# Harmonic Oscillator I

Lecture 8

Physics 342
Quantum Mechanics I

Wednesday, February 10th, 2010

We can manipulate operators, to a certain extent, as we would algebraic expressions. By considering a factorization of the Hamiltonian, it is possible to efficiently generate quantum mechanical solutions to the harmonic oscillator potential – today we will begin that process by finding the ground state and an operator prescription for generating excited states (that is, wavefunctions satisfying the time-independent Schrödinger equation with successively higher energy).

This algebraic approach is meant to complement the analytical approach we used for the infinite square well. There, energy quantization manifest itself through a boundary condition. For our algebraic construction, energy quantization comes from the existence of a ground state[1], and a procedure for building excited states that brings with it a natural, finite energy scale.

## 8.1 Operators

We are now viewing the replacement of momentum: $p \longrightarrow \frac{\hbar}{i}\frac{\partial}{\partial x}$ as a quantum mechanical assignment. Instead of being a dynamical variable, even a constant of the motion at times, momentum in quantum mechanics is an operator that acts on the wave function. There is a still more abstract view of operators that we will discuss at the appropriate time, but for now, if we have a wavefunction (or a piece of one) $f(x)$, then $p f(x) = \frac{\hbar}{i} f'(x)$. Similarly, $x$ itself is an operator in this context, although it is not as obvious – $x$ tells us to "multiply by $x$". This makes sense when we think of expectation values and variances, where $x$ is the variable over which integration is

[1] The existence of a lowest energy state (ground state) is equivalent to the requirement that the wavefunction vanish at spatial infinity, in this case.

performed.

It is interesting to discuss these operators in the language of linear algebra – from this point of view, $p$ is Hermitian – that is to say that it can act on either the right or the left in an inner product – for any $f(x)$ and $g(x)$ that vanish at spatial infinity[2] :

$$\int_{-\infty}^{\infty} f(x)^* \, p \, g(x) \, dx = \int_{-\infty}^{\infty} (p \, f(x))^* \, g(x) \, dx \tag{8.2}$$

in loose language. In the same way, $x$ is also Hermitian, and both operators have continuous spectra (indeed, the eigenvector equation for $p$ now reads: $\frac{\hbar}{i} \frac{\partial}{\partial x} f(x) = \bar{p} \, f(x)$ for continuous $\bar{p}$).

From any pair of operators, we can form the commutator – remember that the commutator in linear algebra is the difference between the product of two matrices taken in both orderings: $[\mathbb{A}, \mathbb{B}] = \mathbb{A}\,\mathbb{B} - \mathbb{B}\,\mathbb{A}$. The same is true for the functional generalization here – but we need to be careful – what does:

$$[x, p] = x \, \frac{\hbar}{i} \, \frac{\partial}{\partial x} - \frac{\hbar}{i} \, \frac{\partial}{\partial x} \, x \tag{8.3}$$

mean? To keep track, we can put a "test function" $f(x)$ to the right of the commutator operator:

$$[x, p] \, f(x) = x \, \frac{\hbar}{i} \, f'(x) - \frac{\hbar}{i} \left( f(x) + x \, f'(x) \right) = i \, \hbar \, f(x), \tag{8.4}$$

and we say that $[x, p] = i \, \hbar$ for short. The point is that when we manipulate the quantum mechanical operators $x$ and $p$, we can do so while ignoring the differential operator nature of $p$, provided we understand that "order counts". So, unlike classical mechanics, our algebraic manipulations involve this added complexity, or "fun factor", depending on your point of view (you can always leave $\frac{\hbar}{i} \frac{\partial}{\partial x}$ in for $p$ and get the correct expressions, of course).

[2] This can be established via integration-by-parts – for:

$$\begin{aligned} \int_{-\infty}^{\infty} \left( \frac{\hbar}{i} \, \frac{df(x)}{dx} \right)^* g(x) \, dx &= i \, \hbar \int_{-\infty}^{\infty} \frac{df^*(x)}{dx} \, g(x) \, dx \\ &= -i \, \hbar \int_{-\infty}^{\infty} f^*(x) \, \frac{dg(x)}{dx} \, dx \\ &= \int_{-\infty}^{\infty} f^*(x) \left( \frac{\hbar}{i} \, \frac{dg(x)}{dx} \right) dx, \end{aligned} \tag{8.1}$$

where we have assumed $f^*(x)$ and/or $g(x)$ vanish at spatial infinity.

