The Simple Harmonic Oscillator II

In a previous lecture we solved the Schrödinger equation for the harmonic Oscillator using the traditional technology for solving ODEs.

In this lecture we shall revisit the SHO but solve it using a different algebraic tool known as ladder operators. This method was invented P. A. M. Dirac and its generalizations have found wide range applications in both physics and mathematics.

Rewriting the Hamiltonian in terms of creation/annihilation operators.

One of the key observations about the SHO hamiltonian is that it is a quadratic operator:

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

We saw in a previous lecture that it implies that the energy eigenvalues of H are positive definite. If ψ is a state then

$$(\psi, H\psi) = \frac{1}{2m} \|p\psi\|^2 + \frac{1}{2} m\omega^2 \|x\psi\|^2$$

$$\geq 0 .$$

The stroke of genius by Dirac was to introduce re-write the Hamiltonian in terms of the following non-Hermitian operators:

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

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

a and $a^\dagger$ are not Hermitian but they are conjugate of each other:

$$[a]^\dagger = \left[\sqrt{\frac{m\omega}{2\hbar}} \left(x + \frac{iP}{m\omega}\right)\right]^\dagger$$

$$= \sqrt{\frac{m\omega}{2\hbar}} \left(x^\dagger - i p^\dagger\right)$$

$$= \sqrt{\frac{m\omega}{2\hbar}} \left(x - i P\right)$$

$$= a^\dagger.$$

Now recall the fundamental commutation relation

$$[x, p] = i\hbar.$$

as well as $[x, x] = [p, p] = 0$.

Using these we get

$$[a, a^\dagger] = \left(\frac{m\omega}{2\hbar}\right)\left[x + \frac{ip}{m\omega}, x - \frac{ip}{m\omega}\right]$$

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

$$= \frac{+i}{2\hbar}\left\{-i\hbar + i\hbar\right\}$$

$$= 1$$

And so $\boxed{[a, a^\dagger] = 1}$

Let us introduce $N = a^\dagger a$. Then it is not hard to see that

$$H = \left(N + \frac{1}{2}\right)\hbar\omega \quad [\text{show}].$$

Note that $[H, N] = 0$. Thus if ψ is an eigenfunction of H with eigenvalue E then ψ is also an eigenfunction of N. This is true in general.

Let A & B be two operators such that they commute i.e.

$$[A, B] = 0$$

Let ψ be an eigenfunction of A with eigenvalue a (assumed to be non-degenerate). Then ψ is also an eigenfunction of B.

Proof:

$$A\psi = a\psi$$

If we apply B to this we get:

$$\begin{aligned} B(A\psi) &= B(a\psi) \\ (BA)\psi &= aB\psi \quad \left[\begin{array}{c}\text{Since } a \text{ is a number} \\ \text{it commutes with } B\end{array}\right] \\ (AB)\psi &= a(B\psi) \\ A(B\psi) &= a(B\psi) \end{aligned}$$

So we see $(B\psi)$ is also an eigenfunction of A with the same eigenvalue a. Since a is a non-degenerate eigenvalue it implies that $B\psi$ and ψ are proportional to each other:

$$B\psi \propto \psi$$

Let us call the constant of proportionality b:

$$B\psi = b\psi$$

Thus we see that ψ is an eigenfunction of both A and B. Such eigenfunctions are called simultaneous eigenfunctions. ■

So the eigenfunctions of H are also eigenfunctions of N.

$$N\psi_n = n\psi_n, \quad \text{let } n \text{ be eigenvalues of } N.$$

Then $H\psi_n = \left(n+\frac{1}{2}\right)\hbar\omega\, \psi_n$

Interpretation of N, a and $a^\dagger$:

N is obviously Hermitian: $N^\dagger = (a^\dagger a)^\dagger = a^\dagger (a^\dagger)^\dagger = a^\dagger a$.

[This uses the fact that $(AB)^\dagger = B^\dagger A^\dagger$.]

