PHYS 3803: Quantum Mechanics I, Spring 2021

Lecture 16, March 25, 2021 (Thursday)

- Reading: Harmonic Oscillator, My Notes and Griffiths 2.3
- Assignments:
  Problem Set 7 due March 26 (Friday).
  Problem Set 8 due April 07 (Wednesday).
  Submit your homework assignments to Canvas.

Topics for Today: Harmonic Oscillator [Griffiths 2.3]

4.2 Energy Eigenstates of the Harmonic Oscillator [Griffiths 2.3.1]

Topics for Next Lecture: Harmonic Oscillator

4.3 The Harmonic Oscillator in the Coordinate Basis [Griffiths 2.3.2]

4.2 Energy Eigenstates of the Harmonic Oscillator

The energy eigenvalue equation for the harmonic oscillator is

$$H|E_n\rangle = \left(\frac{P^2}{2m} + \frac{1}{2}m\omega^2 X^2\right)|E_n\rangle = E_n|E_n\rangle\,.$$

Apart from scaling factors, the Hamiltonian has the following form

$$H \sim X^2 + P^2 = (X+iP)(X-iP) \quad \text{N.B.} \quad A^2 - B^2 = (A+B)(A-B)\,.$$

Let us define two new operators

$$a = \sqrt{\frac{m\omega}{2\hbar}}\left(X + \frac{i}{m\omega}P\right) \quad \text{and} \quad a^\dagger = \sqrt{\frac{m\omega}{2\hbar}}\left(X - \frac{i}{m\omega}P\right)\,.$$

The operator $a^\dagger a$ is related to the Hamiltonian

$$\begin{aligned} a^\dagger a &= \frac{1}{\hbar\omega}\left(\frac{P^2}{2m} + \frac{1}{2}m\omega^2 X^2\right) + \frac{i}{2\hbar}[X,P] \\ &= \frac{1}{\hbar\omega}H - \frac{1}{2} \quad \text{with} \quad [X,P] = i\hbar\,. \end{aligned}$$

The Hamiltonian becomes

$$H = \hbar\omega \left(a^\dagger a + \frac{1}{2} \right) .$$

The operators a and $a^\dagger$ has the following commutation relation

$$\begin{aligned}
[a, a^\dagger] &= \left(\frac{m\omega}{2\hbar}\right) \left(-\frac{i}{m\omega}[X, P] + \frac{i}{m\omega}[P, X] \right) \\
&= \left(\frac{m\omega}{2\hbar}\right) \left(\frac{2\hbar}{m\omega}\right) \\
&= 1 .
\end{aligned}$$

That is

$$[a, a^\dagger] = 1 ,$$

where a is the annihilation operator and $a^\dagger$ is the creation operator.

Let us define the operator $a^\dagger a$ as the number operator

$$N \equiv a^\dagger a$$

and the Hamiltonian can be expressed as

$$H = \hbar\omega(N + \frac{1}{2}).$$

Applying the commutation relations

$$[a, a^\dagger] = 1\,,$$

and

$$[a, a] = 0\,, \quad \text{and} \quad [a^\dagger, a^\dagger] = 0\,,$$

we obtain

- $[N, a] = \,?$ and $[N, a^\dagger] = \,?$
- $[H, a] = \,?$ and $[H, a^\dagger] = \,?$
- $[H, N] = \,?$

Applying the commutation relations among a and $a^\dagger$, we obtain

$$
\begin{aligned}
\left[N, a^\dagger\right] &= \left[a^\dagger a, a^\dagger\right] \;=\; a^\dagger\,, \\
[N, a] &= \left[a^\dagger a, a\right] \;=\; -a\,, \\
\left[H, a^\dagger\right] &= (\hbar\omega)\left[(N + \frac{1}{2}), a^\dagger\right] \;=\; (\hbar\omega) a^\dagger\,, \\
[H, a] &= (\hbar\omega)\left[(N + \frac{1}{2}), a\right] \;=\; -(\hbar\omega) a\,,
\end{aligned}
$$

and

$$[H, N] = 0.$$

This implies that H and N can be simultaneous diagonalized or that they have a common set of eigenvectors.