The commutator is useful in algebraic manipulation – if we had a form like $x\,p\,f(x)$ and we wanted to reverse the order of $x$ and $p$ as they operate on $f(x)$, then we know:

$$\begin{aligned} x\,p\,f(x) &= p\,x\,f(x) + [x,p]\,f(x) \\ &= p\,x\,f(x) + i\,\hbar\,f(x) \longrightarrow p\,x\,f(x) = x\,p\,f(x) - i\,\hbar\,f(x). \end{aligned} \tag{8.5}$$

## 8.2 Factoring Operators

Factoring a differential operator is not trivial – take the wave equation (with fundamental velocity set to one):

$$\left(-\frac{\partial^2}{\partial t^2} + \frac{\partial^2}{\partial x^2}\right) f(x,t) = 0, \tag{8.6}$$

for some function $f(x,t)$. This looks like "the difference of two squares", so we are tempted to factor the wave operator:

$$\left(\frac{\partial}{\partial x} - \frac{\partial}{\partial t}\right)\left(\frac{\partial}{\partial x} + \frac{\partial}{\partial t}\right) \underbrace{\text{“=”}}_{?} \left(-\frac{\partial^2}{\partial t^2} + \frac{\partial^2}{\partial x^2}\right). \tag{8.7}$$

Again, it is useful to introduce a test function $f(x,t)$, then we can figure out what we mean unambiguously. The above is

$$\left(\frac{\partial}{\partial x} - \frac{\partial}{\partial t}\right)\left(\frac{\partial f}{\partial x} + \frac{\partial f}{\partial t}\right) = \frac{\partial^2 f}{\partial x^2} + \frac{\partial^2 f}{\partial x \partial t} - \frac{\partial^2 f}{\partial t \partial x} - \frac{\partial^2 f}{\partial t^2}, \tag{8.8}$$

so indeed, this is a legitimate factorization of the wave equation. In fact, a very useful one – it is easy to see that the other order is also a factorization:

$$\left(\frac{\partial}{\partial x} - \frac{\partial}{\partial t}\right)\left(\frac{\partial}{\partial x} + \frac{\partial}{\partial t}\right) f(x,t) = \left(\frac{\partial}{\partial x} + \frac{\partial}{\partial t}\right)\left(\frac{\partial}{\partial x} - \frac{\partial}{\partial t}\right) f(x,t), \tag{8.9}$$

so that if either "root" of the wave equation is satisfied, we have a valid solution:

$$\left(\frac{\partial}{\partial x} - \frac{\partial}{\partial t}\right) f(x,t) = 0 \qquad \text{or} \qquad \left(\frac{\partial}{\partial x} + \frac{\partial}{\partial t}\right) f(x,t) = 0 \tag{8.10}$$

where the first equation has solution $f(x,t) = \phi(x+t)$ and the second has $f(x,t) = \phi(x-t)$ for any scalar $\phi(y)$, so we conclude that the solutions to the wave equation are of the form $\phi(x \pm t)$, as we know they are.

It is hard to see what the big deal is – but now consider an operator of the form:

$$\alpha^2 \frac{\partial^2}{\partial x^2} - q(x)^2, \tag{8.11}$$

or, acting on our "test function" $f(x)$:

$$\left(\alpha^2 \frac{\partial^2}{\partial x^2} - q(x)^2\right) f(x) = \alpha^2 f''(x) - q(x)^2 f(x). \tag{8.12}$$

It is clear, because of the $x$-dependence in $q(x)$ that the "obvious" factorization will not work:

$$\begin{aligned}\left(\alpha \frac{\partial}{\partial x} + q(x)\right)\left(\alpha \frac{\partial}{\partial x} - q(x)\right) f(x) &= \left(\alpha \frac{\partial}{\partial x} + q(x)\right) \left(\alpha f'(x) - q(x) f(x)\right) \\ &= \alpha^2 f''(x) - \alpha q'(x) f(x) - \alpha q(x) f'(x) + \alpha q(x) f'(x) - q(x)^2 f(x) \\ &= \alpha^2 f''(x) - \alpha q'(x) f(x) - q(x)^2 f(x).\end{aligned} \tag{8.13}$$

