\ 0 & 0 & \sqrt{12} & 0 & 9 & \cdots \\ \vdots & & & & & \end{pmatrix}, \quad (11)$$

which can also be obtained by squaring the matrix representing x (Try it! Although the matrix is infinite-dimensional, there are only 2 non-zero elements in each row or column, so the pattern becomes simple.)

The diagonal entries of $\boldsymbol{X}^2$ have a particular meaning. Recalling the definition of expectation value ($\langle \hat{O} \rangle = \langle \Psi | \hat{O} | \Psi \rangle$ for any operator $\hat{O}$ in state $|\Psi\rangle$), we see that each diagonal element of the matrix is equal to the expectation value of the operator in the corresponding basis state. Thus x^2 has the expectation value $\langle x^2 \rangle = \frac{1}{M\omega^2}\frac{2n+1}{2}\hbar\omega = \frac{1}{M\omega^2}E_n$ in state n.

Recall that for the harmonic oscillator the potential energy is given as $V(x) = ½M\omega^2 x^2$. Thus the matrix representing $V(x)$ is proportional to $\boldsymbol{X}^2$, and the expectation value of the potential energy is given by

$$\langle V(x) \rangle = ½M\omega^2 \langle x^2 \rangle = ½E_n \quad . \tag{12}$$

A similar analysis can be carried out to construct the matrix representation of the operators for the momentum p, p^2, and kinetic energy T, using (6) to write the momentum operator in terms of the ladder operators.

Exercise: Do this, and show that the matrix $\boldsymbol{P}$ is Hermitian.

The analysis of the matrix $\boldsymbol{P}^2$ shows that the expectation value of the kinetic energy T is also equal to half the total energy:

$$\langle V \rangle = \langle T \rangle = ½\langle E \rangle. \tag{13}$$

This same relationship is also true for the *classical* harmonic oscillator if we take the average over a full cycle of oscillation. (Remember that the average of $\sin^2(\omega t)$ over a full cycle is ½.) Equation (13) is a special case of the so-called "virial theorem" (Griffiths [3.97], Problem 3.31)

$$2\langle T \rangle = \langle x \frac{dV}{dx} \rangle \ , \tag{14}$$

which is true for any stationary state, and which is one of the many useful results which can be derived from Griffiths's Eq. [3.71]:

$$\frac{d}{dt}\langle Q \rangle = \frac{i}{\hbar}\langle [\hat{H}, \hat{Q}] \rangle + \langle \frac{\partial Q}{\partial t} \rangle. \tag{15}$$