

## HARMONIC OSCILLATOR: MATRIX ELEMENTS

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References: Griffiths, David J. (2005), *Introduction to Quantum Mechanics*, 2nd Edition; Pearson Education - Problem 3.33.

Shankar, R. (1994), *Principles of Quantum Mechanics*, Plenum Press. Section 7.4, Exercise 7.4.1.

In analyzing the harmonic oscillator, we used the raising and lowering operators to calculate  $\langle x \rangle$  and  $\langle p \rangle$ , finding that they are both zero for all stationary states. These quantities are really the diagonal elements of the matrices  $X$  and  $P$ . That is

$$\langle x \rangle_{nn} = \langle n|x|n \rangle \quad (1)$$

$$= X_{nn} \quad (2)$$

We can use the same technique to calculate the off-diagonal elements.

We review the equations involving the raising and lowering operators first:

$$x = \sqrt{\frac{\hbar}{2m\omega}}(a_+ + a_-) \quad (3)$$

$$p = i\sqrt{\frac{\hbar m\omega}{2}}(a_+ - a_-) \quad (4)$$

$$a_+ \psi_n = \sqrt{n+1} \psi_{n+1} \quad (5)$$

$$a_- \psi_n = \sqrt{n} \psi_{n-1} \quad (6)$$

The general matrix elements for the operator  $x$  can then be calculated:

$$\langle n|x|n' \rangle = \sqrt{\frac{\hbar}{2m\omega}}(\sqrt{n'+1}\langle n|n'+1 \rangle + \sqrt{n'}\langle n|n'-1 \rangle) \quad (7)$$

$$= \sqrt{\frac{\hbar}{2m\omega}}(\sqrt{n'+1}\delta_{n,n'+1} + \sqrt{n'}\delta_{n,n'-1}) \quad (8)$$

By similar reasoning we get the matrix elements for  $p$ :

$$\langle n|p|n'\rangle = i\sqrt{\frac{\hbar m\omega}{2}}(\sqrt{n'+1}\delta_{n,n'+1} - \sqrt{n'}\delta_{n,n'-1}) \quad (9)$$

These results agree with those found by doing the integrals involving Hermite polynomials.

We now have all the matrix elements of X and P so it would be interesting to calculate the full hamiltonian matrix, which is

$$H = \frac{1}{2m}P^2 + \frac{m\omega^2}{2}X^2 \quad (10)$$

In order to calculate the squares of the two matrices, we observe that both X and P are *tridiagonal* matrices with the added condition that their main diagonals are all zero. That is, the two diagonals above and below the main diagonal are the only places with non-zero elements. The square of such a matrix will have non-zero elements only on the main diagonal, and on the diagonals *two* above and below the main diagonal (you can verify this by drawing out such a matrix and seeing where the non-zero elements lie, or by doing tedious calculations with indices).

We can demonstrate how these elements can be calculated by considering the diagonal elements of  $X^2$ .

$$X_{nn}^2 = \sum_{n'} \langle n|x|n'\rangle \langle n'|x|n\rangle \quad (11)$$

$$= \frac{\hbar}{2m\omega} \sum_{n'} [\sqrt{n'+1}\delta_{n,n'+1} + \sqrt{n'}\delta_{n,n'-1}] [\sqrt{n+1}\delta_{n',n+1} + \sqrt{n}\delta_{n',n-1}] \quad (12)$$

$$= \frac{\hbar}{2m\omega} (2n+1) \quad (13)$$

The last line is obtained by noting that all the terms in the sum contain the product of two Kronecker deltas, so only in those cases where *both* deltas are non-zero is there a non-zero contribution to the sum. This happens only in the terms involving the product of the first and fourth terms (where  $n' = n - 1$ ) and the second and third terms (where  $n' = n + 1$ ).

By a similar argument, we get

$$P_{nn}^2 = \frac{\hbar m\omega}{2} (2n+1) \quad (14)$$

Therefore the *diagonal* elements of  $(1/2m)P^2 + (m\omega^2/2)X^2$  are

$$H_{nn} = \hbar\omega \left( n + \frac{1}{2} \right) \quad (15)$$

which is what you would expect, as these are the energy levels of the harmonic oscillator.

It remains only to show that the off-diagonal elements of  $H$  are zero.

$$X_{nm}^2 = \sum_{n'} \langle n|x|n'\rangle \langle n'|x|m\rangle \quad (16)$$

$$= \frac{\hbar}{2m\omega} \sum_{n'} [\sqrt{n'+1}\delta_{n,n'+1} + \sqrt{n'}\delta_{n,n'-1}] [\sqrt{m+1}\delta_{n',m+1} + \sqrt{m}\delta_{n',m-1}] \quad (17)$$

To see which non-zero elements exist on row  $n$ , we note that for a given value of  $n$ , we must have either  $n' = n - 1$  or  $n' = n + 1$  in order for one of the deltas in the first term to be non-zero. If  $n' = n - 1$ , then in the second term, we must have either  $n - 1 = m + 1$  or  $n - 1 = m - 1$ . The second case results in a diagonal element which we have already considered, so we need consider only the case  $m = n - 2$ . In this case, the matrix element is

$$X_{n,n-2}^2 = \frac{\hbar}{2m\omega} \sqrt{n(n-1)} \quad (18)$$

Similarly, if  $n' = n + 1$ , the non-diagonal term is  $n + 1 = m - 1$  or  $m = n + 2$ , and we get

$$X_{n,n+2}^2 = \frac{\hbar}{2m\omega} \sqrt{(n+1)(n+2)} \quad (19)$$

Similar reasoning gives us the elements from  $P^2$ :

$$P_{n,n-2}^2 = -\frac{\hbar m\omega}{2} \sqrt{n(n-1)} \quad (20)$$

$$P_{n,n+2}^2 = -\frac{\hbar m\omega}{2} \sqrt{(n+1)(n+2)} \quad (21)$$

Combining these two results, we see that the *non-diagonal* elements of  $(1/2m)P^2 + (m\omega^2/2)X^2$  are all zero.

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