

Lecture notes: QM 05
The Harmonic Oscillator

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The classical harmonic oscillator is a rich and interesting dynamical system. It is one of those few problems that are important to all branches of physics. It allows us to understand many kinds of oscillations in complex systems. The harmonic oscillator provides a useful model for a variety of vibrational phenomena that are encountered, for instance, in classical mechanics, electrodynamics, statistical mechanics, solid state, atomic, nuclear, and particle physics. In quantum mechanics, it serves as an invaluable tool to illustrate the basic concepts and the formalism.

1 The Hamiltonian

The total energy E of a particle of mass m moving in one dimension under the action of a restoring force $F = -kx$ ($k > 0$) is usually written as

$$E = \frac{1}{2}mv^2 + \frac{1}{2}kx^2 = \frac{p^2}{2m} + \frac{1}{2}m\omega^2x^2. \quad (1)$$

Here $\omega = \sqrt{k/m}$ is angular frequency of the oscillation. The Hamiltonian of the one-dimensional harmonic potential is therefore given by

$$\hat{H} = \frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega^2\hat{x}^2. \quad (2)$$

The harmonic oscillator potential in here is

$$V(\hat{x}) = \frac{1}{2}m\omega^2\hat{x}^2. \quad (3)$$

The problem is how to find the energy eigenvalues and eigenstates of this Hamiltonian. This problem can be studied by means of two separate methods. The first method, called the analytic method, consists in solving the time-independent Schrödinger equation for the Hamiltonian (2). The second method, called the *ladder* or *algebraic method*, does not deal with solving the Schrödinger equation, but deals instead with operator algebra involving operators known as the *creation* and *annihilation* or *ladder operators*. We shall discuss the second method, for it is more straightforward, more elegant and much simpler than solving the Schrödinger equation.

2 Factorizing the Hamiltonian

To proceed we rewrite the Hamiltonian (2) as

$$\hat{H} = \frac{1}{2}m\omega^2 \left(\hat{x}^2 + \frac{\hat{p}^2}{m^2\omega^2} \right). \quad (4)$$

The expression in the parenthesis is the sum of two squares. Motivated by the identity $a^2 + b^2 = (a - ib)(a + ib)$, holding for numbers a and b , we examine if the expression in the parenthesis can be written as a product

$$\begin{aligned} \left(\hat{x} - \frac{i\hat{p}}{m\omega} \right) \left(\hat{x} + \frac{i\hat{p}}{m\omega} \right) &= \hat{x}^2 + \frac{\hat{p}^2}{m^2\omega^2} + \frac{i}{m\omega}(\hat{x}\hat{p} - \hat{p}\hat{x}) \\ &= \hat{x}^2 + \frac{\hat{p}^2}{m^2\omega^2} + \frac{i}{m\omega}[\hat{x}, \hat{p}] \\ &= \hat{x}^2 + \frac{\hat{p}^2}{m^2\omega^2} - \frac{\hbar}{m\omega}, \end{aligned} \quad (5)$$

where the extra terms arise because \hat{x} and \hat{p} do not commute, opposite to numbers. We now define the right-most factor in the above product to be \hat{A} :

$$\hat{A} = \hat{x} + \frac{i\hat{p}}{m\omega}. \quad (6)$$

Since \hat{x} and \hat{p} are Hermitian operators, we have the Hermitian conjugate of \hat{A} as

$$\hat{A}^\dagger = \hat{x} - \frac{i\hat{p}}{m\omega}, \quad (7)$$

and this is the left-most factor in the product! We can therefore rewrite (5) as

$$\hat{x}^2 + \frac{\hat{p}^2}{m^2\omega^2} = \hat{A}^\dagger \hat{A} + \frac{\hbar}{m\omega}, \quad (8)$$

Therefore, in terms of $\hat{A}^\dagger \hat{A}$ we rewrite the Hamiltonian (2) as

$$\hat{H} = \frac{1}{2}m\omega^2 \hat{A}^\dagger \hat{A} + \frac{1}{2}\hbar\omega. \quad (9)$$

This is a factorized form of the Hamiltonian: up to an additive constant E_0 , \hat{H} is the product of a positive constant times the operator product $\hat{A}^\dagger \hat{A}$. We note that the commutator of \hat{A} and \hat{A}^\dagger is

$$[\hat{A}, \hat{A}^\dagger] = \left[\hat{x} + \frac{i\hat{p}}{m\omega}, \hat{x} - \frac{i\hat{p}}{m\omega} \right] = -\frac{i}{m\omega}[\hat{x}, \hat{p}] + \frac{i}{m\omega}[\hat{p}, \hat{x}] = \frac{2\hbar}{m\omega} \quad (10)$$