N is also positive definite:

$$(\psi, N\psi) = (\psi, a^\dagger a\psi) = ((a^\dagger)^\dagger\psi, a\psi)$$
$$= (a\psi, a\psi) = \|a\psi\|^2 \geq 0$$

Since ψ is arbitrary we write $N \geq 0$.

Next consider $[N, a]$:

$$[N, a] = [a^\dagger a, a] = a^\dagger[a, a] + [a^\dagger, a]a$$

[This uses the identity $[AB, C] = ABC - CAB$

$= ABC - ACB + ACB - CAB = A[B, C] + [A, C]B$]

So $[N, a] = a^\dagger \cdot 0 + (-1)a \Rightarrow [N, a] = -a.$

Similarly, $[N, a^\dagger] = +a^\dagger$.

Let ψ_n be an eigenfunction of N with eigenvalue n.

$$N\psi_n = n\psi_n.$$

What is the effect of a on ψ_n?

$$N(a\psi_n) = (aN - a)\psi_n \text{ , [we have used } [N, a] = -a \text{]}$$

$$= aN\psi_n - a\psi_n$$
$$= a \cdot n \cdot \psi_n - a\psi_n$$
$$= (n-1)(a\psi_n)$$

Thus $a\psi_n$ is <u>also</u> an eigenfunction of N but with eigenvalue $(n-1)$. Thus we can write:

$$a\psi_n = c_{n-1}\psi_{n-1}$$

c_n is a constant of proportionality.

Similarly $a^\dagger\psi_n$ is also an eigenfunction of N but with eigenvalue $n+1$.

$$a^\dagger\psi_n = D_{n+1}\psi_{n+1} \text{ , } D_{n+1} \rightarrow \text{constant of proportionality}$$

Observations: $a^\dagger$ raises the N eigenvalue by 1 unit while a lowers the N eigenvalue by 1 unit.

$$\left.\begin{array}{l} a^\dagger \to \text{raising operator} \\ a \to \text{lowering operator} \end{array}\right\} \text{ladder operators}$$

Determination of C_n and D_n.

Let us assume that ψ_n are normalized and orthogonal:

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

Then

$$(a\psi_n, a\psi_n) = |C_{n-1}|^2 (\psi_{n-1}, \psi_{n-1})$$

or $(a^\dagger a \psi_n, \psi_n) = |C_{n-1}|^2 \cdot 1$

or $(N\psi_n, \psi_n) = |C_{n-1}|^2$

or $n(\psi_n, \psi_n) = |C_{n-1}|^2$

or $|C_{n-1}|^2 = n$

or $C_{n-1} = \sqrt{n}$.

$C_n = \sqrt{n+1}$

Similarly $(a^\dagger\psi_n, a^\dagger\psi_n) = |D_{n+1}|^2 (\psi_{n+1}, \psi_{n+1})$

or $(aa^\dagger\psi_n, \psi_n) = |D_{n+1}|^2 \cdot 1$

$((a^\dagger a+1)\psi_n, \psi_n) = |D_{n+1}|^2$

or $((N+1)\psi_n, \psi_n) = |D_{n+1}|^2$

or $(n+1)(\psi_n, \psi_n) = |D_{n+1}|^2$

or $|D_{n+1}|^2 = (n+1)$

$D_{n+1} = \sqrt{n+1}$

What happens if we keep on applying a ?

$$a\,\psi_n = \sqrt{n}\,\psi_{n-1}$$
$$a\,a\,\psi_n = \sqrt{n}\,a\,\psi_{n-1}$$
$$= \sqrt{n}\sqrt{n-1}\,\psi_{n-2}$$

$\vdots$

$$(a)^m \psi_n = \sqrt{n\cdot(n-1)\cdots(n-m+1)}\,\psi_{n-m}$$

This process cannot continue indefinitely since otherwise for some integer m the N eigenvalue of the state will become negative.

