Physics 195a
Course Notes
The Simple Harmonic Oscillator: Creation and Destruction Operators
021105 F. Porter

1 Introduction

The harmonic oscillator is an important model system pervading many areas in classical physics; it is likewise ubiquitous in quantum mechanics. The non-relativistic Scrödinger equation with a harmonic oscillator potential is readily solved with standard analytic methods, whether in one or three dimensions. However, we will take a different tack here, and address the one-dimension problem more as an excuse to introduce the notion of "creation" and "annihilation" operators, or "step-up" and "step-down" operators. This is an example of a type of operation which will repeat itself in many contexts, including the theory of angular momentum.

2 Harmonic Oscillator in One Dimension

Consider the Hamiltonian:

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

This is the Hamiltonian for a particle of mass m in a harmonic oscillator potential with spring constant $k = m\omega^2$, where ω is the "classical frequency" of the oscillator. We wish to find the eigenstates and eigenvalues of this Hamiltonian, that is, we wish to solve the Schrödinger equation for this system. We'll use an approach due to Dirac.

Define the operators:

$$a \equiv \sqrt{\frac{m\omega}{2}}x + i\frac{1}{\sqrt{2m\omega}}p \tag{2}$$

$$a^\dagger \equiv \sqrt{\frac{m\omega}{2}}x - i\frac{1}{\sqrt{2m\omega}}p. \tag{3}$$

Note that $a^\dagger$ is the Hermitian adjoint of a. We can invert these equations to obtain the x and p operators:

$$x = \frac{1}{\sqrt{2m\omega}}(a + a^\dagger), \tag{4}$$

$$p = -i\sqrt{\frac{m\omega}{2}}(a - a^\dagger). \tag{5}$$

Further, define

$$N \equiv a^\dagger a \tag{6}$$
$$= \frac{m\omega}{2}x^2 + \frac{1}{2m\omega}p^2 - \frac{1}{2}, \tag{7}$$

where we have made use of the commutator $[x, p] = i$. Thus, we may rewrite the Hamiltonian in the form:

$$H = \omega\left(N + \frac{1}{2}\right), \tag{8}$$

and our problem is equivalent to finding the eigenvectors and eigenvalues of N.

3 Algebraic Determination of the Spectrum

Let $|n\rangle$ denote an eigenvector of N, with eigenvalue n:

$$N|n\rangle = n|n\rangle. \tag{9}$$

Then $|n\rangle$ is also an eigenstate of H with eigenvalue $(n + \frac{1}{2})\omega$. Since N is Hermitian,

$$N^\dagger = (a^\dagger a)^\dagger = (a^\dagger)(a^\dagger)^\dagger = a^\dagger a = N, \tag{10}$$

its eigenvalues are real. Also $n \geq 0$, since

$$n = \langle n|N|n\rangle = \langle n|a^\dagger a|n\rangle = \langle an|an\rangle \geq 0. \tag{11}$$

Now consider the commutator:

$$[a, a^\dagger] = \left[\sqrt{\frac{m\omega}{2}}x + i\frac{1}{\sqrt{2m\omega}}p, \sqrt{\frac{m\omega}{2}}x - i\frac{1}{\sqrt{2m\omega}}p\right]$$
$$= \frac{i}{2}\{-[x, p] + [p, x]\} = 1. \tag{12}$$

Next, notice that

$$Na = a^\dagger aa = aa^\dagger a - a = a(N - 1), \tag{13}$$
$$Na^\dagger = a^\dagger aa^\dagger = a^\dagger a^\dagger a + a^\dagger = a^\dagger(N + 1). \tag{14}$$

Thus,

$$Na|n\rangle = a(N-1)|n\rangle = (n-1)a|n\rangle. \tag{15}$$

We see that $a|n\rangle$ is also an eigenvector of N, with eigenvalue $n-1$. Assuming $|n\rangle$ is normalized, $\langle n|n\rangle = 1$, then

$$\langle an|an\rangle = \langle n|N|n\rangle = n, \tag{16}$$

or $a|n\rangle = \sqrt{n}|n-1\rangle$, where we have also normalized the new eigenvector $|n-1\rangle$.