This implies that

$$\left[\sqrt{\frac{m\omega}{2\hbar}} \hat{A}, \sqrt{\frac{m\omega}{2\hbar}} \hat{A}^\dagger \right] = 1 \quad (11)$$

suggesting the definition of unit-free operators \hat{a} and \hat{a}^\dagger :

$$\begin{aligned} \hat{a} &\equiv \sqrt{\frac{m\omega}{2\hbar}} \hat{A}, \\ \hat{a}^\dagger &\equiv \sqrt{\frac{m\omega}{2\hbar}} \hat{A}^\dagger. \end{aligned} \quad (12)$$

Therefore, due to the scaling we have

$$\boxed{[\hat{a}, \hat{a}^\dagger] = 1.} \quad (13)$$

The operator \hat{a} is called *annihilation* operator and \hat{a}^\dagger is called a *creation* operator. The justification for these names will be seen soon. From the above definitions we read the relations of \hat{a} and \hat{a}^\dagger with \hat{x} and \hat{p} :

$$\boxed{\begin{aligned} \hat{a} &= \sqrt{\frac{m\omega}{2\hbar}} \left(\hat{x} + \frac{i\hat{p}}{m\omega} \right), \\ \hat{a}^\dagger &= \sqrt{\frac{m\omega}{2\hbar}} \left(\hat{x} - \frac{i\hat{p}}{m\omega} \right). \end{aligned}} \quad (14)$$

The inverse relations are useful as well:

$$\boxed{\begin{aligned}\hat{x} &= \sqrt{\frac{\hbar}{2m\omega}} (\hat{a} + \hat{a}^\dagger), \\ \hat{p} &= \frac{1}{i} \sqrt{\frac{m\omega\hbar}{2}} (\hat{a} - \hat{a}^\dagger).\end{aligned}} \quad (15)$$

While neither \hat{a} nor \hat{a}^\dagger is hermitian (they are hermitian conjugates of each other), the above equations are consistent with the hermiticity of \hat{x} and \hat{p} . We can now write the Hamiltonian in terms of the \hat{a} and \hat{a}^\dagger operators. Using (12) we have

$$\hat{A}\hat{A}^\dagger = \frac{2\hbar}{m\omega} \hat{a}\hat{a}^\dagger, \quad (16)$$

and therefore from (9) we get

$$\boxed{\hat{H} = \hbar\omega \left(\hat{a}^\dagger\hat{a} + \frac{1}{2} \right) = \hbar\omega \left(\hat{N} + \frac{1}{2} \right), \quad \hat{N} \equiv \hat{a}^\dagger\hat{a}.} \quad (17)$$

The above form of the Hamiltonian is factorized: up to an additive constant \hat{H} is the product of a positive constant times the operator product $\hat{a}^\dagger\hat{a}$. In here we have dropped the identity operator, which is usually understood. We have also introduced the number operator \hat{N} . This is, by construction, a hermitian operator and it is, up to a scale and an additive constant, equal to the Hamiltonian. An eigenstate of \hat{H} is also an eigenstate of \hat{N} and it follows from the above relation that the respective eigenvalues E and N are related by

$$E = \hbar\omega \left(N + \frac{1}{2} \right). \quad (18)$$

3 The ground state

On any state ψ that is normalized we have

$$\langle \hat{H} \rangle_\psi = (\psi, \hat{H}\psi) = \hbar\omega(\psi, \hat{a}^\dagger\hat{a}\psi) + \frac{1}{2}\hbar\omega(\psi, \psi), \quad (19)$$

and moving the \hat{a}^\dagger to the first ψ , we get

$$\langle \hat{H} \rangle_\psi = \hbar\omega(\hat{a}\psi, \hat{a}\psi) + \frac{1}{2}\hbar\omega \geq \frac{1}{2}\hbar\omega. \quad (20)$$

