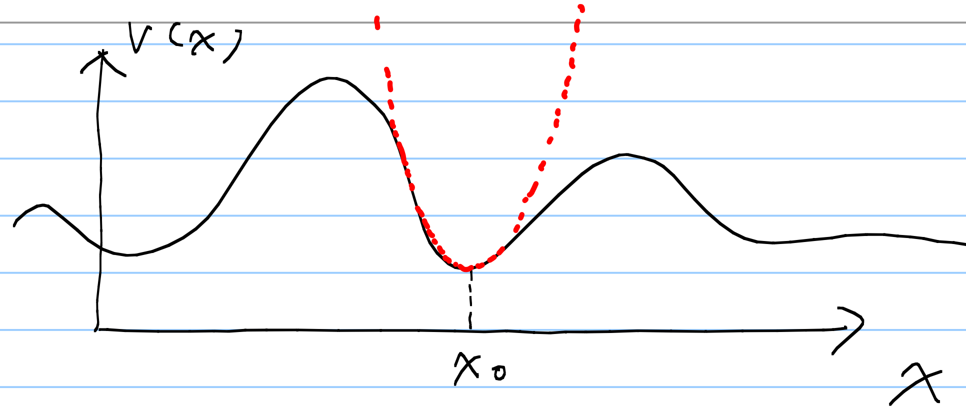
Harmonic Oscillator

4-1

Note Title 9/20/2010



For an arbitrary potential, in the neighborhood of a local minimum, using the taylor series about the minimum

$$V(x) = V(0) + V'(x_0)(x-x_0) + \frac{1}{2}V''(x_0)(x-x_0)^2 + \cdots.$$

Since $V'(x_0)=0$ because x_0 is a local minimum and if we take $V(0)$ also as zero without losing any generality, near the local minimum

$$V(x) \simeq \frac{1}{2}V''(x_0)(x-x_0)^2$$

Or using the spring constant concept based on the Hooke's law

$$V(x) = \frac{1}{2}kx^2, \quad \text{with } x_0 = 0, \quad k = V''(x_0).$$

This is called simple harmonic oscillator or just harmonic oscillator

We know from Newton's second law that the motion governed by this simple harmonic oscillator corresponds to an oscillation with

$$\omega = \sqrt{\frac{k}{m}} \Rightarrow k = m\omega^2$$

So the Hamiltonian of an harmonic oscillator is

$$H = T + V = \frac{p^2}{2m} + \frac{1}{2} m\omega^2 x^2 .$$

Now we want to solve the T.I.S.E.

$$H\psi(x) = E\psi(x)$$

$$\Rightarrow \frac{1}{2m}\left[p^2 + (m\omega x)^2\right]\psi = E\psi(x)$$

There are two ways to solve this :
① power series method (Sect. 2.3.2)
② ladder operator method (Sect. 2.3.1)

We will mostly focus onto the second method, which is more important than the first.

We want to replace the quadratic operators (p^2 and x^2) by linear operators.

Noting that $u^2 + v^2 = (iu + v)(-iu + v)$, Let's define two so called ladder operators : we will see the origin of this name soon

$$\boxed{a_\pm \equiv \frac{1}{\sqrt{\hbar\omega}} \frac{1}{\sqrt{2m}} (\mp ip + m\omega x)}$$

Now

$$a_- a_+ = \frac{1}{2\hbar\omega m} (ip + m\omega x)(-ip + m\omega x)$$

$$= \frac{1}{2\hbar\omega m} \left(p^2 + (m\omega x)^2 - im\omega(xp - px) \right)$$

Here $(xp - px) \equiv [x, p]$ is called the commutator of x and p.
In general, the commutator of any two operators A and B is $[A, B] = AB - BA$

With this notation

$$a_- a_+ = \frac{1}{2\hbar\omega m}\left(p^2 + (m\omega x)^2\right) - \frac{i}{2\hbar}[x, p]$$

The important thing is that $[x, p]$ is not zero, as we see below:

$$[x, p] f(x) = x \frac{\hbar}{i}\frac{d}{dx}(f) - \frac{\hbar}{i}\frac{d}{dx}(xf)$$

$$= \frac{\hbar}{i}\left(\cancel{x\frac{df}{dx}} - x\frac{df}{dx} - \left(\frac{dx}{dx}\right) f \right)$$

$$= i\hbar f(x)$$

$$\therefore \quad \boxed{[x, p] = i\hbar}$$

This is called the "canonical commutation relation."

We usually say that "x" and "p" do not commute. And any non-commuting operators have uncertainty principle involved: we will learn more about this in Chap. 3.