Let us denote the eigenvector by $|n\rangle$ such that

$$N|n\rangle = n|n\rangle$$

where n is the eigenvalue and the eigenvectors $|n\rangle$ form a complete set of orthonormal basis vectors

$$\langle m|n\rangle = \delta_{mn} \quad \text{and} \quad \sum_n |n\rangle\langle n| = \mathrm{I}\,.$$

Then we have

$$\begin{aligned} H|n\rangle &= \hbar\omega(N + \frac{1}{2})|n\rangle \\ &= \hbar\omega(n + \frac{1}{2})|n\rangle \\ &= E_n|n\rangle \end{aligned}$$

The energy associate with the state $|n\rangle$ us

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

Now let us consider $|n'\rangle = a|n\rangle$, and

$$\begin{aligned} H(a|n\rangle) &= aH|n\rangle + [H,a]|n\rangle \\ &= E_n(a|n\rangle) - \hbar\omega(a|n\rangle) \\ &= (E_n - \hbar\omega)(a|n\rangle) \\ &= E_{n-1}(a|n\rangle) \\ H|n'\rangle &= E_{n-1}|n'\rangle\,, \end{aligned}$$

where we have applied

$$[H,a] \equiv Ha - aH \quad \text{and} \quad Ha = aH + [H,a] = aH - (\hbar\omega)a\,.$$

The state $a|n\rangle$ is an eigenstate of the Hamiltonian with the eigenvalue

$$E_n - \hbar\omega = E_{n-1}$$

The effect of the operator a on a state is to lower its energy by one unit of $\hbar\omega$. Therefore, the operator a is called the lowering operator.

The state with energy

$$E_n - \hbar\omega = [(n-1) + \frac{1}{2}]\hbar\omega = E_{n-1}$$

must correspond to to $|n-1\rangle$. We can write

$$\begin{aligned} a|n\rangle &= c_n|n-1\rangle \\ \langle n|a^\dagger &= c_n^*\langle n-1| \end{aligned}$$

Multiplying by the adjoint, we have
$\langle n|a^\dagger a|n\rangle = c_n^* c_n\langle n-1|n-1\rangle = |c_n|^2$:

$$\begin{aligned} |c_n|^2 &= c_n^* c_n \\ &= c_n^* c_n\langle n-1|n-1\rangle \\ &= \langle n|a^\dagger a|n\rangle \\ &= \langle n|N|n\rangle \\ &= n\langle n|n\rangle \\ &= n, \end{aligned}$$

that is $|c_n|^2 = n$. We may choose c_n to be real and obtain

$$c_n = c_n^* = \sqrt{n}\,, \quad a|n\rangle = \sqrt{n}|n-1\rangle\,, \quad \text{and} \quad |n-1\rangle = \frac{1}{\sqrt{n}}a|n\rangle\,.$$

Similarly, we have $|n''\rangle = a^\dagger|n\rangle$, and

$$\begin{aligned} H(a^\dagger|n\rangle) &= a^\dagger H|n\rangle - [a^\dagger, H]|n\rangle \\ &= E_n a^\dagger|n\rangle - (-\hbar\omega a^\dagger)|n\rangle \\ &= (E_n + \hbar\omega)a^\dagger|n\rangle \\ &= E_{n+1}(a^\dagger|n\rangle) \\ H|n''\rangle &= E_{n+1}|n''\rangle\,, \end{aligned}$$

where we have applied

$$[H, a^\dagger] \equiv Ha^\dagger - a^\dagger H \quad \text{and} \quad Ha^\dagger = a^\dagger H + [H, a^\dagger] = a^\dagger H + (\hbar\omega)a^\dagger\,.$$

The operator $(a^\dagger)$ acting on a state raises its energy by one unit of $\hbar\omega$. Therefore, $a^\dagger$ is known as the raising operator.