The inequality follows because any expression of the form (ψ, ψ) is greater than or equal to zero. This shows that for any energy eigenstate with energy E such that $\hat{H}\psi = E\psi$, we have

$$E \geq \frac{1}{2}\hbar\omega. \quad (21)$$

This important result about the spectrum followed directly from the factorization of the Hamiltonian. But we also get the information required to find the ground state wave function. The minimum energy $\frac{1}{2}\hbar\omega$ will be realized for a state ψ if the term $(\hat{a}\psi, \hat{a}\psi)$ in (20) vanishes. For this to vanish $\hat{a}\psi$ must vanish. Therefore, the ground state wave function ψ_0 must satisfy

$$\hat{a}\psi_0 = 0. \quad (22)$$

The operator \hat{a} annihilates the ground state and this why \hat{a} is called the annihilation operator. Using the definition of \hat{a} in (14) and the position space representation of \hat{p} , this becomes

$$\left(\hat{x} + \frac{i}{m\omega} \frac{\hbar}{i} \frac{d}{dx} \right) \psi_0(x) = 0$$

or,

$$\left(\hat{x} + \frac{\hbar}{m\omega} \frac{d}{dx} \right) \psi_0(x) = 0. \quad (23)$$

Remarkably, this is a first order differential equation for the ground state. Not a second order equation, like the Schrödinger equation that determines the general energy eigenstates. This is a dramatic simplification afforded by the factorization of the Hamiltonian into a product of first-order differential operators. The above equation is rearranged as

$$\frac{d\psi_0}{dx} = -\frac{m\omega}{\hbar} x\psi_0. \quad (24)$$

Solving the differential equation yields

$$\boxed{\psi_0(x) = \left(\frac{m\omega}{\pi\hbar} \right)^{\frac{1}{4}} e^{-\frac{m\omega}{2\hbar} x^2}}, \quad (25)$$

where we included a normalization constant to guarantee that $(\psi_0, \psi_0) = 1$. Note that ψ_0 is indeed an energy eigenstate with energy E_0 :

$$\hat{H}\psi_0 = \hbar\omega \left(\hat{a}^\dagger \hat{a} + \frac{1}{2} \right) \psi_0 = \frac{1}{2}\hbar\omega\psi_0 \quad \rightarrow \quad E_0 = \frac{1}{2}\hbar\omega. \quad (26)$$

4 Operator manipulation

We have seen that all energy eigenstates are eigenstates of the Hermitian number operator $\hat{N} = \hat{a}^\dagger \hat{a}$. This is because $\hat{H} = \hbar\omega(\hat{N} + \frac{1}{2})$. Note that since $\hat{a}\psi_0 = 0$ we also have

$$\hat{N}\psi_0 = \hat{a}^\dagger \hat{a}\psi_0 = 0. \quad (27)$$

Thus ψ_0 is an eigenstate of the operator \hat{N} with an eigenvalue $N = 0$. Therefore ψ_0 is an energy eigenstate with energy E_0 given by

$$E_0 = \hbar\omega \left(0 + \frac{1}{2} \right) = \frac{1}{2}\hbar\omega, \quad (28)$$

which we have already shown in (26).

We can quickly check that

$$\begin{aligned} [\hat{N}, \hat{a}] &= [\hat{a}^\dagger \hat{a}, \hat{a}] = [\hat{a}^\dagger, \hat{a}] \hat{a} = -\hat{a}, \\ [\hat{N}, \hat{a}^\dagger] &= [\hat{a}^\dagger \hat{a}, \hat{a}^\dagger] = \hat{a}^\dagger [\hat{a}, \hat{a}^\dagger] = \hat{a}^\dagger. \end{aligned} \quad (29)$$

Similarly we can show

$$\begin{aligned} [\hat{N}, \hat{a}^2] &= [\hat{N}, \hat{a}\hat{a}] = [\hat{N}, \hat{a}]\hat{a} + \hat{a}[\hat{N}, \hat{a}] = -\hat{a}\hat{a} + \hat{a}(-\hat{a}) = -2\hat{a}^2, \\ [\hat{N}, (\hat{a}^\dagger)^2] &= [\hat{N}, \hat{a}^\dagger \hat{a}^\dagger] = [\hat{N}, \hat{a}^\dagger] \hat{a}^\dagger + \hat{a}^\dagger [\hat{N}, \hat{a}^\dagger] = \hat{a}^\dagger \hat{a}^\dagger + \hat{a}^\dagger \hat{a}^\dagger = 2(\hat{a}^\dagger)^2. \end{aligned} \quad (30)$$

and also

$$\begin{aligned} [\hat{N}, (\hat{a})^3] &= -3(\hat{a})^3, \\ [\hat{N}, (\hat{a}^\dagger)^3] &= 3(\hat{a}^\dagger)^3. \end{aligned} \quad (31)$$

Using these identities and induction you should be able to show that:

$$\begin{aligned} [\hat{N}, (\hat{a})^k] &= -k(\hat{a})^k, \\ [\hat{N}, (\hat{a}^\dagger)^k] &= k(\hat{a}^\dagger)^k. \end{aligned} \quad (32)$$