So the only way this lowering operation terminates is if n is an integer so that for some value of m, say m', we have:

$$(a)^{m'}\psi = 0$$

So here are our conclusions:

1. $N\psi_n = n\psi_n$, $n = 0, 1, 2, 3, \ldots$

   $N \rightarrow$ Number operator.

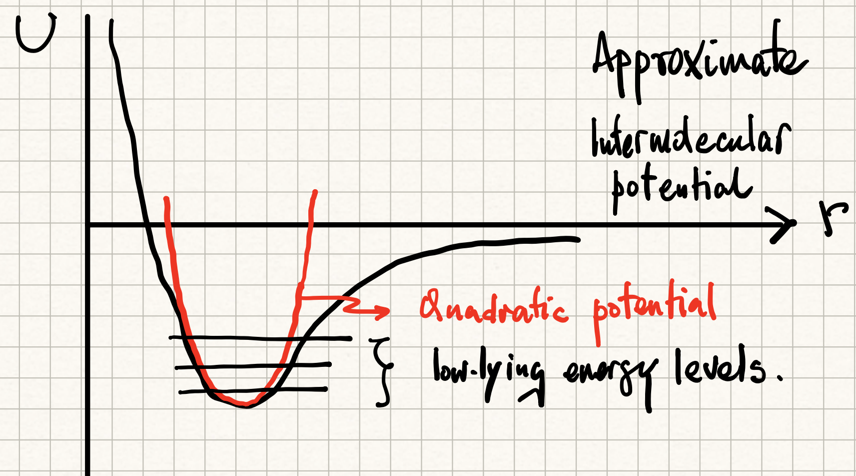
2. $a^\dagger$: raising operator

3. a : lowering operator

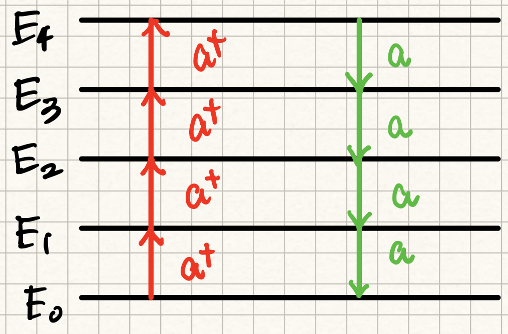
4. The eigenvalue spectrum of the Hamiltonian

$$E_n = \frac{1}{2}\hbar\omega,\ \frac{3}{2}\hbar\omega,\ \frac{5}{2}\hbar\omega,\ \ldots\ldots$$

5. Note that difference in energy of two consecutive energy levels is $\Delta E = \hbar\omega$. As discussed in the previous lecture on the SHO the intermolecular potential roughly looks like that of the SHO:



Graphically :



This is strong evidence that the quanta of energy $\hbar\omega$ can be thought of as a photon. In general, in QFT the harmonic oscillator provides for a model of a quantum field whose excitations can be interpreted as particles.

This motivates the alternative names creation and annihilation operator for the operators a^+ and a, respectively.

Explicit forms of the wave functions

We have solved for the energy eigenvalues of the SHO using the ladder operators. For most purposes we don't need much else apart from the fact that ψ_n form an orthonormal set. But we can derive the explicit forms of ψ_n easily.

We start with the vacuum state ψ_0. Recall that ψ_0 is annihilated by a:

$$a\,\psi_0 = 0$$

Using the representation of a in terms of x & p we get:

$$\sqrt{\frac{m\omega}{2\hbar}}\left[x - \frac{i}{m\omega}\left(-i\hbar\frac{d}{dx}\right)\right]\psi_0(x) = 0$$

or $\left(x + x_0^2\dfrac{d}{dx}\right)\psi_0(x) = 0$, where $x_0^2 = \dfrac{\hbar}{m\omega}$

