

# The Simple Harmonic Oscillator

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This part of the course is based on Refs. [1] – [3].

## 1. Introduction

We return now to the study of a 1-d stationary problem: that of the simple harmonic oscillator (SHO, in short). This is of both an extreme importance in physics, and is very useful in demonstrating the basic concepts of quantum mechanics derived earlier.

We consider a particle of mass  $m$ , that is moving in a potential which depends only on  $x$ , and has the form

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

where  $k$  is some constant.

This particle is therefore attracted to the origin ( $x = 0$ , the center of the potential) by a restoring force given by Hook's law,  $F = -\frac{dV}{dx} = -kx$ .

The parabolic potential in Equation 1 is particularly useful both in classical and in quantum mechanics, since it provides a very good approximations to many arbitrary, continuous potentials close to a stable equilibrium position. The SHO is therefore the prototype for systems in which there exist small motion (vibrations) about a point of stable equilibrium - such as vibrations of atoms in a lattice, etc.

## 2. The harmonic oscillator in classical mechanics

Because of the importance of SHO, it is worth recalling the classical treatment. The equation of motion of a particle is given by

$$m \frac{d^2x}{dt^2} = -\frac{dV}{dx} = -kx \quad (2)$$

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The general solution of this equation is

$$x = X_0 \cos(\omega t - \phi), \quad (3)$$

namely a sinusoidal oscillation around  $x = 0$ . Here,

$$\omega = \sqrt{\frac{k}{m}} \quad (4)$$

is the angular frequency of the motion, and the constants  $X_0$  (the amplitude) and  $\phi$  (the initial phase) are determined by the initial conditions.

The kinetic energy of the particle is

$$T = \frac{1}{2}m \left( \frac{dx}{dt} \right)^2 = \frac{p^2}{2m}, \quad (5)$$

where  $p = m \frac{dx}{dt}$  is the momentum of the particle, while the potential energy is given by Equation 1,

$$V = \frac{1}{2}kx^2 = \frac{1}{2}m\omega^2x^2.$$

The total energy is thus

$$E = T + V = \frac{p^2}{2m} + \frac{1}{2}m\omega^2x^2 = \frac{1}{2}m\omega^2X_0^2 \quad (6)$$

which is a constant of motion. (Note that we used Equation 3). The energy of the particle is therefore time-independent, and depends only on  $X_0$ , which is arbitrary (see Figure 1).

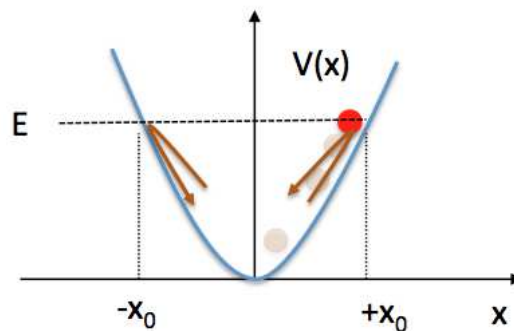


Fig. 1.— The potential energy,  $V(x)$  in a 1-d simple harmonic oscillator. The amplitude of the classical motion of particle with energy  $E$  is  $X_0$ .

The motion of the particle is limited between  $-X_0 \leq x \leq X_0$ . At  $x = \pm X_0$  the kinetic energy is zero, while the potential energy is maximal, while at  $x = 0$ , the kinetic energy is maximal and the potential energy is zero.

For ease of comparison between the classical and quantum results, let us calculate the classical probability  $p(x)dx$  of finding the particle in the interval  $dx$  around  $x$ , when a random observation is carried out. This probability is equal to the fraction of the total time that the particle spends in this interval.

Denote the period of oscillation by  $T_{\text{osc}} = 2\pi/\omega$ , this probability is given by

$$p(x)dx = \frac{1}{T_{\text{osc}}} \frac{2dx}{v(x)} = \frac{\omega}{2\pi} \frac{2dx}{(-1)\omega X_0 \sin(\omega t - \phi)} = \frac{dx}{\pi (X_0^2 - x^2)^{1/2}} \quad (7)$$

Obviously,  $p(x)dx$  is largest near the turning points,  $x = \pm X_0$ , where the speed of the classical particle vanishes.

### 3. Quantum mechanical treatment - I: wave functions

Since the potential is time-independent, we obtain a time-independent Schrödinger equation. The Hamiltonian operator is

$$\hat{H} = -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + \frac{1}{2}kx^2, \quad (8)$$

and the time-independent Schrödinger equation reads

$$-\frac{\hbar^2}{2m} \frac{d^2\phi(x)}{dx^2} + \frac{1}{2}kx^2\phi(x) = E\phi(x). \quad (9)$$

where clearly the energy  $E$  is the eigenvalue of the Hamiltonian operator. It is convenient to introduce the dimensionless eigenvalue

$$\lambda \equiv \frac{2E}{\hbar\omega}, \quad (10)$$

where  $\omega = \sqrt{k/m}$  is the angular frequency of the corresponding classical oscillator.