Now with this commutator

$$a_- a_+ = \frac{1}{2\hbar\omega m}\left(p^2 + (m\omega x)^2\right) + \frac{1}{2}$$

$$= \frac{1}{\hbar\omega} \cdot H + \frac{1}{2}$$

$$\Rightarrow \boxed{H = \hbar\omega\left(a_- a_+ - \frac{1}{2}\right)}$$

If we go through similar steps,

$$a_+ a_- = \frac{1}{\hbar\omega} H - \frac{1}{2}$$

In particular, $[a_-, a_+] = 1$

Now the T.I.S.E. reduces to

$$H\psi = E\psi$$

$$\Rightarrow \quad \hbar\omega\left(a_\pm a_\mp \pm \frac{1}{2}\right)\psi = E\psi$$

* Now comes a crucial step:
If ψ is an eigenfcn with E, then $a_+\psi$ is another eigenfcn with $E+\hbar\omega$.

In other words, if $H\psi = E\psi$, then

$$H(a_+\psi) = (E+\hbar\omega)(a_+\psi).$$

Let's see how this happens:

$$H(a_+\psi) = \hbar\omega\left(a_+a_- + \frac{1}{2}\right)(a_+\psi)$$
$$= \hbar\omega\left(a_+a_-a_+ + \frac{1}{2}a_+\right)\psi$$
$$= \hbar\omega \cdot a_+\left(a_-a_+ + \frac{1}{2}\right)\psi$$
$$= \hbar\omega \cdot a_+\left(a_-a_+ - \frac{1}{2} + 1\right)\psi$$
$$= a_+\left(\hbar\omega\left(a_-a_+ - \frac{1}{2}\right)\psi + \hbar\omega\psi\right)$$
$$= a_+\left(H\psi + \hbar\omega\psi\right) = a_+\left(E\psi + \hbar\omega\psi\right)$$
$$= a_+(E+\hbar\omega)\psi = (E+\hbar\omega)(a_+\psi)$$
$$\therefore \text{ Q.E.D.}$$

The same way, if $H\psi = E\psi$, then

$$H(a_-\psi) = (E-\hbar\omega)(a_-\psi)$$

So we call a_+ : raising operator
a_- : lowering operator

Or

both of them ladder operators

* Here, because the lowest energy cannot be lower than zero, if the lowest rung corresponds to ψ_0 with E_0, $a_-\psi_0$ should not exist. In other words, $a_-\psi_0$ should not be normalizable.

There are two possibilities for the non-normalizability : ① zero
② square-integral is infinite.

We cannot prove which one of these two is correct, but from consistency with the power-series method, we find "①" is the case.

In other words $a_-\psi_0 = 0$

We can use this to determine ψ_0 as follows.

$$a_- \equiv \frac{1}{\sqrt{\hbar\omega}}\frac{1}{\sqrt{2m}}(ip + m\omega x)$$
$$= \frac{1}{\sqrt{\hbar\omega}}\frac{1}{\sqrt{2m}}\left(\hbar\frac{d}{dx} + m\omega x\right)$$

$\Rightarrow$ $a_-\psi_0 = 0$ gives

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

$$\Rightarrow \frac{d}{dx}\psi_0 = -\frac{m\omega}{\hbar}x\psi_0 \Rightarrow \frac{d\psi_0}{\psi_0} = -\frac{m\omega}{\hbar}x\,dx$$

$$\Rightarrow \ln\psi_0 = -\frac{m\omega}{2\hbar}x^2 + \text{const}$$

$$\Rightarrow \psi_0 = A e^{-\frac{m\omega}{2\hbar}x^2}$$

Normalize it

$$1 = A^2\int_{-\infty}^{\infty} e^{-\frac{m\omega}{\hbar}x^2}dx = A^2\sqrt{\frac{\pi\hbar}{m\omega}}$$

$$\Rightarrow A = \left(\frac{m\omega}{\pi\hbar}\right)^{\frac{1}{4}}$$

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

How about E_0 ?

$$H\psi_0 = E_0\psi_0 \Rightarrow \hbar\omega(a_+a_- + \tfrac{1}{2})\psi_0 = E_0\psi_0$$

$$\Rightarrow \hbar\omega(a_+\cdot 0 + \tfrac{1}{2}\psi_0) = E_0\psi_0$$

$$\Rightarrow (\tfrac{1}{2}\hbar\omega)\psi_0 = E_0\psi_0 \Rightarrow E_0 = \tfrac{1}{2}\hbar\omega$$

Now, all the higher eigen energies can be obtained through $E_1 = E_0 + \hbar\omega = (1+\frac{1}{2})\hbar\omega$
$E_2 = E_1 + \hbar\omega = (2+\frac{1}{2})\hbar\omega$

--- $E_n = (n+\frac{1}{2})\hbar\omega$, with the eigenfcts
$\psi_n(x) = A_n(a_+)^n\psi_0(x)$ with proper normalization constants.

