

Harmonic Oscillator Physics

Lecture 9

Physics 342 Quantum Mechanics I

Friday, February 12th, 2010

For the harmonic oscillator potential in the time-independent Schrödinger equation:

$$\frac{1}{2m} \left(-\hbar^2 \frac{d^2\psi(x)}{dx^2} + m^2 \omega^2 x^2 \psi(x) \right) = E \psi(x), \quad (9.1)$$

we found a ground state

$$\psi_0(x) = A e^{-\frac{m\omega x^2}{2\hbar}} \quad (9.2)$$

with energy $E_0 = \frac{1}{2} \hbar \omega$. Using the raising and lowering operators

$$\begin{aligned} a_+ &= \frac{1}{\sqrt{2\hbar m \omega}} (-ip + m\omega x) \\ a_- &= \frac{1}{\sqrt{2\hbar m \omega}} (ip + m\omega x), \end{aligned} \quad (9.3)$$

we found we could construct additional solutions with increasing energy using a_+ , and we could take a state at a particular energy E and construct solutions with lower energy using a_- . The existence of a minimum energy state ensured that no solutions could have negative energy and was used to define ψ_0 ¹:

$$a_- \psi_0 = 0 \quad H(a_+^n \psi_0) = \left(\frac{1}{2} + n \right) \hbar \omega a_+^n \psi_0. \quad (9.4)$$

The operators a_+ and a_- are Hermitian conjugates of one another – for any

¹I am leaving the “hats” off, from here on – we understand that H represents a differential operator given by $H(x, \frac{\hbar}{i} \frac{\partial}{\partial x})$ for a classical Hamiltonian.

$f(x)$ and $g(x)$ (vanishing at spatial infinity), the inner product:

$$\begin{aligned} \int_{-\infty}^{\infty} f(x)^* a_{\pm} g(x) dx &= \int_{-\infty}^{\infty} f(x)^* \left(\mp \hbar \frac{\partial g(x)}{\partial x} + m \omega x g(x) \right) dx \\ &= \int_{-\infty}^{\infty} \left(\pm \hbar \frac{\partial f(x)^*}{\partial x} g(x) + f(x)^* m \omega x g(x) \right) dx \\ &= \int_{-\infty}^{\infty} (a_{\mp} f(x))^* g(x) dx, \end{aligned} \tag{9.5}$$

(integration by parts) or, in words, we can “act on $g(x)$ with a_{\pm} or act on $f(x)$ with a_{\mp} ” in the inner product.

9.1 Normalization

The state ψ_n that comes from n applications of a_{\pm}^n is not normalized, nor does the eigenvalue form of the time-independent Schrödinger equation demand that it be. Normalization is the manifestation of our probabilistic interpretation of $|\Psi(x, t)|^2$. Consider the ground state, that has an undetermined constant A . If we want $|\Psi(x, t)|^2$ to represent a probability density, then

$$\int_{-\infty}^{\infty} A^2 e^{-\frac{m\omega x^2}{\hbar}} dx = 1, \tag{9.6}$$

and the left-hand side is a Gaussian integral:

$$\int_{-\infty}^{\infty} A^2 e^{-\frac{m\omega x^2}{\hbar}} dx = A^2 \sqrt{\frac{\pi \hbar}{m\omega}}, \tag{9.7}$$

so the normalization is $A = \left(\frac{m\omega}{\pi \hbar}\right)^{1/4}$. Just because we have normalized the ground state does not mean that $\psi_1 \sim a_{+}\psi_0(x)$ is normalized. Indeed, we have to normalize each of the $\psi_n(x)$ separately. Fortunately, this can be done once (and for all).

