Harmonic Oscillator ala Dirac and Linear Algebra

Differential equation Approach

The Schrodinger equation for the 1-dimensional harmonic oscillator with a potential function

$$V(x) = \frac{1}{2}kx^2$$

is given by

$$-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} + \frac{1}{2}kx^2\psi(x) = E\psi(x)$$

The standard ODE solution of this equations goes as follows. Let

$$\xi = \alpha x \qquad \alpha^4 = \frac{mk}{\hbar^2}$$

$$\lambda = \frac{2E}{\hbar\omega_0} \qquad \omega_0 = \left(\frac{k}{m}\right)^{1/2}$$

This gives the new equation

$$\frac{d^2\psi}{d\xi^2} + (\lambda - \xi^2)\psi = 0$$

If we consider the behavior of the equation as $\xi \to \pm\infty$ we can neglect λ and the equation becomes

$$\frac{d^2\psi}{d\xi^2} - \xi^2\psi = 0$$

which says that the large ξ behavior of the solution is

$$\psi = e^{-\xi^2/2}$$

This suggests that we try a solution of the form

$$\psi = H(\xi)e^{-\xi^2/2}$$

which should remove the large ξ behavior from the equation. We get the equation

$$H'' - 2\xi H' + (\lambda - 1)H = 0$$

This is Hermite's equation and provided we choose $\lambda = 2n + 1$.

If we do not terminate the series the solutions are not square integrable and cannot represent wave functions.

The series solutions we found earlier have the recursion relation

$$a_{k+2} = \frac{(2k+1-\lambda)}{(k+2)(k+1)} a_k$$

If the series does not terminate, then its dominant asymptotic behavior can be inferred from the coefficients of its high terms

$$\lim_{k\to\infty} \frac{a_{k+2}}{a_k} \to \frac{2}{k}$$

This ratio is the same as that of the series for $\xi^n e^{\xi^2}$ with any finite value of n.

This means that the solution $\psi = H(\xi)e^{-\xi^2/2}$ will not be square-integrable unless the series is terminated.

So we terminate the series and the solutions are the Hermite polynomials H_n .

For this choice of λ we get energy eigenvalues

$$E_n = \hbar\omega_0\left(n + \frac{1}{2}\right)$$

with associated wave functions

$$\psi_n(x) = H(\alpha x)e^{-\alpha^2 x^2/2}$$

Linear Algebra Approach

Alternatively, we can look at this problem from a purely linear algebra point of view.

In this case, we write the Schrodinger equation as an energy eigenvalue/eigenvector equation. The linear operator involved is the energy operator or the Hamiltonian, which we write as

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

where the ^ over a symbol designates a linear operator. We also assume the fundamental commutation relation

$$[\hat{x},\hat{p}] = i\hbar$$

We also have

$$[\hat{x},\hat{x}] = 0 = [\hat{p},\hat{p}]$$

All operators in QM that represent observables like energy , momentum and position are Hermitian operators, hence

$$\hat{H}^{+} = \hat{H}\,, \hat{p}^{+} = \hat{p}\,, \hat{x}^{+} = \hat{x}$$

We now define two new operator as follows:

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

$$\hat{a}^{+} = \sqrt{\frac{m\omega}{2\hbar}}\hat{x}^{+} - i\frac{\hat{p}^{+}}{\sqrt{2m\omega\hbar}} = \sqrt{\frac{m\omega}{2\hbar}}\hat{x} - i\frac{\hat{p}}{\sqrt{2m\omega\hbar}}$$

or $\hat{a}^{+}$ is the Hermitian conjugate of $\hat{a}$, i.e., $\hat{a}$ is not Hermitian.

