A short introduction to quantum mechanics IX: 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. We postpone our demonstration of solving Schrödinger equation for hydrogen atom to another article.

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

Given this, if you recall Planck relation $E = \hbar\omega$, you will know that H and $h\omega$ have the same dimension, namely, energy. Thus, we might as well write $H = \text{blah} h\omega$ where blah is dimensionless. Thus, (1) can be re-expressed as

$$H = \hbar\omega\left(\frac{m\omega}{2\hbar}x^2 + \frac{p^2}{2m\hbar\omega}\right) \tag{2}$$

where the terms in the parenthesis are dimensionless.

So, how can we factor out the terms in the parenthesis? Note that the terms in the parenthesis are in the form $A^2 + B^2$. If you know some high school mathematics, you know

$$A^2 + B^2 = (A + Bi)(A - Bi) \tag{3}$$

as long as $AB = BA$. In our case,

$$A = \sqrt{\frac{m\omega}{2\hbar}}x, \qquad B = \frac{p}{\sqrt{2m\hbar\omega}} \tag{4}$$

However, we do not have $AB = BA$. Then, we can modify (3) to write

$$A^2 + B^2 = \frac{1}{2}(A + Bi)(A - Bi) + \frac{1}{2}(A - Bi)(A + Bi) \tag{5}$$

which is satisfied, even when $AB \neq BA$. So, let's write $a = A + Bi$. Then, $a^\dagger = A - Bi$ as A and B are Hermitian. In other words, we have

$$a = \frac{m\omega}{2\hbar}x + \frac{p}{\sqrt{2m\hbar\omega}}i \tag{6}$$

and by taking its Hermitian conjugate, we have:

$$a^\dagger = \frac{m\omega}{2\hbar}x - \frac{p}{\sqrt{2m\hbar\omega}}i \tag{7}$$

Thus, we can write (1) as

$$H = \frac{1}{2}(aa^\dagger + a^\dagger a)\hbar\omega \tag{8}$$

Furthermore, using $[x, p] = xp - px = i\hbar$, it is easy to show the following (**Problem 1.** Hint[1]):

$$[a, a^\dagger] = 1 \tag{9}$$

Using all these relations, we can re-express the Hamiltonian (8) as follows:

$$H = (a^\dagger a + \frac{1}{2})\hbar\omega = (N + \frac{1}{2})\hbar\omega \tag{10}$$

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:

$$\begin{aligned}[N, a] &= [a^\dagger a, a] = a^\dagger aa - aa^\dagger a \\ &= (a^\dagger a - aa^\dagger)a = (-1)a = -a \end{aligned} \tag{11}$$

We conclude:

$$[N, a] = -a \tag{12}$$

Similarly, one can show:

$$[N, a^\dagger] = a^\dagger \tag{13}$$

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

$$N|n\rangle = n|n\rangle \tag{14}$$

Given this, notice the following:

$$\begin{aligned} Na^\dagger|n\rangle &= (a^\dagger N + [N, a^\dagger])|n\rangle \\ &= (a^\dagger N + a^\dagger)|n\rangle = na^\dagger|n\rangle + a^\dagger|n\rangle \\ &= (n+1)a^\dagger|n\rangle \end{aligned} \tag{15}$$

[1]Use the result of Problem 3 in "A short introduction to quantum mechanics III: the equivalence between Heisenberg's matrix method and Schrödinger's differential equation."

Therefore $a^\dagger|n\rangle$ 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:

$$Na|n\rangle = (n-1)a|n\rangle \tag{16}$$

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

Also, from (10), we see that $|n\rangle$ is an eigenvector of the Hamiltonian with eigenvalue $\left(n+\frac{1}{2}\right)\hbar\omega$. Therefore, $a^p|n\rangle$ will have $\left(n-p+\frac{1}{2}\right)\hbar\omega$ as its eigenvalue. At first glance, if we choose $p = n+1$ or larger, $a^p|n\rangle$ can have a negative eigenvalue. In other words, we have

$$H\left(a^p|n\rangle\right) = \left(n-p+\frac{1}{2}\right)\left(a^p|n\rangle\right) \tag{17}$$

where $(n-p+1/2)$ is negative.

But, it can't be, as our Hamiltonian (1) cannot be negative since p^2 and x^2 are always non-negative. If you don't understand what I mean, let me explain it to you. Suppose $|\psi\rangle$ is an arbitrary wave function. Then, we have

$$\langle\psi|H|\psi\rangle = \frac{1}{2m}\langle\psi|p^2|\psi\rangle + \frac{m\omega^2}{2}\langle\psi|x^2|\psi\rangle \tag{18}$$

The first term on the right-hand side is always non-negative, as

$$\langle\psi|p^2|\psi\rangle = \int dx\langle\psi|p|x\rangle\langle x|p|\psi\rangle \int dx(\langle x|p|\psi\rangle)^*(\langle x|p|\psi\rangle) \tag{19}$$

is always non-negative. Similarly, the second term on the right-hand side is also always non-negative, as

$$\langle\psi|x^2|\psi\rangle = \int dx\langle\psi|x|x\rangle\langle x|x|\psi\rangle = \int dx(\langle x|x|\psi\rangle)^*(\langle x|x|\psi\rangle) \tag{20}$$

is always non-negative. Thus, $\langle\psi|H|\psi\rangle \geq 0$.