There is a cross-term in the above that is not in the actual expression (8.12), so this is *not* a valid factorization of the operator (8.11). Of course, the ordering makes a difference – we have no reason to prefer + for the first factor, − for the second in the first line of the above, we might just as easily have written

$$\left(\alpha \frac{\partial}{\partial x} - q(x)\right) \left(\alpha \frac{\partial}{\partial x} + q(x)\right) f(x) \tag{8.14}$$

and expected to get a valid result. Notice what happens for this operator, when we write out its action on $f(x)$

$$\left(\alpha \frac{\partial}{\partial x} - q(x)\right)\left(\alpha \frac{\partial}{\partial x} + q(x)\right) f(x) = \alpha^2 f''(x) + \alpha q'(x) f(x) - q(x)^2 f(x). \tag{8.15}$$

The sum of the two gives us just the right result

$$\begin{aligned}&\frac{1}{2}\left[\left(\alpha \frac{\partial}{\partial x} + q(x)\right) \left(\alpha \frac{\partial}{\partial x} - q(x)\right) + \left(\alpha \frac{\partial}{\partial x} - q(x)\right) \left(\alpha \frac{\partial}{\partial x} + q(x)\right)\right] \\ &\quad = \alpha^2 \frac{\partial^2}{\partial x^2} - q(x)^2.\end{aligned} \tag{8.16}$$

The *anticommutator* of two matrices is, as one might expect: $\{\mathbb{A}, \mathbb{B}\} \equiv \mathbb{A}\,\mathbb{B} + \mathbb{B}\,\mathbb{A}$, and in this notation, the operator analogy allows us to write the above as

$$\frac{1}{2}\left\{\left(\alpha\frac{\partial}{\partial x}+q(x)\right),\left(\alpha\frac{\partial}{\partial x}-q(x)\right)\right\}=\alpha^2\,\frac{\partial^2}{\partial x^2}-q(x)^2. \tag{8.17}$$

The commutator of the two orderings gives the residual ("bad") piece, from which we can still construct the correct operator, of course (by subtracting the offending term from either (8.13) or (8.14))

$$\left[\left(\alpha\,\frac{\partial}{\partial x}+q(x)\right),\left(\alpha\frac{\partial}{\partial x}-q(x)\right)\right]=-2\,\alpha\,q'(x)\,f(x). \tag{8.18}$$

## 8.3 Harmonic Oscillator

Now we can study a new physical system – we saw how the wavefunction was generated by a potential and boundary conditions for the simple case of an infinite square well. What about a "mass on a spring"? We have the obvious potential here $V(x)=\frac{1}{2}\,k\,x^2$, so we can form the Hamiltonian. Then there's the question of boundary conditions: Classically, we would fix the maximal extension of the spring, either from initial values (set $x(t=0)=a$, $\dot{x}(t=0)=0$), or by specifying the energy. On the quantum side, we have no obvious boundary, except the implicit condition that $\psi(x\rightarrow\pm\infty)=0$ for the spatial portion of the wave function. That will lead to some interesting predictions, but for now, let's write out the Hamiltonian for use in Schrödinger's equation.

Remember that for $\Psi(x,t)=\phi(t)\,\psi(x)$, Schrödinger's equation, which reads in general:

$$i\,\hbar\,\frac{\partial\Psi}{\partial t}=-\frac{\hbar^2}{2\,m}\,\frac{\partial^2\Psi}{\partial x^2}+V(x)\,\Psi, \tag{8.19}$$

has the separable solution: $\phi(t)=e^{-i\,\frac{E}{\hbar}\,t}$ with $\psi(x)$ solving the time-independent Schrödinger equation

$$-\frac{\hbar^2}{2\,m}\,\frac{d^2\psi}{dx^2}+\frac{1}{2}\,m\,\omega^2\,x^2\,\psi=E\,\psi \tag{8.20}$$

where we have input the relevant potential, defining $\omega^2=\frac{k}{m}$ as usual.