This equation is easily solved:

$$\frac{d\psi_0}{\psi_0} = -\frac{x}{x_0^2}\,dx$$

$$\psi_0 = c\,e^{-x^2/2x_0^2}$$

which after normalizing leads to

$$\psi_0 = \frac{1}{\sqrt{x_0\sqrt{\pi}}}\,e^{-x^2/2x_0^2}$$

Using a similar logic we can derive the excited states:

$$\sqrt{1}\ \psi_1(x) = a^{\dagger}\psi_0(x)$$
$$= \frac{1}{\sqrt{2}\,x_0}\left(x - x_0^2\frac{d}{dx}\right)\psi_0(x)$$

$\vdots$

And so we get

$$\psi_n(x) = \frac{1}{\sqrt{\sqrt{\pi}\,2^n n!}}\frac{1}{x_0^{n+1/2}}\left(x - x_0^2\frac{d}{dx}\right)^n e^{-\frac{1}{2}\left(\frac{x}{x_0}\right)^2}$$

In terms of the Hermites we can write [show]:

$$\psi_n(x) = \left[\frac{m\omega}{\pi\hbar\,2^{2n}(n!)^2}\right]^{1/4} e^{-\frac{1}{2}\left(\frac{x}{x_0}\right)^2} H_n(x/x_0).$$

In general, we know from the previous lecture:

$$(\Delta x)(\Delta p) \geq \frac{\hbar}{2}.$$

But for the ground state ψ_0, it can be shown that this bound is saturated:

$$(\Delta x)_{\Psi_0} (\Delta p)_{\Psi_0} = \frac{\hbar}{2}.$$

The Gaussian is the only state that saturates the bound.

The Heisenberg Formulation of quantum mechanics: The Schrödinger Picture & The Heisenberg Picture

In quantum mechanics what we observe are the inner products: $(\chi, \hat{O}\Psi)(t)$ which are functions of time.

According to Schrödinger the dynamics is encoded in the wavefunctions whose time evolution is given by the Schrödinger equation:

$$i\hbar \frac{\partial \Psi}{\partial t}(x,t) = H\Psi(x,t)$$

In these formulations the observables are time independent operators. This formulation of quantum mechanics is known as the Schrödinger picture of quantum mechanics.

But there is an alternate description of quantum mechanics in which the opposite is true.

Consider an observable $\hat{O}$ in the Schrödinger picture and two states ψ and ϕ. Then the inner product $(\psi, \hat{O}\phi)(t)$ is time dependent:

$$(\psi(t), \hat{O}\,\phi(t)) = (U(t)\psi(0), \hat{O}\,U(t)\,\phi(0))$$

[The x dependence is suppressed as it has been integrated over].

Define $\hat{O}_H(t) = U^\dagger(t)\,\hat{O}\,U(t)$

and $\psi_H = \psi(0)$ etc.

Then we get $(\psi(t), \hat{O}\,\phi(t)) = (\psi(0), U^\dagger(t)\,\hat{O}\,U(t)\,\phi(0))$

$$= (\psi_H, \hat{O}_H(t)\,\phi_H).$$

Here $\hat{O}_H(t)$ is the time dependent object while

ψ_H is fixed. The dynamics is given by an equation for the operators $\hat{O}_H(t)$ and they are known as the Heisenberg equations:

For systems for which the Hamiltonian is independent of time:

$$\frac{d}{dt}\hat{O}_H = \frac{d}{dt}\left(U^\dagger(t)\,\hat{O}_S\,U(t)\right)$$

[where we denote $\hat{O}_S$ as the operator in Schrödinger picture

$$= \frac{dU^\dagger}{dt}\cdot\hat{O}_S\cdot U + U^\dagger\hat{O}\frac{dU}{dt}$$

Note that $\frac{d}{dt}U = \frac{d}{dt}e^{iHt/\hbar} = \frac{iH}{\hbar}e^{iHt/\hbar} = \frac{iH}{\hbar}U(t)$

and $\frac{dU^\dagger}{dt} = U(t)^\dagger\left(\frac{i}{\hbar}\right)H$

so $\frac{d\hat{O}_H}{dt} = \frac{i}{\hbar}U^\dagger(t)\,H\,\hat{O}_S\,U(t) - \frac{i}{\hbar}U^\dagger(t)\,\hat{O}_S\,H\,U(t)$

But $[U^\dagger(t), H] = 0$ and $[U(t), H] = 0$

and so

$$\boxed{\frac{d\hat{O}_H}{dt} = +\frac{i}{\hbar}\left[\hat{H}, \hat{O}_H(t)\right]}$$

This is the Heisenberg equation of motion.