Suppose we have a normalized set of ψ_n , i.e. $\int_{-\infty}^{\infty} \psi_n^2 dx = 1$ for all $n = 0 \rightarrow \infty$. We know that $\psi_{n\pm 1} = \alpha_{\pm} a_{\pm} \psi_n$ where the goal is to find the constants α_{\pm} associated with raising and lowering while keeping the wavefunctions normalized. Take the norm of the resulting raised or lowered state:

$$\begin{aligned} \int_{-\infty}^{\infty} |\psi_{n\pm 1}|^2 dx &= \alpha_{\pm}^2 \int_{-\infty}^{\infty} (a_{\pm} \psi_n(x))^* (a_{\pm} \psi_n(x)) dx \\ &= \alpha_{\pm}^2 \int_{-\infty}^{\infty} (a_{\mp} a_{\pm} \psi_n(x))^* \psi_n(x) dx, \end{aligned} \tag{9.8}$$

and the operator $a_{\mp} a_{\pm}$ is related to the Hamiltonian, as we saw last time: $H = \hbar \omega (a_{\pm} a_{\mp} \pm \frac{1}{2})$. Then

$$a_{\mp} a_{\pm} \psi_n = \left(\frac{H}{\hbar \omega} \pm \frac{1}{2} \right) \psi_n = \left(\frac{1}{2} + n \pm \frac{1}{2} \right) \psi_n, \quad (9.9)$$

so (9.8) becomes

$$\alpha_{\pm}^2 \int_{-\infty}^{\infty} (a_{\mp} a_{\pm} \psi_n(x))^* \psi_n(x) dx = \alpha_{\pm}^2 \left(\frac{1}{2} + n \pm \frac{1}{2} \right) \int_{-\infty}^{\infty} |\psi_n(x)|^2 dx. \quad (9.10)$$

The integral $\int_{-\infty}^{\infty} |\psi_n(x)|^2 dx = 1$ by assumption, so we have

$$\alpha_+ = \frac{1}{\sqrt{n+1}} \quad \alpha_- = \frac{1}{\sqrt{n}}, \quad (9.11)$$

and our final relation is

$$\boxed{\psi_{n+1} = \frac{1}{\sqrt{n+1}} a_+ \psi_n \quad \psi_{n-1} = \frac{1}{\sqrt{n}} a_- \psi_n.} \quad (9.12)$$

Starting from the ground state, for which we know the normalization,

$$\begin{aligned} \psi_1 &= a_+ \psi_0 \\ \psi_2 &= \frac{1}{\sqrt{2}} a_+ \psi_1 = \frac{1}{\sqrt{1 \times 2}} a_+^2 \psi_0 \\ \psi_3 &= \frac{1}{\sqrt{3}} a_+ \psi_2 = \frac{1}{\sqrt{1 \times 2 \times 3}} a_+^3 \psi_0. \end{aligned} \quad (9.13)$$

The general case is

$$\boxed{\psi_n = \frac{1}{\sqrt{n!}} a_+^n \psi_0} \quad (9.14)$$

for the appropriately normalized ψ_0 ,

$$\boxed{\psi_0(x) = \left(\frac{m \omega}{\pi \hbar} \right)^{1/4} e^{-\frac{m \omega x^2}{2 \hbar}}.} \quad (9.15)$$

9.2 Orthonormality

The states described by ψ_n are complete (we assume) and orthonormal – take our usual inner product for ψ_m and ψ_n :

$$\psi_n \cdot \psi_m = \int_{-\infty}^{\infty} \psi_n(x)^* \psi_m(x) dx = \frac{1}{\sqrt{m!}} \frac{1}{\sqrt{n!}} \int_{-\infty}^{\infty} (a_+^n \psi_0)^* (a_+^m \psi_0) dx. \quad (9.16)$$

Now, suppose $m > n$, then using the fact that a_+ and a_- are Hermitian conjugates, we can flip the a_+^m onto the other term:

$$\frac{1}{\sqrt{m!}} \frac{1}{\sqrt{n!}} \int_{-\infty}^{\infty} (a_+^n \psi_0)^* (a_+^m \psi_0) dx = \frac{1}{\sqrt{m!}} \frac{1}{\sqrt{n!}} \int_{-\infty}^{\infty} (a_-^m a_+^n \psi_0)^* (\psi_0) dx, \quad (9.17)$$