### 8.3.1 Factoring the Hamiltonian

To the extent that the Hamiltonian operator is made up of $x$'s and $p$'s, it can be viewed as a differential operator that acts on a wavefunction. We just saw how to deal with factorization of simple one-dimensional operators. Consider, then, the simple relation provided by taking the Hamiltonian operator

$$\hat{H} = \frac{1}{2\,m}\left(-\hbar^2\,\frac{\partial^2}{\partial x^2} + m^2\,\omega^2\,x^2\right) \tag{8.21}$$

and factoring the term in parentheses with $\alpha = \hbar$, and $q(x) = m\,\omega\,x$ (with obvious sign replacement), we get one ordering:

$$\begin{aligned}\frac{1}{2\,m}\left(-\hbar\,\frac{\partial}{\partial x} + m\,\omega\,x\right)\left(\hbar\,\frac{\partial}{\partial x} + m\,\omega\,x\right) &= \frac{1}{2\,m}\left(-\hbar^2\,\frac{\partial^2}{\partial x^2} - \hbar\,m\,\omega + m^2\,\omega^2\,x^2\right)\\ &= \hat{H} + \frac{i\,\omega}{2}\,[x, p].\end{aligned} \tag{8.22}$$

The other ordering gives:

$$\frac{1}{2\,m}\left(\hbar\,\frac{\partial}{\partial x} + m\,\omega\,x\right)\left(-\hbar\,\frac{\partial}{\partial x} + m\,\omega\,x\right) = \hat{H} - \frac{i\,\omega}{2}\,[x, p]. \tag{8.23}$$

Then we can form the commutator of the two terms:

$$\frac{1}{2\,m}\left[\hbar\frac{\partial}{\partial x} + m\,\omega\,x, -\hbar\,\frac{\partial}{\partial x} + m\,\omega\,x\right] = -i\,\omega[x, p] = \hbar\,\omega, \tag{8.24}$$

and for ease-of-use, we normalize the above to get

$$\left[\frac{1}{\sqrt{2\,m\,\hbar\,\omega}}\left(\hbar\,\frac{\partial}{\partial x} + m\,\omega\,x\right), \frac{1}{\sqrt{2\,m\,\hbar\,\omega}}\left(-\hbar\,\frac{\partial}{\partial x} + m\,\omega\,x\right)\right] = 1. \tag{8.25}$$

These two operators are called $a_-$ and $a_+$ respectively, and can be written in terms of the momentum operator $p = \frac{\hbar}{i}\,\frac{\partial}{\partial x}$

$$\begin{aligned} a_- &= \frac{1}{\sqrt{2\,m\,\hbar\,\omega}}\left(\hbar\,\frac{\partial}{\partial x} + m\,\omega\,x\right) = \frac{1}{\sqrt{2\,m\,\hbar\,\omega}}\,(i\,p + m\,\omega\,x)\\ a_+ &= \frac{1}{\sqrt{2\,m\,\hbar\,\omega}}\left(-\hbar\,\frac{\partial}{\partial x} + m\,\omega\,x\right) = \frac{1}{\sqrt{2\,m\,\hbar\,\omega}}\,(-i\,p + m\,\omega\,x),\end{aligned} \tag{8.26}$$

with $[a_-, a_+] = 1$ and, from (8.23)

$$a_-a_+ = \frac{\hat{H}}{\hbar\,\omega} + \frac{1}{2} \tag{8.27}$$

and

$$a_+a_- = a_-a_+ - 1 = \frac{\hat{H}}{\hbar\,\omega} - \frac{1}{2}. \tag{8.28}$$

There is a point to all of this – using the last two equations, the Hamiltonian operator can be factored into products of $a_-$ and $a_+$

$$\hat{H} = \hbar\,\omega \left( a_\pm\, a_\mp \pm \frac{1}{2} \right). \tag{8.29}$$

Now, using Schrödinger's equation, we have $\hat{H}\,\psi = E\,\psi$. Suppose we have a solution $\psi$ for some energy $E$, then consider the operator $a_-$ acting on $\psi$ (i.e. $a_-\psi$), this state solves Schrödinger's equation with a new energy

$$\begin{aligned} \hat{H}\, a_-\,\psi &= \left[ \hbar\,\omega \left( a_- a_+ - \frac{1}{2} \right) \right] a_-\psi \\ &= \hbar\,\omega a_-\, a_+\, a_-\,\psi - \frac{1}{2}\, a_-\,\psi \\ &= a_- \left[ \left( \hbar\,\omega\, (a_+\, a_- - \frac{1}{2} \right) \right] \psi \\ &= a_-\, (H - \hbar\,\omega)\,\psi \\ &= (E - \hbar\,\omega)\, a_-\,\psi. \end{aligned} \tag{8.30}$$