Comment:

1. H commutes U(t) and so H is the same in both Heisenberg and Schrödinger pictures.

Time dependence of $\langle x \rangle$ for the SHO:

The full time dependent wave function of the SHO has the form:

$$\psi(x,t) = \sum_n c_n \, \psi_n(x) \, e^{-iE_n t/\hbar}$$

where $\psi_n(x)$ are the energy eigenstates and their energy eigenvalues are given by:

$$E_n = (n+\tfrac{1}{2})\hbar\omega$$

More explicitly we can write:

$$\psi(x,t) = e^{-\frac{i}{2}\omega t} \sum_n c_n \, \psi_n(x) \, e^{-in\omega t}$$

with $\quad c_n = (\psi_n, \psi(t=0))$

And so we have:

$$\langle x \rangle = \int dx \, \psi^*(x,t) \, x \, \psi(x,t)$$

$$= \int dx \sum_{n,m} c_m^* c_n \, \psi_m(x) \, x \, \psi_n(x) \, e^{-i(n-m)\omega t}$$

$$= \sum_{n,m} c_m^* c_n e^{-i(n-m)\omega t} \int dx \, \psi_m(x) \, x \, \psi_n(x)$$

But from:

$$a = \sqrt{\frac{m\omega}{2\hbar}} \left(x + \frac{ip}{m\omega} \right)$$

$$a^\dagger = \sqrt{\frac{m\omega}{2\hbar}} \left(x - \frac{ip}{m\omega} \right)$$

we get $x = \sqrt{\frac{\hbar}{2m\omega}} \left(a + a^\dagger \right)$

ands $x \psi_n = \sqrt{\frac{\hbar}{2m\omega}} \left(a + a^\dagger \right) \psi_n$

$$= \sqrt{\frac{\hbar}{2m\omega}} \left(\sqrt{n} \, \psi_{n-1} + \sqrt{n+1} \, \psi_{n+1} \right)$$

And so $\int dx \, \psi_m(x) \, x \, \psi_n(x)$

$$= \sqrt{\frac{\hbar}{2m\omega}} \left(\sqrt{n} \, \delta_{m,n-1} + \sqrt{n+1} \, \delta_{m,n+1} \right)$$

Thus we have

$$\langle x \rangle = \sqrt{\frac{\hbar}{2m\omega}} \sum_{m,n} \left(c_m^* c_n e^{-i(n-m)\omega t} \left(\sqrt{n}\, \delta_{m,n-1} + \sqrt{n+1}\, \delta_{m,n+1} \right) \right)$$

$$= \sqrt{\frac{\hbar}{2m\omega}} \sum_{n=0}^{\infty} \left(c_{n-1}^* c_n e^{-i(\cancel{n}-\cancel{n}+1)\omega t} \sqrt{n} + c_{n+1}^* c_n \cdot e^{-i(\cancel{n}-\cancel{n}-1)\omega t} \sqrt{n+1} \right)$$

$$= \sqrt{\frac{\hbar}{2m\omega}} \sum_{n=1}^{\infty} \left(c_{n-1}^* c_n e^{-i\omega t} \sqrt{n} + c_n^* c_{n-1} e^{i\omega t} \sqrt{n} \right)$$