and we know that $a_+^n \psi_0 \sim \psi_n$ and $a_-^m \psi_n \sim \psi_{n-m}$ – but for $m > n$, we have $a_-^{m-n} \psi_0 = 0$, the defining property of the ground state. In the case $n > m$, we just use the conjugate in the other direction, and make the same argument:

$$\frac{1}{\sqrt{m!}} \frac{1}{\sqrt{n!}} \int_{-\infty}^{\infty} (a_+^n \psi_0)^* (a_+^m \psi_0) dx = \frac{1}{\sqrt{m!}} \frac{1}{\sqrt{n!}} \int_{-\infty}^{\infty} (\psi_0)^* (a_-^n a_+^m \psi_0) dx = 0. \quad (9.18)$$

Only when $m = n$ will we get a non-zero result, and of course, $\int_{-\infty}^{\infty} \psi_m^2 dx = 1$ by construction. So

$$\boxed{\int_{-\infty}^{\infty} \psi_n(x)^* \psi_m(x) dx = \delta_{mn}.} \quad (9.19)$$

9.2.1 Hermite Polynomials

The prescription for generating ψ_n does not provide a particularly easy way to obtain the functional form for an arbitrary n – we have to repeatedly apply the raising operator to the ground state. There is a connection between the Hermite polynomials and our procedure of “lifting up” the ground state. Using the Frobenius method, it is possible to solve Schrödinger’s equation as a power series expansion (described in Griffiths), and we won’t re-live that argument (yet). But it is important to understand the connection between the algebraic, operational approach and the brute force series expansion.

Starting from the ground state, let’s act with a_+ (call the normalization constant A again, just to make the expressions more compact):

$$\begin{aligned} \psi_1 &= a_+ \psi_0 = \frac{1}{\sqrt{2m\omega\hbar}} \left(-\hbar \frac{\partial}{\partial x} + m\omega x \right) \left(A e^{-\frac{m\omega x^2}{2\hbar}} \right) \\ &= \frac{A}{\sqrt{2}} \left(2 \sqrt{\frac{m\omega}{\hbar}} x \right) e^{-\frac{m\omega x^2}{2\hbar}}. \end{aligned} \quad (9.20)$$

Consider the second state,

$$\begin{aligned}
 \psi_2 &= \frac{1}{\sqrt{2}} a_+ \psi_1 = \frac{1}{\sqrt{2}} \frac{1}{\sqrt{2m\omega\hbar}} \left(-\hbar \frac{\partial}{\partial x} + m\omega x \right) \left[\frac{A}{\sqrt{2}} \left(2\sqrt{\frac{m\omega}{\hbar}} x \right) e^{-\frac{m\omega x^2}{2\hbar}} \right] \\
 &= \frac{A}{2\sqrt{2}} e^{-\frac{m\omega x^2}{2\hbar}} \left(-\hbar \frac{\partial}{\partial x} \right) \left(\frac{2x}{\hbar} \right) \\
 &\quad + \frac{1}{\sqrt{2}} \left(2\sqrt{\frac{m\omega}{\hbar}} x \right) \frac{1}{\sqrt{2m\omega\hbar}} \left(-\hbar \frac{\partial}{\partial x} + m\omega x \right) \left[\frac{A}{\sqrt{2}} e^{-\frac{m\omega x^2}{2\hbar}} \right] \\
 &= \frac{A}{2\sqrt{2}} e^{-\frac{m\omega x^2}{2\hbar}} (-2) + \frac{A}{2\sqrt{2}} \left(2\sqrt{\frac{m\omega}{\hbar}} x \right)^2 e^{-\frac{m\omega x^2}{2\hbar}} \\
 &= \frac{A}{2\sqrt{2}} \left(4\frac{m\omega}{\hbar} x^2 - 2 \right) e^{-\frac{m\omega x^2}{2\hbar}}.
 \end{aligned} \tag{9.21}$$