Let's plug in an eigenvector of H with eigenvalue E to $|\psi\rangle$. Then,

$$\langle\psi|H|\psi\rangle = \langle\psi|E|\psi\rangle = E\langle\psi|\psi\rangle \geq 0 \tag{21}$$

Therefore, the eigenvalue E cannot be negative.

Therefore, we cannot arbitrarily lower the energy eigenvalue by applying the lowering operator repeatedly to $|n\rangle$. Where have we gone wrong? Where is the loophole in our argument? (17) is still correct, even when $(n-p+1/2)$ is negative. The only way this formula is satisfied without $a^p|n\rangle$ being a proper eigenvector is

$$a^p|n\rangle = 0 \tag{22}$$

Then, both the left-hand side and the right-hand side of (17) are zero.

In other words, we see that we reached a zero-vector at a certain point when we applied a repetitively to $|n\rangle$. In other words, there exists $l \leq p-1$, such that $a^l|n\rangle$ is not a zero vector, but

$$a^{l+1}|n\rangle = 0 \tag{23}$$

Now, let's define

$$|\psi_l\rangle \equiv a^l|n\rangle \tag{24}$$

Then, from (23), it satisfies $a|\psi_l\rangle = 0$.

Now, it is easy to see:

$$N|\psi_l\rangle = a^\dagger a|\psi_l\rangle = a^\dagger \cdot 0 = 0 = 0|\psi_l\rangle \tag{25}$$

Therefore, $|\psi_l\rangle$ is an eigenvector of N with eigenvalue 0. It implies $|\psi_l\rangle = c|0\rangle$ up to some normalization factor c, if we use the notation of (14), and want to normalize $|0\rangle$ by $\langle 0|0\rangle = 1$. Now notice that not only H, but also N cannot have a negative eigenvalue, because

$$\langle n|N|n\rangle = (\langle n|a\dagger)(a|n\rangle) = (a|n\rangle)^*(a|n\rangle) \geq 0 \tag{26}$$

Thus, we see that $|0\rangle$ has the lowest eigenvalue for N, which is zero. Therefore, it also has the lowest eigenvalue for the energy operator which is given by $(N+1/2)\hbar\omega$. Thus, it is the ground state, i.e., the lowest energy 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 the 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 $|0\rangle$ as follows. (6) and $a|0\rangle = 0$ implies:

$$\left(x + \frac{\hbar}{m\omega}\frac{d}{dx}\right)\psi_0(x) = 0 \tag{27}$$

The solution is given by:

$$\psi_0(x) = Ce^{-\frac{m\omega}{2\hbar}x^2} \tag{28}$$

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 $|1\rangle$ can be obtained as follows:

$$\psi_1(x) = \left(x - \frac{\hbar}{m\omega}\frac{d}{dx}\right)\psi_0(x) \tag{29}$$

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

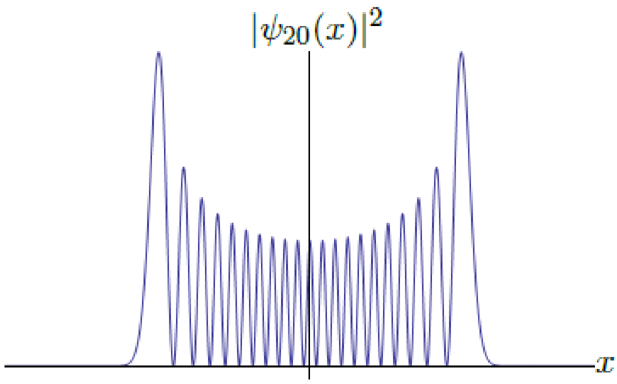

Figure 1: $|\psi_{20}(x)|^2$

will be found at the position between x and $x + dx$. It is naturally given by $|\psi_n(x)|^2 dx$.

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 $|n\rangle$s are normalized (i.e. the norm is 1) show that the following $|n+1\rangle$ and $|n-1\rangle$ are also properly normalized.

$$|n+1\rangle = \frac{a^\dagger}{\sqrt{n+1}}|n\rangle, \quad |n-1\rangle = \frac{a}{\sqrt{n}}|n\rangle \tag{30}$$

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

$$\langle n|x|n\rangle, \quad \langle n|x|n+1\rangle \tag{31}$$

[2]Express x in terms of a and $a^\dagger$ using (6) and (7), and use the result of Problem 2.

Problem 4. How does the expectation value of the position x for a quantum state initially given by $\frac{|3\rangle+|4\rangle}{\sqrt{2}}$ 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 $|0\rangle$). Show that the uncertainty principle would be violated if there existed a state $|\psi\rangle$ of which the energy for harmonic oscillator is zero. (i.e. $\langle\psi|H|\psi\rangle = 0$ 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])

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.
- $|n\rangle$ is defined by $N|n\rangle = n|n\rangle$. The eigenvalues n are always non-negative integers. $a^\dagger|n\rangle$ has an eigenvalue $n+1$. $a|n\rangle$ has an eigenvalue $n-1$, unless $n = 0$. When $n = 0$, we have $a|0\rangle = 0$.

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