$\boxed{\text{Ex.}}$ Find the first excited state of the harmonic oscillator

$$\psi_1(x) = A_1 a_+\psi_0(x)$$

$$= A_1 \frac{1}{\sqrt{\hbar\omega}}\frac{1}{\sqrt{2m}}(-iP + m\omega x)\psi_0(x)$$

$$= A_1 \frac{1}{\sqrt{2m\hbar\omega}}\left(-\hbar\frac{d}{dx} + m\omega x\right)\left(\frac{m\omega}{\pi\hbar}\right)^{\frac{1}{4}} e^{-\frac{m\omega}{2\hbar}x^2}$$

$$= A_1\cdot\frac{1}{\sqrt{2m\hbar\omega}}\cdot\left(\frac{m\omega}{\pi\hbar}\right)^{\frac{1}{4}}\cdot(m\omega x + m\omega x)\, e^{-\frac{m\omega}{2\hbar}x^2}$$

$$= A_1\left(\frac{m\omega}{\pi\hbar}\right)^{\frac{1}{4}}\sqrt{\frac{2m\omega}{\hbar}}\cdot x\, e^{-\frac{m\omega}{2\hbar}x^2}$$

$$1 = \int_{-\infty}^{\infty}|\psi_1|^2 dx \Rightarrow \text{gives } A_1 = 1$$

* Is there an easier way to find A_n?
Yes: see below.

Note that $H\psi_n = E_n \psi_n$

$$\Rightarrow \hbar\omega\left(a_+a_- + \tfrac{1}{2}\right)\psi_n = \hbar\omega\left(n+\tfrac{1}{2}\right)\psi_n$$

$$\Rightarrow \quad a_+a_-\psi_n = n\psi_n .$$

[We also call a_+a_- the "number operator"] because of this property

Also, nothe that $a_\pm$ is the "hermitian conjugate" of $a_\mp$; we will discuss this more in chap. 3.

This implies that for arbitrary functions $f(x)$ and $g(x)$

$$\int f^*(a_\pm g)\,dx = \int (a_\mp f)^* g\,dx$$

; See Griffiths for the proof

Now if $a_+\psi_n = c_n\psi_{n+1}$,

$$\int (a_+\psi_n)^*(a_+\psi_n)\,dx = |c_n|^2 \int \psi_{n+1}^*\psi_{n+1}\,dx$$

$$\Leftrightarrow \int \psi_n^*(a_-a_+\psi_n)\,dx = |c_n|^2$$

$$\Leftrightarrow \int \psi_n^*(a_+a_- + 1)\psi_n\,dx = |c_n|^2$$

$$\Leftrightarrow \int \psi_n^* n\psi_n\,dx + \int \psi_n^*\psi_n\,dx = |c_n|^2$$

$$\Rightarrow |c_n|^2 = n+1 \Rightarrow c_n = \sqrt{n+1}$$

$\Rightarrow$ $\boxed{\begin{aligned} a_+ \psi_n &= \sqrt{n+1}\ \psi_{n+1} \\ a_- \psi_n &= \sqrt{n}\ \psi_{n-1} \end{aligned}}$, and similarly

Then $a_+ \psi_{n-1} = \sqrt{n}\ \psi_n$

$$\Rightarrow \psi_n = \frac{1}{\sqrt{n}} a_+ \psi_{n-1} = \frac{1}{\sqrt{n}} \cdot \frac{1}{\sqrt{n-1}} a_+^2 \psi_{n-2} = \cdots$$

$$= \frac{1}{\sqrt{n!}} (a_+)^n \psi_0$$

e.g., $\psi_1 = a_+ \psi_0$ just as we found in the previous example.

* Some more useful properties are :

$\int_{-\infty}^{\infty} \psi_m^* \psi_n \, dx = \delta_{mn}$, as they should be ; see Griffiths for proof.