We may continue this process to higher powers of a, *e.g.*,

$$a^2|n\rangle = a\sqrt{n}|n-1\rangle = \sqrt{n(n-1)}|n-2\rangle. \tag{17}$$

If n is an eigenvalue of N, then so are $n-1, n-2, n-3, \ldots$. But we showed that all of the eigenvalues of N are ≥ 0, so this sequence cannot go on forever. In order for it to terminate, we must have n an integer, so that we reach the value 0 eventually, and conclude with the states

$$a|1\rangle = \sqrt{1}|0\rangle, \tag{18}$$

$$a|0\rangle = 0. \tag{19}$$

Hence, the spectrum of N is $\{0, 1, 2, 3, \ldots, n, ?\}$.

To investigate further, we similarly consider:

$$Na^\dagger|n\rangle = (n+1)a^\dagger|n\rangle. \tag{20}$$

Hence $a^\dagger|n\rangle$ is also an eigenvector of N with eigenvalue $n+1$:

$$a^\dagger|n\rangle = \sqrt{n+1}|n+1\rangle. \tag{21}$$

The spectrum of N is thus the set of all non-negative integers. The energy spectrum is:

$$E_n = \omega\left(n + \frac{1}{2}\right), \quad n = 0, 1, 2, \ldots. \tag{22}$$

We notice two interesting differences between this spectrum and our classical experience. First, of course, is that the energy levels are quantized. Second, the ground state energy is $E_0 = \omega/2 > 0$. Zero is not an allowed energy. This lowest energy value is referred to as "zero-point motion". We cannot give the particle zero energy and be consistent with the uncertainty principle, since this would require $p = 0$ and $x = 0$, simultaneously.

We may give a "physical" intuition to the operators a and $a^\dagger$: The energy of the oscillator is quantized, in units of ω, starting at the ground state with energy $\frac{1}{2}\omega$. The $a^\dagger$ operator "creates" a quantum of energy when operating on a state – we call it a "creation operator" (alternatively, a "step-up operator"). Similarly, the a operator "destroys" a quantum of of energy – we call it a "destruction operator" (or "step-down", or "annihilation operator"). This idea takes on greater significance when we encounter the subject of "second quantization" and quantum field theory.

4 The Eigenvectors

We have determined the eigenvalues; let us turn our attention now to the eigenvectors. Notice that we can start with the ground state $|0\rangle$ and generate all eigenvectors by repeated application of $a^\dagger$:

$$\begin{aligned} |1\rangle &= a^\dagger|0\rangle \\ |2\rangle &= \frac{(a^\dagger)^2}{\sqrt{2}}|0\rangle \\ &\vdots \\ |n\rangle &= \frac{(a^\dagger)^n}{\sqrt{n!}}|0\rangle. \end{aligned} \tag{23}$$

So, if we can find the ground state wave function, we have a prescription for determining any other state.

We wish to find the ground state wave function, in the position representation (for example). If $|x\rangle$ represents the amplitude describing a particle at position x, then $\langle x|0\rangle = \psi_0(x)$ is the ground state wave function in postition space.[1] Consider:

$$\begin{aligned} \langle x|a|0\rangle &= 0 \\ &= \langle x|\sqrt{\frac{m\omega}{2}}x + \frac{ip}{\sqrt{2m\omega}}|0\rangle \\ &= \left(\sqrt{\frac{m\omega}{2}}x + \frac{1}{\sqrt{2m\omega}}\frac{d}{dx}\right)\langle x|0\rangle. \end{aligned} \tag{24}$$

[1]The notion here is that the wave function of a particle at position x is (proportional to) a δ-function in position. Hence, $\psi_0(x) = \langle x|0\rangle = \int \delta(x-x')\psi_0(x')\,dx'$.