These relations suggest why \hat{N} is called the number operator. Acting on powers of creation or annihilation operators by commutation it gives the same object multiplied by (plus or minus) the number of creation or annihilation operators, k in the above. Closely related commutators are also useful:

$$\begin{aligned} [\hat{a}^\dagger, (\hat{a})^k] &= -k(\hat{a})^{k-1}, \\ [\hat{a}, (\hat{a}^\dagger)^k] &= k(\hat{a}^\dagger)^{k-1}. \end{aligned} \quad (33)$$

These commutators are analogous to $[\hat{p}, (\hat{x})^k]$ and $[\hat{x}, (\hat{p})^k]$. We will also make use of the following Lemma which helps in evaluations where we have an operator \hat{A} that kills a state ψ and we aim to simplify the action of $\hat{a}\hat{B}$, where \hat{B} is another operator, acting on ψ .

$$\boxed{\text{If } \hat{A}\psi = 0, \text{ then } \hat{A}\hat{B}\psi = [\hat{A}, \hat{B}]\psi} \quad (34)$$

This is easily proved. First note that

$$\hat{A}\hat{B} = [\hat{A}, \hat{B}] + \hat{B}\hat{A}, \quad (35)$$

as can be quickly checked expanding the right-hand side. It then follows that

$$\hat{A}\hat{B}\psi = ([\hat{A}, \hat{B}] + \hat{B}\hat{A})\psi = [\hat{A}, \hat{B}]\psi, \quad (36)$$

because $\hat{B}\hat{A}\psi = \hat{B}(\hat{A}\psi) = 0$. This is what we wanted to show. This is all we need to know about commutators and we can now proceed to construct the states of the harmonic oscillator.

5 Excited states

Since \hat{a} annihilates ψ_0 consider acting on the ground state with \hat{a}^\dagger . It is clear that \hat{a}^\dagger cannot also annihilate ψ_0 . If that would happen then acting with both sides of the commutator identity $[\hat{a}, \hat{a}^\dagger] = 1$ on ψ_0 would lead to a contradiction: the left-hand side would vanish but the right-hand side would not. Thus consider the wave function

$$\psi_1 \equiv \hat{a}^\dagger \psi_0. \quad (37)$$

We are going to show that this is an energy eigenstate. For this purpose we act on it with the number operator:

$$\hat{N}\psi_1 = \hat{N}\hat{a}^\dagger\psi_0 = [\hat{N}, \hat{a}^\dagger]\psi_0, \quad (38)$$

where we used the fact that $\hat{N}\psi_0 = 0$ and Lemma (34). Given that $[\hat{N}, \hat{a}^\dagger] = \hat{a}^\dagger$, we get

$$\hat{N}\psi_1 = \hat{a}^\dagger\psi_0 = \psi_1. \quad (39)$$

Thus ψ_1 is an eigenstate of the operator \hat{N} with eigenvalue $N = 1$. Since the eigenvalue of the operator \hat{N} for the state ψ_0 is zero, the effect of acting \hat{a}^\dagger on ψ_0 was to increase the eigenvalue of the number operator by one unit. The operator \hat{a}^\dagger is called the *creation* operator because it creates a state out of the ground state. Alternatively, it is called the *raising* operator, because it raises (by one unit) the eigenvalue of \hat{N} . Since $N = 1$ for ψ_1 it follows that ψ_1 is an energy eigenstate with energy E_1 given by

$$E_1 = \hbar\omega \left(1 + \frac{1}{2}\right) = \frac{3}{2}\hbar\omega. \quad (40)$$

It also turns out that ψ_1 is properly normalized:

$$(\psi_1, \psi_1) = (\hat{a}^\dagger\psi_0, \hat{a}^\dagger\psi_0) = (\psi_0, \hat{a}\hat{a}^\dagger\psi_0), \quad (41)$$

where we used the Hermitian conjugation property to move the \hat{a}^\dagger acting on the left input into the right input, where it goes as $(\hat{a}^\dagger)^\dagger = \hat{a}$. We then have

$$(\psi_1, \psi_1) = (\psi_0, \hat{a}\hat{a}^\dagger\psi_0) = (\psi_0, [\hat{a}, \hat{a}^\dagger]\psi_0) = (\psi_0, \psi_0) = 1, \quad (42)$$

where we used (34) in the evaluation of $\hat{a}\hat{a}^\dagger\psi_0$. Indeed the state ψ_1 is correctly normalized.

