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

$$\langle x\rangle_{nn} = \langle n|x|n\rangle \tag{0.1}$$
$$= X_{nn} \tag{0.2}$$

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

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

$$x = \sqrt{\frac{\hbar}{2m\omega}}(a_+ + a_-) \tag{0.3}$$
$$p = i\sqrt{\frac{\hbar m\omega}{2}}(a_+ - a_-) \tag{0.4}$$
$$a_+\psi_n = \sqrt{n+1}\psi_{n+1} \tag{0.5}$$
$$a_-\psi_n = \sqrt{n}\psi_{n-1} \tag{0.6}$$

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

$$\langle n|x|n'\rangle = \sqrt{\frac{\hbar}{2m\omega}}(\sqrt{n'+1}\langle n|n'+1\rangle + \sqrt{n'}\langle n|n'-1\rangle) \tag{0.7}$$
$$= \sqrt{\frac{\hbar}{2m\omega}}(\sqrt{n'+1}\delta_{n,n'+1} + \sqrt{n'}\delta_{n,n'-1}) \tag{0.8}$$

By similar reasoning we get the matrix elements for p:

$$\langle n|p|n'\rangle = i\sqrt{\frac{\hbar m\omega}{2}}(\sqrt{n'+1}\delta_{n,n'+1} - \sqrt{n'}\delta_{n,n'-1}) \tag{0.9}$$

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

$$\mathsf{H} = \frac{1}{2m}\mathsf{P}^2 + \frac{m\omega^2}{2}\mathsf{X}^2 \tag{0.10}$$

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.

$$\mathsf{X}^2_{nn} = \sum_{n'} \langle n|x|n'\rangle\langle n'|x|n\rangle \tag{0.11}$$

$$= \frac{\hbar}{2m\omega}\sum_{n'}[\sqrt{n'+1}\delta_{n,n'+1} + \sqrt{n'}\delta_{n,n'-1}][\sqrt{n+1}\delta_{n',n+1} + \sqrt{n}\delta_{n',n-1}] \tag{0.12}$$

$$= \frac{\hbar}{2m\omega}(2n+1) \tag{0.13}$$

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

$$\mathsf{P}^2_{nn} = \frac{\hbar m\omega}{2}(2n+1) \tag{0.14}$$

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

$$\mathsf{H}_{nn} = \hbar\omega\left(n + \frac{1}{2}\right) \tag{0.15}$$

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.

$$\mathsf{X}^2_{nm} = \sum_{n'} \langle n|x|n'\rangle\langle n'|x|m\rangle \tag{0.16}$$

$$= \frac{\hbar}{2m\omega}\sum_{n'}[\sqrt{n'+1}\delta_{n,n'+1} + \sqrt{n'}\delta_{n,n'-1}][\sqrt{m+1}\delta_{n',m+1} + \sqrt{m}\delta_{n',m-1}] \tag{0.17}$$

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

$$\mathsf{X}^2_{n,n-2} = \frac{\hbar}{2m\omega}\sqrt{n(n-1)} \tag{0.18}$$

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

$$\mathsf{X}^2_{n,n+2} = \frac{\hbar}{2m\omega}\sqrt{(n+1)(n+2)} \tag{0.19}$$

Similar reasoning gives us the elements from P^2:

$$\mathsf{P}^2_{n,n-2} = -\frac{\hbar m\omega}{2}\sqrt{n(n-1)} \tag{0.20}$$

$$\mathsf{P}^2_{n,n+2} = -\frac{\hbar m\omega}{2}\sqrt{(n+1)(n+2)} \tag{0.21}$$

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

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