Thus, we have the (first order!) differential equation:

$$\frac{d}{dx}\psi_0(x) = -m\omega x\psi_0(x), \tag{25}$$

with solution:

$$\ln\psi_0(x) = -m\omega\frac{x^2}{2} + \text{constant}. \tag{26}$$

The constant is determined (up to an arbitrary phase) by normalizing, to obtain:

$$\psi_0(x) = \left(\frac{m\omega}{\pi}\right)^{1/4}\exp\left(-\frac{1}{2}m\omega x^2\right). \tag{27}$$

This is a Gaussian form. The Fourier transform of a Gaussian is also a Gaussian, so the momentum space wave function is also of Gaussian form. In this case, the position-momentum uncertainty relation is an equality, $\Delta x\Delta p = 1/2$. This is sometimes referred to as a "minimum wave packet".

Now that we have the ground state, we may follow our plan to obtain the excited states. For example,

$$\langle x|1\rangle = \langle x|a^\dagger|0\rangle = \left(\sqrt{\frac{m\omega}{2}}x - \frac{1}{\sqrt{2m\omega}}\frac{d}{dx}\right)\langle x|0\rangle \tag{28}$$

Substituting in our above result for ψ_0, we thus obtain:

$$\psi_1(x) = \sqrt{2m\omega}\left(\frac{m\omega}{\pi}\right)^{1/4} x\exp\left(-\frac{1}{2}m\omega x^2\right). \tag{29}$$

To express the general eigenvector, it is convenient to define $y = \sqrt{m\omega}x$, and

$$a^\dagger = \frac{1}{\sqrt{2}}(y - d_y), \tag{30}$$

where d_y is a shorthand notation meaning d/dy. The general eigenfunctions are clearly all polynomials times $e^{-y^2/2}$, since

$$\psi_n(y) = \frac{(a^\dagger)^n}{\sqrt{n!}}\psi_0(n) = \frac{1}{\sqrt{2^n n!}}(y - d_y)^n\frac{1}{\pi^{1/4}}e^{-y^2/2}. \tag{31}$$

Thus, we may let

$$\psi_n(y) = \frac{1}{\sqrt{2^n n!}}\frac{1}{\pi^{1/4}}H_n(y)e^{-y^2/2}, \tag{32}$$

where H_n is a polynomial, to be determined.

We may derive a recurrence relation which these polynomials satisfy. First, use

$$\psi_{n+1}(y) = \frac{a^\dagger}{\sqrt{n+1}}\psi_n(y) = \frac{1}{\sqrt{2(n+1)}}(y - d_y)\psi_n(y), \tag{33}$$

to obtain:

$$H_{n+1}(y) = 2yH_n(y) - d_y H_n(y). \tag{34}$$

On the other hand,

$$\psi_{n-1}(y) = \frac{a}{\sqrt{n}}\psi_n(y) = \frac{1}{\sqrt{2n}}(y + d_y)\psi_n(y), \tag{35}$$

or,

$$d_y H_n(y) = 2nH_{n-1}(y). \tag{36}$$

Combining Eqns. 34 and 36 to eliminate the derivative, we find:

$$H_{n+1}(y) = 2yH_n(y) - 2nH_{n-1}(y). \tag{37}$$

This result is the familiar *recurrence relation* for the **Hermite polynomials** (hence our choice of symbol).

We could go on to determine other properties of these polynomials, such as *Rodrigues' formula*:

$$H_n(x) = (-)^n e^{x^2}\frac{d^n}{dx^n}e^{-x^2}, \quad n = 0, 1, 2, \ldots \tag{38}$$

But we'll conclude here only by noting that the harmonic oscillator wave functions are also eigenstates of parity:

$$P\psi_n(x) = \psi_n(-x) = (-)^n\psi_n(x), \tag{39}$$

wherer P is the parity (space reflection) operator. This fact shouldn't be surprising, since $[H, P] = 0$.

In Fig. 1 we show the first five harmonic oscillator wave functions. It is worth noting several characteristics of these curves, which are representative of wave functions for one-dimensional potential problems.

- The ground state wave function has no nodes (at finite y); the first excited state has one node. In general, the n-th wave function has $n - 1$ nodes.