Next consider the state

$$\psi'_2 \equiv \hat{a}^\dagger\hat{a}^\dagger\psi_0. \quad (43)$$

This has

$$\hat{N}\psi'_2 = \hat{N}\hat{a}^\dagger\hat{a}^\dagger\psi_0 = [\hat{N}, \hat{a}^\dagger\hat{a}^\dagger]\psi_0 = 2\hat{a}^\dagger\hat{a}^\dagger\psi_0 = 2\psi'_2, \quad (44)$$

so ψ'_2 is a state with number $N = 2$ and energy $E_2 = \frac{5}{2}\hbar\omega$. Now we check whether ψ'_2 is properly normalized or not. We find

$$\begin{aligned} (\psi'_2, \psi'_2) &= (\hat{a}^\dagger\hat{a}^\dagger\psi_0, \hat{a}^\dagger\hat{a}^\dagger\psi_0) = (\psi_0, \hat{a}\hat{a}\hat{a}^\dagger\hat{a}^\dagger\psi_0) = (\psi_0, \hat{a}[\hat{a}, \hat{a}^\dagger\hat{a}^\dagger]\psi_0) \\ &= (\psi_0, 2\hat{a}\hat{a}^\dagger\psi_0) = 2(\psi_0, \psi_0) = 2. \end{aligned} \quad (45)$$

The properly normalized wave function is therefore

$$\psi_2 \equiv \frac{1}{\sqrt{2}} \hat{a}^\dagger \hat{a}^\dagger \psi_0. \quad (46)$$

Similarly we can show that the properly normalized third excited state would be

$$\begin{aligned} \psi_3 &\equiv \frac{1}{\sqrt{2}} \frac{1}{\sqrt{3}} \hat{a}^\dagger \hat{a}^\dagger \hat{a}^\dagger \psi_0 \\ &= \frac{1}{\sqrt{3!}} (\hat{a}^\dagger)^3 \psi_0 \end{aligned} \quad (47)$$

We now claim that the properly normalized n -th excited state of the simple harmonic oscillator is (you may find it is interesting to prove the claim as an exercise)

$$\boxed{\psi_n \equiv \frac{1}{\sqrt{n!}} \underbrace{\hat{a}^\dagger \cdots \hat{a}^\dagger}_n \psi_0 = \frac{1}{\sqrt{n!}} (\hat{a}^\dagger)^n \psi_0.} \quad (48)$$

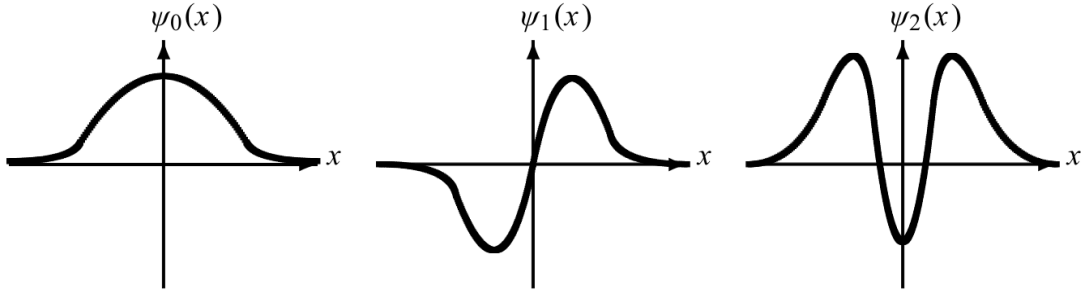


Figure 1: Shapes of the first three wave functions of the harmonic oscillator [1].

We also show that the eigenvalue of ψ_n for the operator \hat{N} is n :

$$\begin{aligned} \hat{N}\psi_n &= \frac{1}{\sqrt{n!}} \hat{N} (\hat{a}^\dagger)^n \psi_0 \\ &= \frac{1}{\sqrt{n!}} \hat{a}^\dagger \hat{a} (\hat{a}^\dagger)^n \psi_0 \\ &= \frac{1}{\sqrt{n!}} \hat{a}^\dagger [\hat{a}, (\hat{a}^\dagger)^n] \psi_0 \\ &= \frac{1}{\sqrt{n!}} \hat{a}^\dagger n (\hat{a}^\dagger)^{n-1} \psi_0 \\ &= \frac{n}{\sqrt{n!}} (\hat{a}^\dagger)^n \psi_0 \\ &= n \psi_n \end{aligned} \quad (49)$$