Inverting we have

$$\hat{x}^{+} = \sqrt{\frac{\hbar}{2m\omega}}(\hat{a} + \hat{a}^{+})$$

$$\hat{p} = -i\sqrt{\frac{m\omega\hbar}{2}}(\hat{a} - \hat{a}^{+})$$

Using these relations we find

$$[\hat{a},\hat{a}^{+}] = \frac{m\omega}{2\hbar}[\hat{x},\hat{x}] + \frac{1}{2m\omega\hbar}[\hat{p},\hat{p}] - i\frac{1}{2\hbar}[\hat{x},\hat{p}] + i\frac{1}{2\hbar}[\hat{p},\hat{x}]$$

$$= \frac{i}{2\hbar}[[\hat{p},\hat{x}] - [\hat{x},\hat{p}]] = \frac{i}{2\hbar}[\hat{p}\hat{x} - \hat{x}\hat{p} - \hat{x}\hat{p} + \hat{p}\hat{x}]$$

$$= -\frac{i}{\hbar}[\hat{x}\hat{p} - \hat{p}\hat{x}] = -\frac{i}{\hbar}[\hat{x},\hat{p}] = -\frac{i}{\hbar}i\hbar = 1$$

We thus have

$$[\hat{a},\hat{a}^{+}] = 1 \quad \text{and} \quad [\hat{a},\hat{a}] = [\hat{a}^{+},\hat{a}^{+}] = 0$$

In addition, we have

$$\hat{H} = \frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega^2\hat{x}^2 = \frac{1}{2m}\left(-i\sqrt{\frac{m\omega\hbar}{2}}(\hat{a}-\hat{a}^{+})\right)^2 + \frac{1}{2}m\omega^2\left(\sqrt{\frac{\hbar}{2m\omega}}(\hat{a}+\hat{a}^{+})\right)^2$$

$$= \frac{1}{2m}\left(-\frac{m\omega\hbar}{2}\right)(\hat{a}\hat{a} - \hat{a}\hat{a}^{+} - \hat{a}^{+}\hat{a} + \hat{a}^{+}\hat{a}^{+}) + \frac{1}{2}m\omega^2\left(\frac{\hbar}{2m\omega}\right)(\hat{a}\hat{a} + \hat{a}\hat{a}^{+} + \hat{a}^{+}\hat{a} + \hat{a}^{+}\hat{a}^{+})$$

$$= \frac{\hbar\omega}{2}[\hat{a}\hat{a}^{+} + \hat{a}^{+}\hat{a}] = \frac{\hbar\omega}{2}[2\hat{a}^{+}\hat{a} + 1] = \hbar\omega\left[\hat{a}^{+}\hat{a} + \frac{1}{2}\right]$$

We now define

$$\hat{N} = \hat{a}^{+}\hat{a}$$

so that

$$\hat{H} = \hbar\omega\left[\hat{N} + \frac{1}{2}\right]$$

This means that the problem of finding the eigenstates of $\hat{H}$ is equivalent to finding the eigenstates of $\hat{N}$ (since these two operators differ only by a constant).

Let us write the eigenvalue/eigenvector equation for $\hat{N}$ as

$$\hat{N}|n\rangle = n|n\rangle$$

where

$|n\rangle$ = eigenvector of $\hat{N}$ with eigenvalue n

If we can solve for the eigenvalues n , we then have

$$\hat{H}|n\rangle = \hbar\omega\left(\hat{N} + \frac{1}{2}\right)|n\rangle = \hbar\omega\left(n + \frac{1}{2}\right)|n\rangle$$

so that

$$|n\rangle \text{ = eigenvector of } \hat{H} \text{ with eigenvalue } \hbar\omega\left(n + \frac{1}{2}\right)$$

i.e., the energy eigenvalues are $E_n = \hbar\omega\left(n + \frac{1}{2}\right)$.

Now we need to determine the eigenvalues n .

We have

$$\hat{N}^+ = (\hat{a}^+\hat{a})^+ = \hat{a}^+\hat{a} = \hat{N}$$

which means that $\hat{N}$ is a Hermitian operator and thus its eigenvalues are real.