Writing $c_n = |c_n| e^{i\phi_n}$ we get

$$\langle x \rangle = \sqrt{\frac{\hbar}{2m\omega}} \sum_{n=1}^{\infty} |c_{n-1}||c_n| \sqrt{n} \left(e^{-i(\omega t - \phi_n + \phi_{n-1})} + e^{i(\omega t - \phi_n + \phi_{n-1})} \right)$$

$$= \sqrt{\frac{\hbar}{2m\omega}} \sum_{n=1}^{\infty} |c_n||c_{n-1}|\, 2\sqrt{n} \cos(\omega t - \phi_n + \phi_{n-1})$$

$$\boxed{\langle x \rangle(t) = \sqrt{\frac{2\hbar}{m\omega}} \sum_{n=1}^{\infty} |c_n||c_{n-1}| \sqrt{n} \cos(\omega t + \phi_{n-1} - \phi_n)}$$

One can also derive this result using the Heisenberg picture:

Recall $x_H(t) = U(t)^\dagger x_H(0)\, U(t)$ with $U(t) = e^{-\frac{i}{\hbar}Ht}$ and $x_H(0) = x_S$.

We can use the BCH formula:

$$U^\dagger(t)\, x_H(0)\, U(t) = e^{-\frac{i}{\hbar}Ht}\, x_H(0)\, e^{\frac{i}{\hbar}Ht}$$

$$= \sum_{n=0}^{\infty} \frac{\left(-\frac{i}{\hbar}t\right)^n}{n!} [H,[H,[H,[H \ldots,[H,x_H(0)]] \ldots]$$

This power series breaks up into two power series, one with even power and the other with odd power:

Now recall: $[H,x] = \frac{1}{2m}[p^2, x] = -\frac{2i\hbar}{2m} p$

$$= -\frac{i\hbar}{m} p$$

and $[H,p] = \frac{1}{2}m\omega^2 [x^2, p] = i\hbar m\omega^2 x$

1. $[H,[H,x]] = -\frac{i\hbar}{m}[H,p] = \frac{(-i\hbar)}{m}(i\hbar) m\omega^2 x$

$$= +\hbar^2 \omega^2 x$$

2. $[H,[H,[H,x]]] = \hbar^2 \omega^2 [H,x]$

$$= \hbar^2 \omega^2 \left(\frac{-i\hbar}{m}\right) p$$

$$= -i\hbar^3 \omega^2 \frac{p}{m}$$

3. $[H,[H,[H,[H,x]]]] = \frac{-i\hbar^3 \omega^2}{m} [H,p]$

$$= -i\frac{\hbar^3 \omega^2}{\cancel{m}} \, i\hbar \cancel{m} \omega^2 x = + \hbar^4 \omega^4 x$$

4. $[H,[H,[H,[H,[H,x]]]]] = \hbar^4 \omega^4 [H,x]$

$$= \hbar^4 \omega^4 \left(\frac{-i\hbar}{m}\right) p$$

$$= -i \hbar^5 \omega^4 \frac{p}{m}$$

Recall:

$$\cos\theta = 1 - \frac{\theta^2}{2!} + \frac{\theta^4}{4} - \cdots$$

$$\sin\theta = \theta - \frac{\theta^3}{3!} + \frac{\theta^5}{5!} - \cdots$$

$$X_H(t) = X_H(0)\left(1 + \frac{(-it/\hbar)^2}{2!}\hbar^2\omega^2 + \frac{(-it/\hbar)^4}{4!}\hbar^4\omega^4 + \cdots\right)$$

$$-\frac{p}{m}\left(\frac{-it}{\hbar}\cdot(-i\hbar) + \left(\frac{-it}{\hbar}\right)^3\frac{1}{3!}(-i\hbar^3)\,\omega^2 + \left(\frac{-it}{\hbar}\right)^5\frac{1}{5!}(-i\hbar^5)\,\omega^4\right)$$

$$= x_H(0)\cos\omega t + \frac{p_H(0)}{m\omega}\sin\omega t$$

Thus we get:

$$\boxed{\langle x\rangle(t) = \langle x_H(0)\rangle\cos\omega t + \frac{\langle p_H(0)\rangle}{m\omega}\sin\omega t}$$

I leave it as an exercise to show that this is equivalent to the previous result.