Since for the operator \hat{N} the eigenvalue of ψ_n is n , the energy eigenvalue E_n is given by

$$E_n = \hbar\omega \left(n + \frac{1}{2} \right). \quad (50)$$

Also as the various states ψ_n are eigenstates of a Hermitian operator \hat{H} with different eigenvalues, they are orthonormal

$$(\psi_m, \psi_n) = \delta_{mn}. \quad (51)$$

We now note that ψ_n is the state with n operators \hat{a}^\dagger acting on ψ_0 and $\hat{a}\psi_0$ is the state with $n-1$ operators \hat{a}^\dagger acting on ψ_0 because the \hat{a} eliminates one of the creation operator in ψ_n . Thus we expect $\hat{a}\psi_n \sim \psi_{n-1}$. We can make this precise

$$\hat{a}\psi_n = \hat{a} \frac{1}{\sqrt{n!}} (\hat{a}^\dagger)^n \psi_0 = \frac{1}{\sqrt{n!}} [\hat{a}, (\hat{a}^\dagger)^n] \psi_0 = \frac{n}{\sqrt{n!}} (\hat{a}^\dagger)^{n-1} \psi_0. \quad (52)$$

At this point we use (48) with n set equal to $n-1$ and thus we get

$$\hat{a}\psi_n = \frac{n}{\sqrt{n!}} \sqrt{(n-1)!} \psi_{n-1} = \sqrt{n} \psi_{n-1}. \quad (53)$$

By the action of \hat{a}^\dagger on ψ_n we get

$$\begin{aligned} \hat{a}^\dagger \psi_n &= \hat{a}^\dagger \frac{1}{\sqrt{n!}} (\hat{a}^\dagger)^n \psi_0 = \frac{1}{\sqrt{n!}} (\hat{a}^\dagger)^{n+1} \psi_0 \\ &= \frac{1}{\sqrt{n!}} \sqrt{(n+1)!} \psi_{n+1} = \sqrt{(n+1)} \psi_{n+1} \end{aligned} \quad (54)$$

Collecting the results we have

$$\boxed{\begin{aligned} \hat{a}\psi_n &= \sqrt{n} \psi_{n-1}, \\ \hat{a}^\dagger \psi_n &= \sqrt{(n+1)} \psi_{n+1}. \end{aligned}} \quad (55)$$

These relations make it clear that \hat{a} lowers the number of any energy eigenstate by one unit, except for the vacuum ψ_0 which it kills. The raising operator \hat{a}^\dagger increases the number of any eigenstate by one unit. one unit.

6 Expectation values of operators

The expectation value $\langle \hat{x} \rangle_{\psi_n}$ vanishes for any energy eigenstate since we are integrating x , which is odd, against $|\psi_n(x)|^2$, which is always even. Still, it is instructive to see how this happens explicitly:

$$\begin{aligned} \langle \hat{x} \rangle_{\psi_n} &= (\psi_n, \hat{x}\psi_n) = \sqrt{\frac{\hbar}{2m\omega}} (\psi_n, (\hat{a} + \hat{a}^\dagger)\psi_n) \\ &= \sqrt{\frac{\hbar}{2m\omega}} (\psi_n, \hat{a}\psi_n + \hat{a}^\dagger\psi_n) \\ &= \sqrt{\frac{\hbar}{2m\omega}} (\psi_n, \hat{a}\psi_n) + \sqrt{\frac{\hbar}{2m\omega}} (\psi_n, \hat{a}^\dagger\psi_n) \\ &= \sqrt{\frac{\hbar}{2m\omega}} (\psi_n, \sqrt{n} \psi_{n-1}) + \sqrt{\frac{\hbar}{2m\omega}} (\psi_n, \sqrt{(n+1)} \psi_{n+1}) \\ &= \sqrt{\frac{\hbar}{2m\omega}} \sqrt{n} (\psi_n, \psi_{n-1}) + \sqrt{\frac{\hbar}{2m\omega}} \sqrt{(n+1)} (\psi_n, \psi_{n+1}) \\ &= 0. \end{aligned} \quad (56)$$

Since both ψ_{n-1} and ψ_{n+1} are orthonormal to ψ_n . Now we compute the expectation value of \hat{a}^2 :

$$\begin{aligned}
\langle \hat{x}^2 \rangle_{\psi_n} &= (\psi_n, \hat{x}^2 \psi_n) = \frac{\hbar}{2m\omega} (\psi_n, (\hat{a} + \hat{a}^\dagger)^2 \psi_n) \\
&= \frac{\hbar}{2m\omega} (\psi_n, (\hat{a} + \hat{a}^\dagger)(\hat{a} + \hat{a}^\dagger) \psi_n) \\
&= \frac{\hbar}{2m\omega} (\psi_n, (\hat{a}\hat{a} + \hat{a}\hat{a}^\dagger + \hat{a}^\dagger\hat{a} + \hat{a}^\dagger\hat{a}^\dagger) \psi_n) \\
&= \frac{\hbar}{2m\omega} (\psi_n, (\hat{a}\hat{a}^\dagger + \hat{a}^\dagger\hat{a}) \psi_n). \tag{57}
\end{aligned}$$