Now

$$\langle n|\hat{N}|n\rangle = \langle n|n|n\rangle = n\langle n|n\rangle = n$$

where we have used

$$\hat{N}|n\rangle = n|n\rangle \,,\, \langle n|n\rangle = 1 \,,\, \langle n| = (|n\rangle)^+$$

But we also have

$$\langle n|\hat{N}|n\rangle = \langle n|\hat{a}^+\hat{a}|n\rangle = n$$

If we assume that

$$\hat{a}|n\rangle = |\alpha\rangle$$

since it must equal some vector in the space, then we get

$$(\hat{a}|n\rangle)^+ = (|n\rangle)^+\hat{a}^+ = \langle n|\hat{a}^+ = (|\alpha\rangle)^+ = \langle\alpha|$$

Therefore,

$$\langle n|\hat{N}|n\rangle = \langle n|\hat{a}^+\hat{a}|n\rangle = n = (\langle n|\hat{a}^+)(\hat{a}|n\rangle) = \langle\alpha|\alpha\rangle$$

or

n = length squared of some vector

This means that

$$n \geq 0 \quad , \quad real$$

Now

$$\hat{N}\hat{a} = \hat{a}^{+}\hat{a}\hat{a} = \left[\hat{a}\hat{a}^{+} - 1\right]\hat{a} = \hat{a}\left[\hat{a}^{+}\hat{a} - 1\right] = \hat{a}\left[\hat{N} - 1\right]$$

and similarly

$$\hat{N}\hat{a}^{+} = \hat{a}^{+}\left[\hat{N} + 1\right]$$

These are relations among the operators. If we now apply these operator relations to the vectors we find

$$\hat{N}\hat{a}|n\rangle = \hat{a}\left[\hat{N} - 1\right]|n\rangle = (n-1)\hat{a}|n\rangle$$

or

$\hat{a}|n\rangle$ = eigenvector of $\hat{N}$ with eigenvalue (n-1)

Therefore, we can write

$$\hat{a}|n\rangle = \beta|n-1\rangle$$

We then find

$$\langle n|\hat{a}^{+}\hat{a}|n\rangle = n = (\langle n|\hat{a}^{+})(\hat{a}|n\rangle) = \beta^{2}\langle n-1|n-1\rangle = \beta^{2}$$

or

$$\beta^2 = n \to \beta = \sqrt{n}$$

and

$$\hat{a}|n\rangle = \sqrt{n}|n-1\rangle$$

Using this result we have

$$\hat{a}^2|n\rangle = \hat{a}\hat{a}|n\rangle = \sqrt{n}\hat{a}|n-1\rangle = \sqrt{n(n-1)}|n-2\rangle$$

If we keep on going, this implies that if an eigenstate $|n\rangle$ exists with eigenvalue n , then eigenstates for eigenvalues n-1, n-2, n-3, ... must also exist.

Now we already proved that n ≥ 0, so this process must stop before n becomes negative. This means that we must have a situation where we come to some eigenstate, say $|1\rangle$, where

$$\hat{a}|1\rangle = |0\rangle \quad \text{and} \quad \hat{a}|0\rangle = 0$$

so that the sequence would terminate.

Were we to come down to the eigenstate $|\xi\rangle$, $0 < \xi < 1$, then the relation

$$\hat{a}|\xi\rangle = \sqrt{\xi}|\xi - 1\rangle$$

would give an eigenstate with a negative eigenvalue.

The only way to make this work out is to assume that the eigenvalues of $\hat{N}$ are integers going down to zero.

In this case the sequence terminates naturally at eigenvalue = 0.

In a similar way we find

$$\hat{N}\hat{a}^{+}|n\rangle = \hat{a}^{+}\left[\hat{N} + 1\right]|n\rangle = (n+1)\hat{a}^{+}|n\rangle$$

or

$\hat{a}^{+}|n\rangle$ = eigenvector of $\hat{N}$ with eigenvalue (n+1)

Therefore, we can write

$$\hat{a}^{+}|n\rangle = \beta|n+1\rangle$$

In this case we find

$$\hat{a}^+|n\rangle = \sqrt{n+1}|n+1\rangle$$

Putting this all together we have the following result:

> the eigenvalues of $\hat{N}$ are the
> non-negative integers n = 0,1,2,3,4,....