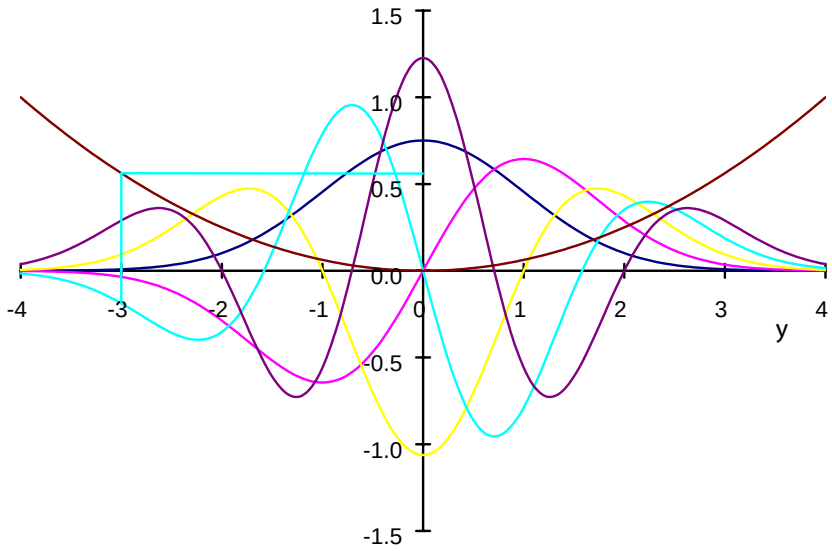

Figure 1: The first five harmonic oscillator wave functions, $\psi_0(y), \ldots, \psi_4(y)$, from Eqn. 32. Also shown is the quadratic potential, $V(y)$, for $\omega = 1/8$. The classical turning point (point of inflection) for ψ_4 is projected to the x-axis at $x = 3$. The projection is extended to the potential curve, and thence to the y-axis, where it may be seen that the energy of this state is $9/16 = (4 + \frac{1}{2})\omega$.

- Correlating with the increase in nodes, the higher the excited state, the greater the spatial frequency of the wave function oscillations. This corresponds to higher momenta, as expected from the deBroglie relation.

- Each wave function has a region around $y = 0$ of oscillatory behavior, in which the curve is concave towards the horizontal axis (the sign of the second derivative is opposite that of the wave function), and a region at larger values of $|y|$ of "decay", in which the curve is convex towards the horizontal axis. This feature may be understood as follows: Wherever the total energy, E, is larger than the potential energy, V, the kinetic energy, T, is positive, and $p = \sqrt{2mT}$ is real. This is the "classically allowed" region, and the wave function really looks like a wave. On the other hand, wherever $E < V$, $T < 0$, and the corresponding "momentum" is imaginary. This is the classically forbidden region. In this region, the probability to find the particle falls off rapidly. Mea-

surements of the particle's position and momentum (yielding a real number) are restricted according to the uncertainty principle such that no internal contradictions occur.

The point of inflection in the wave function between the classically allowed and forbidden regions is the "classical turning point" of the system. This is where the classical momentum is zero, and $E = V$.

5 Exercises

1. We have noticed some things about the qualitative behavior of wave functions in our discussion of Fig. 1. Consider the one-dimensional problem with potential function given by:

$$V(x) = \begin{cases} 0 & \text{for } |x| \leq a, \\ V_0 & \text{for } |x| > a, \end{cases} \tag{40}$$

where $V_0 > 0$ and $a > 0$.

   (a) Suppose that there are four bound states. Make a qualitative, but careful, drawing of what you expect the first four wave functions to look like, in the spirit of Fig. 1.

   (b) Make a qualitative drawing for the wave function of a state with energy above V_0.

2. Let us generalize the discussion of the simple harmonic oscillator to three dimensions. In this case, the Hamiltonian is:

$$H = \frac{1}{2m}(p_1^2 + p_2^2 + p_3^2) + \frac{1}{2}m(\Omega \mathbf{x})^2, \tag{41}$$

where Ω is a 3×3 symmetric real matrix.

   (a) Determine the energy spectrum and eigenvectors of this system.

   (b) Suppose the potential is spherically symmetric. Using the equivalent one-dimensional potential approach, find the eigenvalues and eigenvectors of H corresponding to the possible values of orbital angular momentum.