The pattern continues – we always have some polynomial in x multiplying the exponential factor. That polynomial, for the n^{th} wave function is called H_n , the n^{th} Hermite polynomial. In the dimensionless variable $\xi = \sqrt{\frac{m\omega}{\hbar}} x$, we can read off the first two – $H_1(\xi) = 2\xi$, and $H_2(\xi) = 4\xi^2 - 2$. Normalized, we have the expression

$$\psi_n(x) = \left(\frac{m\omega}{\pi\hbar} \right)^{1/4} \frac{1}{\sqrt{2^n n!}} H_n(\xi) e^{-\frac{\xi^2}{2}} \tag{9.22}$$

with

$$\begin{aligned}
 H_0(\xi) &= 1 \\
 H_1(\xi) &= 2\xi \\
 H_2(\xi) &= 4\xi^2 - 2 \\
 H_3(\xi) &= 8\xi^3 - 12\xi \\
 &\vdots
 \end{aligned} \tag{9.23}$$

This set of polynomials is well-known, and they have a number of interesting recursion and orthogonality properties (many of which can be developed from the a_+ and a_- operators). One still needs a table of these in order to write down a particular ψ_n , but that's better than taking n successive derivatives of ψ_0 – in essence, the Hermite polynomials have accomplished that procedure for you.

Once again, we can plot the first few wavefunctions (see Figure 9.1), and as we increase in energy, we see a pattern similar to the infinite square well case (note that for the harmonic oscillator, we start with $n = 0$ as the ground state rather than 1).

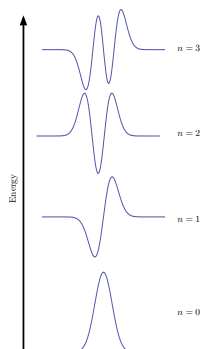


Figure 9.1: The first four stationary states: $\psi_n(x)$ of the harmonic oscillator.

9.3 Expectation Values

9.3.1 Classical Case

The classical motion for an oscillator that starts from rest at location x_0 is

$$x(t) = x_0 \cos(\omega t). \quad (9.24)$$

The probability that the particle is at a particular x at a particular time t is given by $\rho(x, t) = \delta(x - x(t))$, and we can perform the temporal average to get the spatial density. Our natural time scale for the averaging is a half cycle, take $t = 0 \rightarrow \frac{\pi}{\omega}$,

$$\rho(x) = \frac{1}{\frac{\pi}{\omega}} \int_0^{\frac{\pi}{\omega}} \delta(x - x_0 \cos(\omega t)) dt. \quad (9.25)$$

We perform the change of variables to allow access to the δ , let $y = x_0 \cos(\omega t)$ so that

$$\begin{aligned} \rho(x) &= -\frac{\omega}{\pi} \int_{x_0}^{-x_0} \frac{\delta(x - y)}{x_0 \omega \sin(\omega t)} dy \\ &= \frac{1}{\pi} \int_{-x_0}^{x_0} \frac{\delta(x - y)}{x_0 \sqrt{1 - \cos^2(\omega t)}} dy \\ &= \frac{1}{\pi} \int_{-x_0}^{x_0} \frac{\delta(x - y)}{\sqrt{x_0^2 - y^2}} dy \\ &= \frac{1}{\pi \sqrt{x_0^2 - x^2}}. \end{aligned} \quad (9.26)$$

This has $\int_{-x_0}^{x_0} \rho(x) dx = 1$ as expected (note that classically, the particle remains between $-x_0$ and x_0). The expectation value for position is then zero, since $\rho(x)$ is symmetric, $x\rho(x)$ antisymmetric, and the limits of integration are symmetric. The variance is

$$\sigma_x^2 = \langle x^2 \rangle - \langle x \rangle^2 = \int_{-x_0}^{x_0} \frac{x^2}{\pi \sqrt{x_0^2 - x^2}} dx = \frac{1}{2} x_0^2. \quad (9.27)$$