We must have

$$\begin{aligned} a^\dagger|n\rangle &= d_n|n+1\rangle \\ \langle n|a &= d_n^*\langle n+1| \end{aligned}$$

and $\langle n|aa^\dagger|n\rangle = d_n^* d_n\langle n+1|n+1\rangle = |d_n|^2$:

$$\begin{aligned} |d_n|^2 &= d_n^* d_n \\ &= d_n^* d_n\langle n+1|n+1\rangle \\ &= \langle n|aa^\dagger|n\rangle \\ &= \langle n|N+1|n\rangle \\ &= (n+1)\langle n|n\rangle \\ &= n+1, \end{aligned}$$

that is $|d_n|^2 = n+1$.

Choosing d_n to be real, we obtain

$$
\begin{aligned}
d_n = d_n^* &= \sqrt{n+1} \\
a^\dagger|n\rangle &= \sqrt{n+1}|n+1\rangle \\
|n+1\rangle &= \frac{1}{\sqrt{n+1}} a^\dagger|n\rangle
\end{aligned}
$$

Let us consider the expectation value of the number operator N

$$
\begin{aligned}
\langle n|N|n\rangle &= n\langle n|n\rangle = n \\
\langle n|a^\dagger a|n\rangle &= \langle an|an\rangle \geq 0
\end{aligned}
$$

Thus all eigenvalues of N are $n \geq 0$.

Let's denote the smallest eigenvalue of N as n_0. Then

$$a|n_0\rangle = c_{n_0}|n_0 - 1\rangle.$$

Since n_0 is the smallest eigenvalue, we must have

$$\begin{aligned} c_{n_0} &= 0 \\ a|n_0\rangle &= 0 \end{aligned}$$

and

$$n_0|n_0\rangle = N|n_0\rangle = a^\dagger a|n_0\rangle = 0$$

That is $n_0 = 0$.

We can express the ground state as $|0\rangle$ and obtain

$$E_0|0\rangle = H|0\rangle = (N + \frac{1}{2})\hbar\omega|0\rangle = \frac{\hbar\omega}{2}|0\rangle$$

that is $E_0 = \hbar\omega/2$.

The energy eigenstates are the eigenstates of the number operator N:

(a) the ground state $|0\rangle : a|0\rangle = 0$,

(b) 1st excited state $|1\rangle = (1/d_0)a^\dagger|0\rangle = a^\dagger|0\rangle$,

(c) 2nd excited state $|2\rangle = (1/d_1)a^\dagger|1\rangle = (1/\sqrt{2!})(a^\dagger)^2|0\rangle$,

(d) nth excited state $|n\rangle : (1/d_{n-1})a^\dagger|n-1\rangle = (1/\sqrt{n!})(a^\dagger)^n|0\rangle$,

where $d_n = \sqrt{n+1}$.

In the $|n\rangle$ basis,

$$\begin{aligned} a|n\rangle &= \sqrt{n}|n-1\rangle \\ \langle m|a|n\rangle &= \sqrt{n}\langle m|n-1\rangle = \sqrt{n}\delta_{m,n-1} \\ a^\dagger|n\rangle &= \sqrt{n+1}|n+1\rangle \\ \langle m|a^\dagger|n\rangle &= \sqrt{n+1}\langle m|n+1\rangle = \sqrt{n+1}\delta_{m,n+1}. \end{aligned}$$

Furthermore,

$$
\begin{aligned}
X &= \sqrt{\frac{\hbar}{2m\omega}}(a + a^\dagger) \\
P &= -i\sqrt{\frac{\hbar m\omega}{2}}(a - a^\dagger)
\end{aligned}
$$

Thus the matrix elements of X and P becomes

$$
\begin{aligned}
\langle m|X|n\rangle &= \sqrt{\frac{\hbar}{2m\omega}}\langle m|(a + a^\dagger)|n\rangle \\
&= \sqrt{\frac{\hbar}{2m\omega}}[\sqrt{n}\delta_{m,n-1} + \sqrt{n+1}\delta_{m,n+1}] \\
\langle m|P|n\rangle &= -i\sqrt{\frac{\hbar m\omega}{2}}\langle m|(a - a^\dagger)|n\rangle \\
&= -i\sqrt{\frac{\hbar m\omega}{2}}[\sqrt{n}\delta_{m,n-1} - \sqrt{n+1}\delta_{m,n+1}] \, .
\end{aligned}
$$