Since $\hat{a}\hat{a}\psi_n \sim \psi_{n-2}$ and $\hat{a}^\dagger\hat{a}^\dagger\psi_n \sim \psi_{n+2}$ and ψ_{n-2} and ψ_{n+2} are orthonormal to ψ_n , the $\hat{a}\hat{a}$ and $\hat{a}^\dagger\hat{a}^\dagger$ terms do not contribute. At this point we recognize that $\hat{a}^\dagger\hat{a} = \hat{N}$ and

$$\hat{a}\hat{a}^\dagger = [\hat{a}, \hat{a}^\dagger] + \hat{a}^\dagger\hat{a} = 1 + \hat{N}. \tag{58}$$

As a result

$$\begin{aligned}
\langle \hat{x}^2 \rangle_{\psi_n} &= \frac{\hbar}{2m\omega} (\psi_n, (1 + 2\hat{N}) \psi_n) \\
&= \frac{\hbar}{2m\omega} (1 + 2n). \tag{59}
\end{aligned}$$

Similarly it can also be shown that $\langle \hat{p} \rangle_{\psi_n} = 0$ and

$$\langle \hat{p}^2 \rangle_{\psi_n} = \frac{m\hbar\omega}{2} (1 + 2n). \tag{60}$$

Comparing (59) and (60) we see that the expectation values of the potential and kinetic energies are equal and are also equal to half the total energy:

$$\boxed{\frac{m\omega^2}{2} \langle \hat{x}^2 \rangle_{\psi_n} = \frac{1}{2m} \langle \hat{p}^2 \rangle_{\psi_n} = \frac{1}{2} \langle \hat{H} \rangle_{\psi_n}.} \tag{61}$$

This result is known as the *Virial* theorem.

We can now easily calculate the product $\Delta x \Delta p$ and show that

$$\Delta x \Delta p = \left(n + \frac{1}{2} \right) \hbar \quad \implies \quad \Delta x \Delta p \geq \frac{\hbar}{2}, \tag{62}$$

since $n \geq 0$; this is the Heisenberg uncertainty principle.

7 Harmonic oscillator in 3D

The time-independent Schrödinger equation for a spin-less particle of mass m moving under the influence of a three-dimensional potential is

$$\left[-\frac{\hbar^2}{2m} \nabla^2 + V(x, y, z) \right] \psi(x, y, z) = E\psi(x, y, z), \tag{63}$$

where ∇^2 is the Laplacian operator

$$\nabla^2 \equiv \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}. \quad (64)$$

This partial differential equation is generally difficult to solve. But, for those cases where the potential $V(x, y, z)$ separates into the sum of three independent, one-dimensional terms (which should not be confused with a vector)

$$V(x, y, z) = V_x(x) + V_y(y) + V_z(z), \quad (65)$$

we can solve (63) by means of the technique of separation of variables. This technique consists of separating the three-dimensional Schrödinger equation (63) into three independent one-dimensional Schrödinger equations. Let us examine how to achieve this. Note that (63), in conjunction with (65), can be written as

$$\left[\hat{H}_x + \hat{H}_y + \hat{H}_z \right] \psi(x, y, z) = E\psi(x, y, z), \quad (66)$$

where

$$\begin{aligned} \hat{H}_x &= -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V_x(x), \\ \hat{H}_y &= -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial y^2} + V_y(y), \\ \hat{H}_z &= -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial z^2} + V_z(z). \end{aligned} \quad (67)$$

As $V(x, y, z)$ separates into three independent terms, we can also write $\psi(x, y, z)$ as a product of three functions of a single variable each:

$$\psi(x, y, z) = X(x)Y(y)Z(z). \quad (68)$$

Substituting (68) into (66) and dividing by $X(x)Y(y)Z(z)$, we obtain

$$\left[-\frac{\hbar^2}{2m} \frac{1}{X} \frac{d^2 X}{dx^2} + V_x(x) \right] + \left[-\frac{\hbar^2}{2m} \frac{1}{Y} \frac{d^2 Y}{dy^2} + V_y(y) \right] + \left[-\frac{\hbar^2}{2m} \frac{1}{Z} \frac{d^2 Z}{dz^2} + V_z(z) \right] = E. \quad (69)$$