The normalized eigenstates are

$$n=0 \qquad |0\rangle$$

$$n=1 \qquad |1\rangle = \frac{\hat{a}^+}{\sqrt{1}}|0\rangle$$

$$n=2 \qquad |2\rangle = \frac{\hat{a}^+}{\sqrt{2}}|1\rangle = \frac{(\hat{a}^+)^2}{\sqrt{2!}}|0\rangle$$

$$n=3 \qquad |3\rangle = \frac{\hat{a}^+}{\sqrt{3}}|2\rangle = \frac{(\hat{a}^+)^3}{\sqrt{3!}}|0\rangle$$

or, in general

$$|n\rangle = \frac{(\hat{a}^+)^n}{\sqrt{n!}}|0\rangle \quad , \quad E_n = \hbar\omega\left(n + \frac{1}{2}\right) \quad , \quad n = 0,1,2,3,......$$

We note that $E_0 > 0$.

This is the quantum mechanical zero-point energy. It arises from the vector nature of the state vectors(or in old language from the uncertainty principle).

Where are the Schrodinger wave functions?

How did we do this without ever mentioning the Schrodinger equation?

The vector space approach is more general than the Schrodinger approach to quantum mechanics. It can handle significantly more real physical systems than the Schrodinger approach. The Schrodinger approach is, in fact, just a subset of the vector space approach.

Let me illustrate this now by deriving the Schrodinger equation and then generating the old wave functions from our new state vectors.

Derivation of Schrodinger Equation

Assume that we have these eigenvalue/eigenvector equations

$$\hat{p}|p\rangle = p|p\rangle$$
$$\hat{x}|x\rangle = x|x\rangle$$

which define the properties of the eigenvalues/eigenvectors of the momentum and position operators.

These are Hermitian operators and the eigenstates of any Hermitian operator always form a complete set or a basis for the vector space.

This means that we can use the any of the sets

$$\{|n\rangle\} \quad , \quad \{|x\rangle\} \quad , \quad \{|p\rangle\}$$

as a basis for the vector space.

The main difference is that the $\{|n\rangle\}$ states have discrete eigenvalues (the eigenvalues n are the non-negative integers) while the $\{|p\rangle\}$ or $\{|x\rangle\}$ states have continuous eigenvalues (the eigenvalues range continuously over the interval $[-\infty,+\infty]$).

Let us expand an arbitrary state vector in terms of both the discrete and continuous basis vectors, i.e., we write

$$|\psi\rangle = \sum_m \psi_m |m\rangle$$

or

$$|\psi\rangle = \int dx' \psi(x')|x'\rangle$$

or

$$|\psi\rangle = \int dp' \phi(p')|p'\rangle$$

We then have in the discrete case

$$\langle n|\psi\rangle = \sum_m \psi_m \langle n|m\rangle = \sum_m \psi_m \delta_{nm} = \psi_n$$

Now the continuous case is more complicated. We have by analogy

$$\langle x|\psi\rangle = \int dx' \psi(x')\langle x|x'\rangle = \psi(x)$$

This requires that

$$\langle x|x'\rangle = \delta(x - x')$$

and similarly

$$\langle p|\psi\rangle = \int dp' \phi(p')\langle p|p'\rangle = \phi(p)$$

requires that

$$\langle p | p' \rangle = \delta(p - p')$$

This implies that

$$|\psi\rangle = \sum_m |m\rangle\langle m|\psi\rangle \to \sum_m |m\rangle\langle m| = \hat{I}$$

and

$$|\psi\rangle = \int dx' |x'\rangle\langle x'|\psi\rangle \to \int dx' |x'\rangle\langle x'| = \hat{I}$$

and

$$|\psi\rangle = \int dp' |p'\rangle\langle p'|\psi\rangle \to \int dp' |p'\rangle\langle p'| = \hat{I}$$

which is just the sum over all projection operators in each case, which we talked about in an earlier lecture.