Since the application of $a^\dagger$ gives us a higher state, we can construct all higher states from the ground state. For example,

$$\begin{aligned} |1\rangle &= \frac{a^\dagger}{\sqrt{1}}|0\rangle = a^\dagger|0\rangle \\ |2\rangle &= \frac{a^\dagger}{\sqrt{1+1}}|1\rangle = \frac{(a^\dagger)^2}{\sqrt{2}}|0\rangle \\ |n+1\rangle &= \frac{a^\dagger}{\sqrt{n+1}}|n\rangle = \frac{a^\dagger}{\sqrt{n+1}}\frac{a^\dagger}{\sqrt{n}}|n-1\rangle = \frac{(a^\dagger)^{n+1}}{\sqrt{(n+1)!}}|0\rangle \end{aligned}$$

The fact that any higher state can be written as a product of creation operators acting on the ground state and the fact that

$$a|0\rangle = 0 = \langle 0|a^\dagger$$

greatly simplifies the calculation of matrix elements of operators between different states.

Example 1:

$$
\begin{aligned}
\langle 2|X^2|0\rangle &= \langle 2|\left(\frac{\hbar}{2m\omega}\right)^{2/2}(a+a^\dagger)^2|0\rangle \\
&= \left(\frac{\hbar}{2m\omega}\right)\langle 2|a^2+aa^\dagger+a^\dagger a+(a^\dagger)^2|0\rangle \\
&= \left(\frac{\hbar}{2m\omega}\right)\langle 2|aa^\dagger+(a^\dagger)^2|0\rangle \quad (a|0\rangle=0) \\
&= \left(\frac{\hbar}{2m\omega}\right)\langle 2|a+a^\dagger|1\rangle \\
&= \left(\frac{\hbar}{2m\omega}\right)\left(\langle 2|0\rangle+\langle 2|\sqrt{2}|2\rangle\right) \\
&= \frac{\sqrt{2}\hbar}{2m\omega},
\end{aligned}
$$

where we have applied $a^\dagger|n\rangle=\sqrt{n+1}|n+1\rangle$, $a|n\rangle=\sqrt{n}|n-1\rangle$, and $\langle n|n'\rangle=\delta_{n,n'}$.

Relations between the $E-$basis and the $x-$basis

Let us define the wave function

$$\psi_n(x) = \langle x|n\rangle$$

This measures the probability amplitude for finding the oscillator at x with an energy E_n. The ground state satisfies

$$a|0\rangle = 0\,.$$

In the x basis, it becomes

$$\langle x|a|0\rangle = \int dy \langle x|a|y\rangle\langle y|0\rangle = 0\,,$$

with

$$a = \sqrt{\frac{m\omega}{2\hbar}}(X + \frac{i}{m\omega}P)\,.$$

We know that

$$\langle x|X|y\rangle = y\delta(x-y) \quad \text{and} \quad \langle x|P|y\rangle \quad = \quad -i\hbar\frac{d}{dx}\delta(x-y)\,.$$

Thus

$$\langle x|a|y\rangle = \sqrt{\frac{m\omega}{2\hbar}}\left[y\delta(x-y) + \frac{\hbar}{m\omega}\frac{d}{dx}\delta(x-y)\right]$$

And the equation becomes

$$\sqrt{\frac{m\omega}{2\hbar}}\int\left[y\delta(x-y) + \frac{\hbar}{m\omega}\frac{d}{dx}\delta(x-y)\right]\psi_0(y)\,dy = 0$$

or

$$\begin{aligned}\sqrt{\frac{m\omega}{2\hbar}}(x + \frac{\hbar}{m\omega}\frac{d}{dx})\psi_0(x) \quad &= \quad 0 \\ \frac{d\psi_0(x)}{dx} \quad &= \quad -\frac{m\omega}{\hbar}\left[x\psi_0(x)\right].\end{aligned}$$