This shows that $a_-\psi$ is itself a solution to the Schrödinger equation, and that the energy of this new state is the energy of the $\psi$ state minus $\hbar\,\omega$. That's fine, but we still have the problem of finding a single $\psi$ that solves $\hat{H}\,\psi = E\,\psi$ (and, of course, the value of $E$ associated with this). We know that the energy $E$ must be greater than zero for any physically accessible wavefunction (i.e. one that is normalizable, and hence can be interpreted in the statistical sense). If we continually apply $a_-$ to a state $\psi$, we will eventually achieve a state with negative energy, which will then not be a valid solution. In this case, then, there must exist a state $\psi_0$ such that $a_-\,\psi_0 = 0$, but from the definition of the $a_-$ operator, $\psi_0$ solves the differential equation:

$$\frac{1}{\sqrt{2\,m\,\hbar\,\omega}} \left( \hbar\,\frac{\partial}{\partial x} + m\,\omega\,x \right) \psi = 0 \longrightarrow A\,e^{-\frac{m\,\omega\,x^2}{2\,\hbar}}, \tag{8.31}$$

and the procedure stops – we have a lowest energy state $\psi_0$ with energy:

$$H\,\psi_0 = \hbar\,\omega \left( a_+ a_- + \frac{1}{2} \right) \psi_0 = \frac{1}{2}\,\hbar\,\omega\,\psi_0 = E_0\,\psi_0, \tag{8.32}$$

allowing us to set $E_0 = \frac{1}{2}\,\hbar\,\omega$.

With a bit of notational foreshadowing, it will come as no surprise that for a solution $\psi$ with energy $E$, $a_+\,\psi$ is another solution with energy $E + \hbar\,\omega$, and we can start with the lowest state $\psi_0$ and work our way up in energy. For this reason, $a_\pm$ are called raising/lowering operators. If we apply the raising operator to $\psi_0$, we will obtain arbitrarily large energy solutions to Schrödinger's equation.

Keep in mind, though, that the eigenvalue equation itself tells us nothing about normalization – the fact that a particular $\psi_n$ has $\hat{H}\,\psi_n = E_n\,\psi_n$ is independent of the normalization of the wave function, and so we must work directly with the $\psi_n$ state to ensure that it is appropriately normalized.

**Homework**

Reading: Griffiths, pp. 40–47.

**Problem 8.1**

Here are a few quick problems providing practice with commutators (remember the game plan: Put in a test function $T(x)$, evaluate the commutator acting on $T(x)$, then remove $T(x)$ to write your answers in terms of the $x$ and $p$ operators):

**a.** Evaluate $[\hat{H}, x]$ for a generic potential $V(x)$.

**b.** Evaluate $[x^n, p]$ using $[x, p] = i\,\hbar$ successively (to move the $p$ in $x^n\,p$ through all the $x$'s, for example).

**c.** Show that $[p, f(x)] = p\,f(x)$, and use this to reproduce your result from part b.

**Problem 8.2**

Griffiths 2.8. Here we are interested in the decomposition of an initial wavefunction in the eigenfunctions of the infinite square well.

**Problem 8.3**

For an eigenstate: $\Psi(x,t) = \Psi_n(x,t)$ of the infinite square well:

$$\Psi_n(x,t) = \sqrt{\frac{2}{a}}\,\sin\!\left(\frac{n\,\pi\,x}{a}\right)\,e^{-i\,\frac{E_n\,t}{\hbar}}. \tag{8.33}$$

Find $\langle p^2\rangle$, and use this, together with $\langle p\rangle$ to compute $\sigma_p^2 = \langle p^2\rangle - \langle p\rangle^2$. We know that $\sigma_x^2 = \frac{a^2}{12} - \frac{a^2}{2\,n^2\,\pi^2}$. What is the value of the product of these two, $\sigma_x^2\,\sigma_p^2 = \boxed{?}$ What is the minimum value this product can take?