Since each expression in the square brackets depends on only one of the variables x , y , z , and since the sum of these three expressions is equal to a constant, E , each separate expression must then be equal to a constant such that the sum of these three constants is equal to E . For instance, the x -dependent expression is given by

$$\left[-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + V_x(x) \right] X(x) = E_x X(x). \quad (70)$$

Similar equations hold for the y and z coordinates, with

$$E_x + E_y + E_z = E. \quad (71)$$

The separation of variables technique consists in essence of reducing the three-dimensional Schrödinger equation (63) into three separate one-dimensional equations (70).

Now, for the harmonic oscillator in three-dimension, we begin with the anisotropic oscillator, which displays no symmetry, and then consider the isotropic oscillator where the x , y and z axes are all equivalent.

7.1 Anisotropic harmonic oscillator

Consider a particle is moving in a three-dimensional anisotropic oscillator potential

$$V(x, y, z) = \frac{1}{2}m\omega_x^2\hat{x}^2 + \frac{1}{2}m\omega_y^2\hat{y}^2 + \frac{1}{2}m\omega_z^2\hat{z}^2. \quad (72)$$

Its Schrödinger equation separates into three equations similar to (70):

$$\begin{aligned} -\frac{\hbar^2}{2m} \frac{d^2X(x)}{dx^2} + \frac{1}{2}m\omega_x^2\hat{x}^2 X(x) &= E_x X(x), \\ -\frac{\hbar^2}{2m} \frac{d^2Y(y)}{dy^2} + \frac{1}{2}m\omega_y^2\hat{y}^2 Y(y) &= E_y Y(y), \\ -\frac{\hbar^2}{2m} \frac{d^2Z(z)}{dz^2} + \frac{1}{2}m\omega_z^2\hat{z}^2 Z(z) &= E_z Z(z). \end{aligned} \quad (73)$$

The energy eigenvalues corresponding to the potential (72) can be expressed as

$$E_{n_x n_y n_z} = E_{n_x} + E_{n_y} + E_{n_z} = \left(n_x + \frac{1}{2}\right) \hbar\omega_x + \left(n_y + \frac{1}{2}\right) \hbar\omega_y + \left(n_z + \frac{1}{2}\right) \hbar\omega_z, \quad (74)$$

with $n_x, n_y, n_z = 0, 1, 2, 3, \dots$. The corresponding stationary state wave functions are

$$\psi_{n_x n_y n_z}(x, y, z) = X_{n_x}(x) Y_{n_y}(y) Z_{n_z}(z), \quad (75)$$

where $X_{n_x}(x)$, $Y_{n_y}(y)$, and $Z_{n_z}(z)$ are one-dimensional harmonic oscillator wave functions. These states are not degenerate, because the potential (72) has no symmetry (it is anisotropic).

7.2 Isotropic harmonic oscillator

Consider now an isotropic harmonic oscillator potential. Its energy eigenvalues can be inferred from (74) by substituting $\omega_x = \omega_y = \omega_z = \omega$,

$$E_{n_x n_y n_z} = \left(n_x + n_y + n_z + \frac{3}{2}\right) \hbar\omega. \quad (76)$$

Since the energy depends on the sum of n_x, n_y, n_z , any set of quantum numbers having the same sum will represent states of equal energy.

The ground state, whose energy is $E_{000} = 3\hbar\omega/2$, is not degenerate. The first excited state is threefold degenerate, since there are three different states, $\psi_{100}, \psi_{010}, \psi_{001}$ that correspond to the same energy $5\hbar\omega/2$. The second excited state is sixfold degenerate; its energy is $7\hbar\omega/2$.

Table 1 displays the first few energy levels along with their degeneracies, where g_n represents the number of degeneracy of the n th excited state.

Table 1: Energy levels and their degeneracies for an isotropic harmonic oscillator.

n	$2E_n/(\hbar\omega)$	$(n_x n_y n_z)$	g_n
0	3	(000)	1
1	5	(100), (010), (001)	3
1	7	(200), (020), (002)	6
		(110), (101), (001)	
3	9	(300), (030), (003)	10
		(210), (201), (021)	
		(120), (102), (012)	
		(111)	

Note: Most of the materials in this lecture note are taken from the lecture on Quantum Physics by Prof. Barton Zwiebach for the course 8.04 in the year of 2016 at MIT, USA.

References

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