A short introduction to quantum mechanics XIII: Harmonic oscillators

So far, we haven't dealt with any non-trivial examples in quantum mechanics. All our earlier discussions rested on somewhat abstract formalism. Therefore, in this article, we present a non-trivial example of quantum dynamics, albeit the simplest one. Harmonic oscillator. Other interesting example would be hydrogen atom, whose solution showed the triumph of quantum mechanics, as it agreed with experiments. Nevertheless, we will not introduce it in this series, since it is a bit complicated and requires the knowledge of many mathematical special functions. Moreover, one can easily learn it from virtually any quantum mechanics textbooks.

Let's begin. What is the Hamiltonian of harmonic oscillators? It has kinetic energy and potential energy given as follows:

$$H = \frac{p^2}{2m} + \frac{1}{2}m\omega^2 x^2 \tag{1}$$

where $\omega = \sqrt{\frac{k}{m}}$

Now, for a future purpose, let's introduce the following operator.

$$a = \sqrt{\frac{m\omega}{2\hbar}}(x + \frac{i}{m\omega}p) \tag{2}$$

Then, by taking its Hermitian conjugate, the following is clear:

$$a^\dagger = \sqrt{\frac{m\omega}{2\hbar}}(x - \frac{i}{m\omega}p) \tag{3}$$

Furthermore, by being careful to the fact that the order matters when multiplying (i.e. $xp \neq px$) and using $[x, p] = xp - px = i\hbar$, it is easy to show the following (**Problem 1.**):

$$[a, a^\dagger] = 1 \tag{4}$$

Using all these relations, we can re-express the Hamiltonian (1) as follows:

$$H = \frac{1}{2}(aa^\dagger + a^\dagger a)\hbar\omega = (a^\dagger a + \frac{1}{2})\hbar\omega = (N + \frac{1}{2})\hbar\omega \tag{5}$$

where we have used the notation $N \equiv a^\dagger a$ which will turn out to be convenient for our purpose.

Given this, let's calculate the following expression:

$$\begin{aligned} [N, a] &= [a^\dagger a, a] = a^\dagger a a - a a^\dagger a \\ &= (a^\dagger a - a a^\dagger) a = (-1) a = -a \end{aligned} \tag{6}$$

We conclude:

$$[N, a] = -a \tag{7}$$

Similarly, one can show:

$$[N, a^\dagger] = a^\dagger \tag{8}$$

Now, let $|n>$ be the eigenvector of the operator N with eigenvalue n. In other words:

$$N|n>= n|n> \tag{9}$$

Given this, notice the following:

$$\begin{aligned} N a^\dagger |n> &= (a^\dagger N + [N, a^\dagger])|n> \\ &= (a^\dagger N + a^\dagger)|n>= n a^\dagger |n> + a^\dagger |n> \\ &= (n+1) a^\dagger |n> \end{aligned} \tag{10}$$

Therefore $a^\dagger |n>$ is an eigenvector of N with eigenvalue $(n+1)$. From this reason, we call $a^\dagger$ a "raising operator;" it raises the eigenvalue. Similarly, one can show:

$$N a|n>= (n-1) a|n> \tag{11}$$

Therefore $a|n>$ is an eigenvector of N with eigenvalue $(n-1)$. From this reason, we call a a "lowering operator;" it lowers the eigenvalue.

Also, from (5), we see that $|n>$ is an eigenvector of the Hamiltonian with eigenvalue $(n+\frac{1}{2})\hbar\omega$. Therefore, $a^p|n>$ will have $(n-p+\frac{1}{2})\hbar\omega$ as its energy. At first glance, if we choose $p = n+1$ or larger, $a^p|n>$ can have a negative energy. But, it can't be as our Hamiltonian (1) cannot be negative since p^2 and x^2 are always non-negative. Therefore, we cannot arbitrarily lower the energy eigenvalue of $|n>$ by applying the lowering operator repeatedly. It must stop at certain point. It can stop if it becomes a zero vector. Therefore, at certain point of applying the lowering operator repeatedly, there must exist a vector $|\psi_l>$ such that $a|\psi_l>= 0$ while $|\psi_l>$ is not a zero vector. Such a vector has necessarily the lowest eigenvalue of N. Then, it is easy to see:

$$N|\psi_l>= a^\dagger a|\psi_l>= a^\dagger \cdot 0 = 0 = 0|\psi_l> \tag{12}$$

Therefore, the eigenvalue of N for the eigenvector $|\psi_l>$ is 0. It implies $|\psi_l>= |0>$ if we use the notation of (9). As this eigenvector has the

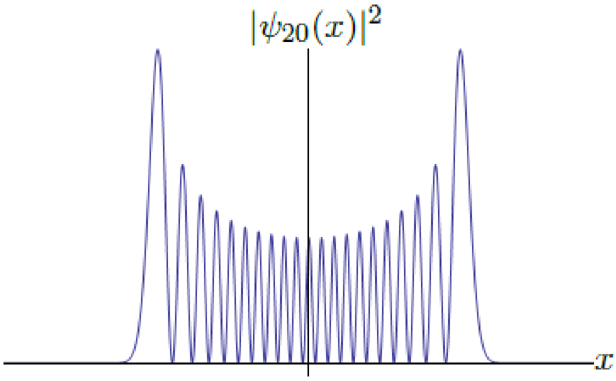

Figure 1: $|\psi_{20}(x)|^2$

lowest eigenvalue for N, it apparently has the lowest eigenvalue for the energy operator which is given by $(N+1/2)\hbar\omega$. Therefore, it is the ground state. Furthermore, one can easily check that the ground state satisfies the condition that its energy must be non-negative as $(0+1/2)\hbar\omega$ is non-negative. As all other states have higher energy, we can easily conclude that all the states have non-negative energy as expected.