We will prove shortly that the quantity $\psi(x) = \langle x | \psi \rangle$ is the Schrodinger wave function.

We note that

$$\int \psi^*(x)\psi(x)dx = \int \langle \psi | x \rangle\langle x | \psi \rangle dx = \langle \psi | \left[\int dx |x\rangle\langle x| \right] | \psi \rangle$$

$$= \langle \psi | \hat{I} | \psi \rangle = \langle \psi | \psi \rangle = 1$$

which is the way Schrodinger wave functions should behave!

Note that we have used

$$\psi(x) = \langle x|\psi\rangle \rightarrow \langle x|\psi\rangle^{+} = \psi^{*}(x) = \langle\psi|x\rangle$$

Now consider

$$|\psi\rangle = \int dp|p\rangle\langle p|\psi\rangle$$

$$\langle x|\psi\rangle = \int dp\langle x|p\rangle\langle p|\psi\rangle$$

$$\psi(x) = \int dp\langle x|p\rangle\phi(p)$$

$$|\psi\rangle = \int dx|x\rangle\langle x|\psi\rangle$$

$$\langle p|\psi\rangle = \int dp\langle p|x\rangle\langle x|\psi\rangle$$

$$\phi(p) = \int dp\langle p|x\rangle\psi(x)$$

Using

$$\langle x|x'\rangle = \delta(x - x')$$

we have

$$\langle x|\hat{I}|x'\rangle = \langle x\left[\left[\int dp|p\rangle\langle p|\right]\right]x'\rangle = \delta(x - x')$$

$$\int\langle x|p\rangle\langle p|x'\rangle dp = \delta(x - x')$$

But we know from Fourier transform theory that

$$\int e^{i\frac{p}{\hbar}(x-x')} dp = \delta(x-x')$$

Therefore we can identify

$$\langle x|p\rangle = e^{i\frac{p}{\hbar}x}$$

We then have the result that $\phi(p)$ is the Fourier transform of $\psi(x)$.

Now

$$\hat{p}|p\rangle = p|p\rangle \rightarrow \hat{p}|\psi\rangle = \hat{I}\hat{p}|\psi\rangle = \int dp|p\rangle\langle p|\hat{p}|\psi\rangle$$

$$= \int dp|p\rangle\langle\psi|\hat{p}|p\rangle^* = \int dp|p\rangle p\langle\psi|p\rangle^* = \int dp|p\rangle p\langle p|\psi\rangle$$

or

$$\hat{p} = \int dp\, p|p\rangle\langle p|$$

This is a general statement about operators. They can be represented by a sum of the products of the eigenvalues and the corresponding projection operators.

Continuing we get

$$\langle x|\hat{p}|p\rangle = p\langle x|p\rangle = pe^{i\frac{p}{\hbar}x} = \frac{\hbar}{i}\frac{d}{dx}e^{i\frac{p}{\hbar}x} = \frac{\hbar}{i}\frac{d}{dx}\langle x|p\rangle$$

and

$$\langle x|\hat{p}|\psi\rangle = \langle x|\hat{p}\left[\int dp|p\rangle\langle p|\psi\rangle\right] = \int dp\, p\langle x|p\rangle\langle p|\psi\rangle$$

$$= \int dp\frac{\hbar}{i}\frac{d}{dx}\langle x|p\rangle\langle p|\psi\rangle = \frac{\hbar}{i}\frac{d}{dx}\int dp\langle x|p\rangle\langle p|\psi\rangle$$

$$= \frac{\hbar}{i}\frac{d}{dx}\langle x|\left(\int dp|p\rangle\langle p|\right)|\psi\rangle = \frac{\hbar}{i}\frac{d}{dx}\langle x|\hat{I}|\psi\rangle = \frac{\hbar}{i}\frac{d}{dx}\langle x|\psi\rangle$$