The solution to this equation is

$$\psi_0(x) = A_0 e^{-\frac{m\omega}{2\hbar}x^2}.$$

This wave functions is normalized such that

$$\begin{aligned}\int \psi_0^*(x)\psi_0(x) &= A_0^* A_0 \int_{-\infty}^{\infty} e^{-\left(\frac{m\omega}{\hbar}\right)x^2}\, dx \\ &= |A_0|^2 \sqrt{\frac{\pi\hbar}{m\omega}} = 1,\end{aligned}$$

Thus

$$|A_0|^2 = \sqrt{\frac{m\omega}{\pi\hbar}}\,.$$

Choose A_0 to be real, we have

$$A_0 = A_0^* = (\frac{m\omega}{\pi\hbar})^{1/4}$$

and

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

To construct the higher order wave functions, we note that in the x basis,

$$a^\dagger \to \sqrt{\frac{m\omega}{2\hbar}}(x - \frac{\hbar}{m\omega}\frac{d}{dx})$$

Furthermore,

$$|n\rangle = \frac{(a^\dagger)^n}{(n!)^{1/2}}|0\rangle \,.$$

Thus

$$\begin{aligned}\langle x|n\rangle &= \psi_n(x)\\ &= \frac{1}{(n!)^{1/2}}(\frac{m\omega}{2\hbar})^{n/2}(x-\frac{\hbar}{m\omega}\frac{d}{dx})^n\psi_0(x)\\ &= (\frac{m\omega}{\pi\hbar})^{1/4}(\frac{m\omega}{2\hbar})^{n/2}\frac{1}{(n!)^{1/2}}(x-\frac{\hbar}{m\omega}\frac{d}{dx})^n e^{-\frac{m\omega}{2\hbar}x^2}.\end{aligned}$$

This completes our investigation in the matrix formulation.

We have determined the energy levels and the wave functions.

Bonus: Time Evolution Operator

The Schrödinger equation is

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

with the solution for the state vector as

$$|\Psi(t)\rangle = U(t, t_0)|\Psi(t_0)\rangle \,.$$

If the Hamiltonian is time independent, the time evolution operator is

$$U(t, t_0) = e^{-iH(t-t_0)/\hbar} \quad \text{or} \quad U(t) = e^{-iHt/\hbar} \quad \text{for} \quad t_0 = 0 \,.$$

The eigenvectors of the Hamiltonian are stationary states such that

$$\begin{aligned} H|\Psi_n(t)\rangle &= E_n|\Psi_n(t)\rangle \quad \text{and} \\ |\Psi_n(t)\rangle &= U(t)|\Psi_n(0)\rangle = e^{-iHt/\hbar}|\Psi_n(0)\rangle = e^{-iE_nt/\hbar}|\Psi_n(0)\rangle \,. \end{aligned}$$

If the state vector is a linear combination of eigenvectors

$$|\Psi(t)\rangle = \sum_n c_n |\Psi_n(t)\rangle \, .$$

Then

$$\begin{aligned} |\Psi(t)\rangle &= U(t)|\Psi(0)\rangle \; = \; e^{-iHt/\hbar}|\Psi(0)\rangle \\ &= e^{-iHt/\hbar}\left[\sum_n c_n|\Psi_n(0)\rangle\right] \; = \; \left[\sum_n c_n e^{-iE_n t/\hbar}|\Psi_n(0)\rangle\right] \, . \end{aligned}$$

In the x basis, that leads to

$$\langle x|\Psi(t)\rangle = \langle x|U(t)|\Psi(0)\rangle = \left[\sum_n c_n e^{-iE_n t/\hbar}\langle x|\Psi_n(0)\rangle\right] \, .$$

That is

$$\Psi(x,t) = \left[\sum_n c_n e^{-iE_n t/\hbar}\Psi_n(x,0)\right] \, .$$