9.3.2 Quantum Case

Referring to the definition of the a_+ and a_- operators in terms of x and p , we can invert and find x and p in terms of a_+ and a_- – these are all still operators, but we are treating them algebraically. The inversion is simple

$$x = \sqrt{\frac{\hbar}{2m\omega}} (a_+ + a_-) \quad p = i \sqrt{\frac{\hbar m\omega}{2}} (a_+ - a_-), \quad (9.28)$$

and these facilitate the expectation value calculations. For example, we can find $\langle x \rangle$ for the n^{th} stationary state:

$$\langle x \rangle = \sqrt{\frac{\hbar}{2m\omega}} \int_{-\infty}^{\infty} \psi_n(x)^* (a_+ + a_-) \psi_n(x) dx = 0, \quad (9.29)$$

by orthogonality. Similarly, $\langle p \rangle = 0$. Those are not particularly surprising.

The variance for position can be calculated by squaring the position operator expressed in terms of a_{\pm}

$$\begin{aligned} \sigma_x^2 &= \langle x^2 \rangle - \langle x \rangle^2 = \frac{\hbar}{2m\omega} \int_{-\infty}^{\infty} \psi_n(x)^* (a_+ a_+ + a_+ a_- + a_- a_+ + a_- a_-) \psi_n(x) dx \\ &= \frac{\hbar}{2m\omega} \int_{-\infty}^{\infty} \psi_n(x)^* (a_+ a_- + a_- a_+) \psi_n(x) dx \\ &= \frac{\hbar}{2m\omega} \left[\int_{-\infty}^{\infty} (n+1) \psi_{n+1}(x)^2 dx + \int_{-\infty}^{\infty} n \psi_{n-1}(x)^2 dx \right] \\ &= \frac{(2n+1)\hbar}{2m\omega} \end{aligned} \quad (9.30)$$

using (9.12).

It is interesting to compare the quantum variance with the classical one. In the case of the above, we can write σ_x^2 in terms of the energy $E_n =$

$\hbar\omega\left(n + \frac{1}{2}\right)$, just

$$\sigma_x^2 = \frac{E_n}{m\omega^2}. \quad (9.31)$$

For the classical variance, we had $\sigma_x^2 = \frac{1}{2}x_0^2$, but this is related to the classical energy. Remember we start from rest at x_0 , so the total energy (which is conserved) is just $E = \frac{1}{2}m\omega^2x_0^2$, indicating that we can write the variance as

$$\sigma_x^2 = \frac{E}{m\omega^2}. \quad (9.32)$$

This is interesting, but we must keep in mind a number of caveats: 1. the classical density is time-dependent, and we have chosen to average over the “natural” timescale in the system, if no such scale presented itself, we would be out of luck making these comparisons, 2. Our classical temporal averaging is very different in spirit than the statistical information carried in the quantum mechanical wavefunction – remember that “expectation values” and variances refer to observations made multiple times on identically prepared systems, and most definitely *not* observations made over time for a single system. We will return to this point later on, for now, the comparison between quantum and classical probabilities is mainly a vehicle for motivating the notion of density as a good descriptor of physics.

Finally, we should ask where n needs to be to achieve a particular classical energy. For example, if we have a mass m with spring constant $k = m\omega^2$ and initial extension x_0 , then the total energy of the oscillator is $E = \frac{1}{2}m\omega^2x_0^2$. For what n is this equal to $E_n = \left(n + \frac{1}{2}\right)\hbar\omega$? If we put an $m = 1$ kg mass on the end of a spring with frequency $\omega = \frac{2\pi}{5}$ 1/s and full extension at $x_0 = 1$ m, then we can get a sense of the classical energy range ($E \sim .8$ J). At what value of n would a quantum mechanical system approach this energy? Using $\hbar \sim 1.05 \times 10^{-34}$ J s, we have $n \sim 6 \times 10^{33}$. We can compare the classical and quantum probability densities in the “large n ” quantum limit, an example is shown in Figure 9.2.