Finally, we have

$$\langle x|f(\hat{p})|\psi\rangle = f\left(\frac{\hbar}{i}\frac{d}{dx}\right)\langle x|\psi\rangle$$

Similarly we can write

$$\langle x|\hat{x}|\psi\rangle = x\langle x|\psi\rangle \quad \text{and} \quad \langle x|f(\hat{x})|\psi\rangle = f(x)\langle x|\psi\rangle$$

Now we can derive Schrodinger's equation. We start with the energy eigenvalue equation

$$\hat{H}|\psi\rangle = E|\psi\rangle = \left[\frac{\hat{p}^2}{2m} + V(\hat{x})\right]|\psi\rangle$$

Then

$$\langle x|\left[\frac{\hat{p}^2}{2m} + V(\hat{x})\right]|\psi\rangle = \langle x|\left[\frac{\hat{p}^2}{2m}\right]|\psi\rangle + \langle x|[V(\hat{x})]|\psi\rangle = E\langle x|\psi\rangle$$

or

$$\frac{1}{2m}\left(\frac{\hbar}{i}\frac{d}{dx}\right)^2\langle x|\psi\rangle + V(x)\langle x|\psi\rangle = E\langle x|\psi\rangle$$

This is Schrodinger's equation if we identify the wave function with $\psi(x) = \langle x|\psi\rangle$, i.e.,

$$-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} + V(x)\psi(x) = E\psi(x)$$

Ground State Wave Function without the Schrodinger Equation

Consider

$$0 = \langle x|\hat{a}|0\rangle = \langle x|\left(\sqrt{\frac{m\omega}{2\hbar}}\hat{x} + i\frac{\hat{p}}{\sqrt{2m\omega\hbar}}\right)|0\rangle$$

$$= \left(\sqrt{\frac{m\omega}{2\hbar}}x + \sqrt{\frac{\hbar}{2m\omega}}\frac{d}{dx}\right)\langle x|0\rangle = \left(\sqrt{\frac{m\omega}{2\hbar}}x + \sqrt{\frac{\hbar}{2m\omega}}\frac{d}{dx}\right)\psi_0(x)$$

where we have defined the ground state wave function as

$$\psi_0(x) = \langle x|0\rangle$$

This is a simple first order differential equation with solution

$$\psi_0(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} e^{-m\omega x^2/2\hbar} = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} H_0\left(\sqrt{\frac{m\omega}{\hbar}}x\right)e^{-m\omega x^2/2\hbar}$$

which is the ground-state wave function of the harmonic oscillator.

The higher energy wave functions are easily derived using

$$\langle x|1\rangle = \psi_1(x) = \langle x|\hat{a}^+|0\rangle = \langle x|\left(\sqrt{\frac{m\omega}{2\hbar}}\hat{x} - i\frac{\hat{p}}{\sqrt{2m\omega\hbar}}\right)|0\rangle$$

$$= \left(\sqrt{\frac{m\omega}{2\hbar}}x - \sqrt{\frac{\hbar}{2m\omega}}\frac{d}{dx}\right)\langle x|0\rangle = \left(\sqrt{\frac{m\omega}{2\hbar}}x - \sqrt{\frac{\hbar}{2m\omega}}\frac{d}{dx}\right)\psi_0(x)$$

$$= \sqrt{\frac{2m\omega}{\hbar}}x\psi_0(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} H_1\left(\sqrt{\frac{m\omega}{\hbar}}x\right)e^{-m\omega x^2/2\hbar}$$

and in general,

$$\langle x|n\rangle = \psi_n(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4}\frac{1}{\sqrt{2^n n!}}H_n\left(\sqrt{\frac{m\omega}{\hbar}}x\right)e^{-m\omega x^2/2\hbar}$$