We can actually obtain the explicit wave-function $\psi_0(x)$ of $|0>$ as follows. (2) and $a|0>=0$ implies:

$$(x+\frac{\hbar}{m\omega}\frac{d}{dx})\psi_0(x)=0 \tag{13}$$

The solution is given by:

$$\psi_0(x)=Ce^{-\frac{m\omega}{2\hbar}x^2} \tag{14}$$

for a certain C that can be determined by normalizing the wave function. We can obtain the eigenvectors of higher eigenvalues by repeatedly applying the raising operator. For example, the wave-function $\psi_1(x)$ of $|1>$ can be obtained as follows:

$$\psi_1(x)=(x-\frac{\hbar}{m\omega}\frac{d}{dx})\psi_0(x) \tag{15}$$

with a certain suitable overall factor, if $\psi_1(x)$ is normalized. From such a normalized $\psi_n(x)$, we can actually calculate the probability that the object will be found at the position between x and $x+dx$. It is naturally given by $|\psi_n(x)|^2dx$.

Actually, in the limit of very high n, the probability approaches the classical one. Think about an object oscillating due to a spring. It stays long when the object is near the turning point, as it momentarily stops and it doesn't stay long at the midpoint since this is when it moves fastest. Therefore, the probability for the particle to be found at the turning point is high and the probability for the particle to be found at the midpoint is low. On the other hand, the probability that the particle would be found outside the oscillating range (i.e. region farther than the turning point) is zero. In the large n limit, the probability shows such a behavior. See Fig.1. I plotted the probability for the particle with $n = 20$ to be found at given position (i.e. x). It is very wiggly, and actually, there are 21 wiggles. The number of wiggle is always $n+1$. Therefore, if n is bigger there will be more wiggles and the width of wiggle will be smaller, meaning that one can see as if the wiggles are smoothed out (i.e. averaged) in the classical limit in which n is very big. In that way, the probability for the classical case would be given by roughly half of the peaks. Also, as I mentioned, you clearly see that the probability is highest near the turning point (the two highest peaks at the ends) and that the probability is almost zero for x farther than the turning points.

Problem 2. If $|n>$s are normalized (i.e. the norm is 1) show the followings (Hint[1]):

$$|n+1>=\frac{a^\dagger}{\sqrt{n+1}}|n>, \quad |n-1>=\frac{a}{\sqrt{n}}|n> \tag{16}$$

Problem 3. Evaluate the followings. (Hint[2])

$$<n|x|n>, \quad <n|x|n+1> \tag{17}$$

Problem 4. How does the expectation value of the position x for a quantum state initially given by $\frac{|3>+|4>}{\sqrt{2}}$ evolve over time? Obtain an explicit expression.

Problem 5. Classically, the energy of a harmonic oscillator is allowed to be zero, if $x = p = 0$. However, we have seen that quantum mechanically, the lowest energy possible is not zero, but $\frac{1}{2}\hbar\omega$ (for $|0>$). Show that the uncertainty principle would be violated if there existed a state $|\psi>$ of which the energy for harmonic oscillator is zero. (i.e. $<\psi|H|\psi>=0$ where H is given by (1).) In other words, this result shows that uncertainty principle forces the ground state energy for harmonic oscillator to be non-zero. This problem was on an exam during Korean Physics Olympiad camp. (Hint[3])

Problem 6. Find the eigenvalues of the following Hamiltonian (Hint[4]):

$$H=\frac{p_x^2+p_y^2+p_z^2}{2m}+\frac{1}{2}mw_1^2x^2+\frac{1}{2}mw_2^2y^2+\frac{1}{2}mw_3z^3 \tag{18}$$

[1] It is enough to show $<n+1|n+1>=<n-1|n-1>=1$ using $<n|n>=1$.

[2] Express x in terms of a and $a^\dagger$ using (2) and (3), and use the result of Problem 2.

[3] Show $<x^2>=<p^2>=0$. Then, use $\Delta x^2=<x^2>-<x>^2$, $\Delta p^2=<p>^2-<p>^2$. I couldn't solve this problem because I didn't know these relations for standard deviations then.

[4] Use the separation of variables method.

Summary

- $H = \dfrac{p^2}{2m} + \dfrac{1}{2} m\omega^2 x^2$.
- $H = \dfrac{1}{2}(aa^\dagger + a^\dagger a)\hbar\omega = (N + \dfrac{1}{2})\hbar\omega$.
- $[a, a^\dagger] = 1$. a is the lowering operator and $a^\dagger$ is the raising operator. They lower and raise the eigenvalues for the Hamiltonian of harmonic oscillator.