

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

$$(0.1) \quad \langle x \rangle_{mn} = \langle n|x|n \rangle$$

$$(0.2) \quad = X_{nn}$$

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

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

$$(0.3) \quad x = \sqrt{\frac{\hbar}{2m\omega}}(a_+ + a_-)$$

$$(0.4) \quad p = i\sqrt{\frac{\hbar m\omega}{2}}(a_+ - a_-)$$

$$(0.5) \quad a_+ \psi_n = \sqrt{n+1} \psi_{n+1}$$

$$(0.6) \quad a_- \psi_n = \sqrt{n} \psi_{n-1}$$

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

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

$$(0.8) \quad = \sqrt{\frac{\hbar}{2m\omega}}(\sqrt{n'+1}\delta_{n,n'+1} + \sqrt{n'}\delta_{n,n'-1})$$

By similar reasoning we get the matrix elements for p :

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

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

$$(0.10) \quad H = \frac{1}{2m}P^2 + \frac{m\omega^2}{2}X^2$$

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 .

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

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

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

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

$$(0.14) \quad P_{nn}^2 = \frac{\hbar m\omega}{2} (2n+1)$$

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

$$(0.15) \quad H_{nn} = \hbar\omega \left(n + \frac{1}{2} \right)$$

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.

$$\begin{aligned} X_{nm}^2 &= \sum_{n'} \langle n|x|n' \rangle \langle n'|x|m \rangle \\ (0.17) \quad & \frac{\hbar}{2m\omega} \sum_{n'} [\sqrt{n'+1} \delta_{n,n'+1} + \sqrt{n'} \delta_{n,n'-1}] [\sqrt{m+1} \delta_{n',m+1} + \sqrt{m} \delta_{n',m-1}] \end{aligned}$$

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

$$(0.18) \quad X_{n,n-2}^2 = \frac{\hbar}{2m\omega} \sqrt{n(n-1)}$$

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

$$(0.19) \quad X_{n,n+2}^2 = \frac{\hbar}{2m\omega} \sqrt{(n+1)(n+2)}$$

Similar reasoning gives us the elements from P^2 :

$$(0.20) \quad P_{n,n-2}^2 = -\frac{\hbar m \omega}{2} \sqrt{n(n-1)}$$

$$(0.21) \quad P_{n,n+2}^2 = -\frac{\hbar m \omega}{2} \sqrt{(n+1)(n+2)}$$

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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