Also from
$$a_- = \frac{1}{\sqrt{\hbar\omega}} \frac{1}{\sqrt{2m}} (ip + m\omega x)$$
$$a_+ = \frac{1}{\sqrt{\hbar\omega}} \frac{1}{\sqrt{2m}} (-ip + m\omega x)$$

$$\boxed{\begin{aligned} x &= \sqrt{\frac{\hbar}{2m\omega}} (a_+ + a_-) \\ p &= i\sqrt{\frac{\hbar m\omega}{2}} (a_+ - a_-) \end{aligned}}$$

$\boxed{\text{Ex,}}$ $\Psi(x,0) = \frac{1}{\sqrt{2}} (\psi_0(x) + \psi_1(x))$

Find $\langle x \rangle$, $\langle p \rangle$, and $\langle x^2 \rangle$

From $a_+ \psi_0 = \psi_1$, $a_+ \psi_1 = \sqrt{2}\, \psi_2$
$a_- \psi_0 = 0$, $a_- \psi_1 = \psi_0$,

$$\langle a_+\rangle = \frac{1}{2}\langle \psi_0 + \psi_1 | a_+ | \psi_0 + \psi_1\rangle$$
$$= \frac{1}{2}\langle \psi_0 + \psi_1 | \psi_1 + \sqrt{2}\psi_2\rangle$$
$$= \frac{1}{2}\left[\cancel{\langle \psi_0 | \psi_1\rangle}^{0} + \cancel{\langle \psi_0 | \sqrt{2}\psi_2\rangle}^{0} + \langle \psi_1 | \psi_1\rangle + \cancel{\langle \psi_1 | \sqrt{2}\psi_2\rangle}^{0}\right]$$
$$= \frac{1}{2}$$

$$\langle a_-\rangle = \frac{1}{2}\langle \psi_0 + \psi_1 | a_- | \psi_0 + \psi_1\rangle$$
$$= \frac{1}{2}\langle \psi_0 + \psi_1 | 0 + \psi_0\rangle$$
$$= \frac{1}{2}\left[\langle \psi_0 | \psi_0\rangle + \cancel{\langle \psi_1 | \psi_0\rangle}^{0}\right]$$
$$= \frac{1}{2}$$

Thus $\langle x\rangle = \sqrt{\frac{\hbar}{2m\omega}}\left[\langle a_+\rangle + \langle a_-\rangle\right]$

$$= \sqrt{\frac{\hbar}{2m\omega}}\left[\frac{1}{2} + \frac{1}{2}\right] = \sqrt{\frac{\hbar}{2m\omega}}$$

$$\langle p\rangle = i\sqrt{\frac{\hbar m\omega}{2}}\left[\langle a_+\rangle - \langle a_-\rangle\right]$$
$$= i\sqrt{\frac{\hbar m\omega}{2}} \cdot \left[\frac{1}{2} - \frac{1}{2}\right] = 0$$

$$\langle x^2\rangle = \frac{\hbar}{2m\omega}\cdot\frac{1}{2}\langle \psi_0 + \psi_1 | (a_+ + a_-)^2 | \psi_0 + \psi_1\rangle$$

$$(a_+ + a_-)^2 = a_+^2 + a_+a_- + \underbrace{a_-a_+}_{= a_+a_- + 1} + a_-^2$$
$$= a_+^2 + 2a_+a_- + a_-^2 + 1$$

$$a_+^2 | \psi_0 + \psi_1\rangle = C_1 | \psi_2\rangle + C_2 | \psi_3\rangle$$
$$a_+a_- | \psi_0 + \psi_1\rangle = a_+a_- | \psi_1\rangle = | \psi_1\rangle$$
$$a_-^2 | \psi_0 + \psi_1\rangle = 0$$

So $\langle \psi_0 + \psi_1 | (a_+ + a_-)^2 | \psi_0 + \psi_1\rangle$

$$= \langle \psi_0 + \psi_1 | C_1 | \psi_2\rangle + \langle \psi_0 + \psi_1 | C_2 | \psi_3\rangle$$

$$+ 2\langle \psi_0+\psi_1 | \psi_1 \rangle + \langle \psi_0+\psi_1 | 0 \rangle$$
$$+ \langle \psi_0+\psi_1 | \psi_0+\psi_1 \rangle$$

$$= 2\langle \psi_1 | \psi_1 \rangle + \langle \psi_0 | \psi_0 \rangle + \langle \psi_1 | \psi_1 \rangle$$
$$= 4$$

$$\therefore \langle x^2 \rangle = \frac{\hbar}{2m\omega} \cdot \frac{1}{2} \cdot 4 = \frac{\hbar}{m\omega}$$

Here I used the so-called Dirac notation to simplify the algebra.

We will discuss this more in chap. 3.

In short in Dirac notation

$$\langle \psi | Q | \phi \rangle \equiv \int \psi^* Q \phi \, dx$$

$$\langle \psi_1+\psi_2 | Q | \phi_1+\phi_2 \rangle$$
$$= \int (\psi_1+\psi_2)^* Q (\phi_1+\phi_2) \, dx \text{ , etc.}$$