9.4 Mixed States

The stationary states of the harmonic oscillator are useful in characterizing some of the peculiarities of the statistical interpretation, but as with the infinite square well, the utility of these states is in their completeness, and our ability to construct arbitrary initial waveforms. Again, let’s look at

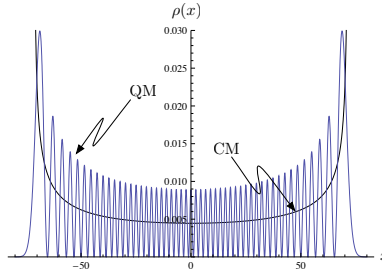


Figure 9.2: The quantum mechanical density (for $n = 50$) compared to the classical density (black).

a two state admixture, just to get a feel for the time-dependence of the expectation values. Take

$$\Psi(x, t) = \alpha e^{-i\frac{3}{2}\omega t} \psi_1(x) + \beta e^{-i\frac{5}{2}\omega t} \psi_2(x) \quad (9.33)$$

with $\alpha^2 + \beta^2 = 1$. Then the expectation value for x is

$$\begin{aligned} \langle x \rangle &= \int_{-\infty}^{\infty} \Psi(x, t)^* x \Psi(x, t) dx \\ &= \int_{-\infty}^{\infty} [\alpha^2 \psi_1 x \psi_1 + \alpha \beta e^{-i\omega t} \psi_1 x \psi_2 + \alpha \beta e^{i\omega t} \psi_2 x \psi_1 + \beta^2 \psi_2 x \psi_2] dx. \end{aligned} \quad (9.34)$$

Using our relation for x in terms of raising and lowering operators: $x = \sqrt{\frac{\hbar}{2m\omega}} (a_+ + a_-)$, we can see that the integral of $\psi_1 x \psi_1$ will be zero (we will end up with a term like $\psi_1 \psi_0$ which integrates to zero by orthogonality, and another term that goes like $\psi_1 \psi_2$, similarly zero). The same is true for $\psi_2 x \psi_2$, so we only need to evaluate the integral of $\psi_1 x \psi_2$

$$\begin{aligned} \int_{-\infty}^{\infty} \psi_1 x \psi_2 dx &= \sqrt{\frac{\hbar}{2m\omega}} \int_{-\infty}^{\infty} \psi_1 (\sqrt{2+1} \psi_3 + \sqrt{2} \psi_1) dx \\ &= \sqrt{\frac{\hbar}{m\omega}} \end{aligned} \quad (9.35)$$

using orthogonality. The integral $\int_{-\infty}^{\infty} \psi_2 x \psi_1 dx$ is also $\sqrt{\frac{\hbar}{m\omega}}$, and we can put these together

$$\langle x \rangle = 2\alpha\beta \sqrt{\frac{\hbar}{m\omega}} \cos(\omega t). \quad (9.36)$$

A similar calculation for the operator $p = i \sqrt{\frac{\hbar m \omega}{2}} (a_+ - a_-)$ gives

$$\langle p \rangle = -2 \alpha \beta \sqrt{\hbar m \omega} \sin(\omega t). \quad (9.37)$$

Notice that this expectation values satisfies Newton's second law:

$$\frac{d\langle p \rangle}{dt} = \left\langle -\frac{dV}{dx} \right\rangle \quad (9.38)$$

for our potential $V = \frac{1}{2} m \omega^2 x^2$ (so that the derivative is linear in x , and $\langle -\frac{dV}{dx} \rangle = -m \omega^2 \langle x \rangle$). This correspondence is an example of Ehrenfest's theorem, relating expectation dynamics to classical dynamics.

Homework

Reading: Griffiths, pp. 47–59 (we will return to the series method later on).

Problem 9.1

- a. For the stationary states of the harmonic oscillator, we know σ_x^2 from (9.31). Rewrite the momentum operator p in terms of the operators a_+ and a_- and use that to calculate σ_p^2 .
- b. Evaluate $\sigma_x^2 \sigma_p^2$, the product of the position and momentum variances – what is the minimum value this product can take?

Problem 9.2

Griffiths 2.15. The probability of finding a quantum mechanically described particle in a harmonic well outside of the classically allowed region.

Problem 9.3

Griffiths 2.13. Given the initial state, normalize the full wavefunction, and compute various expectation values for the harmonic oscillator.