We shall also use the dimensionless variable

$$\xi = \alpha x, \quad (11)$$

where

$$\alpha = \left(\frac{mk}{\hbar^2}\right)^{1/4} = \left(\frac{m\omega}{\hbar}\right)^{1/2}. \quad (12)$$

With simple change of variables, we can write Schrödinger equation (Equation 9) as

$$\frac{d^2\phi(\xi)}{d\xi^2} + (\lambda - \xi^2)\phi(\xi) = 0. \quad (13)$$

Before finding full solution to the Schrödinger equation, let us look first at a limiting case of large  $x$ . This would provide some insight on the asymptotic behaviors. In the limit  $|\xi| \rightarrow \infty$  (and finite total energy,  $E$ ), Equation 13 reduces to:

$$\frac{d^2\phi(\xi)}{d\xi^2} - \xi^2\phi(\xi) = 0. \quad (14)$$

Equation 14 has an **approximate** solution

$$\phi(\xi) \approx \xi^p e^{\pm\xi^2/2}, \quad (15)$$

which is correct in the limit of large  $|\xi|$ , as long as  $p$  is finite. We can add the physical requirement that  $\phi(\xi)$  must remain finite in the limit  $|\xi| \rightarrow \infty$ , to exclude the  $+\xi^2/2$  term in the exponent as a valid solution.

This analysis suggests that the general solution to Schrödinger Equation (13) has the form

$$\phi(\xi) = H(\xi)e^{-\xi^2/2}. \quad (16)$$

Substituting this solution in Schrödinger Equation (13), using

$$\frac{d\phi}{d\xi} = \left( \frac{dH}{d\xi} - \xi H \right) e^{-\xi^2/2}$$

and

$$\frac{d^2\phi}{d\xi^2} = \left( \frac{d^2H}{d\xi^2} - 2\xi \frac{dH}{d\xi} + (\xi^2 - 1)H \right) e^{-\xi^2/2},$$

the Schrödinger equation becomes

$$\frac{d^2H}{d\xi^2} - 2\xi \frac{dH}{d\xi} + (\lambda - 1)H = 0 \quad (17)$$

Equation 17 is called **Hermite equation**. The solutions to this equation are given by *Hermite polynomials*.

In order to solve this equation, the easiest way is to expand  $H(\xi)$  as a power series in  $\xi$ :

$$H(\xi) = a_0 + a_1\xi + a_2\xi^2 + \dots = \sum_{j=0}^{\infty} a_j\xi^j, \quad (18)$$

where  $a_0, a_1, \dots$  are numbers to be determined.

Differentiating Equation 18 term by term, one finds that:

$$\frac{dH}{d\xi} = a_1 + 2a_2\xi + \dots = \sum_{j=0}^{\infty} ja_j\xi^{j-1},$$

and

$$\frac{d^2H}{d\xi^2} = 2a_2 + 2 \cdot 3a_3\xi + 3 \cdot 4a_4\xi^2 + \dots = \sum_{j=0}^{\infty} (j+1)(j+2)a_{j+2}\xi^j,$$

We use this in Equation 17 to find

$$\sum_{j=0}^{\infty} [(j+1)(j+2)a_{j+2} - 2ja_j + (\lambda-1)a_j] \xi^j = 0. \quad (19)$$

Note that this equation is equivalent to our original Schrödinger equation !

A solution is obtained if the coefficient of *each individual power law* of  $\xi$  vanish, namely

$$(j+1)(j+2)a_{j+2} - 2ja_j + (\lambda-1)a_j = 0, \quad (20)$$

or

$$a_{j+2} = \frac{2j+1-\lambda}{(j+1)(j+2)} a_j \quad (21)$$

This is a **recursion formula**, which gives all the coefficients  $a_j$  ( $j > 1$ ) if the first two coefficients:  $a_0$  and  $a_1$  are known. For example:

$$\begin{aligned} a_2 &= \frac{1-\lambda}{2} a_0; & a_4 &= \frac{5-\lambda}{12} a_2 = \frac{(5-\lambda)(1-\lambda)}{24} a_0; \dots \\ a_3 &= \frac{3-\lambda}{6} a_1; & a_5 &= \frac{7-\lambda}{20} a_3 = \frac{(7-\lambda)(3-\lambda)}{120} a_1; \dots \end{aligned} \quad (22)$$

This is exactly what we expect from a second order differential equation.

There is still left the problem of normalization. If we look at large  $j$ ,  $j \gg \lambda$ , the recursion formula (Equation 21) can be written approximately as

$$a_{j+2} \approx \frac{2}{j} a_j. \quad (23)$$

This has the approximate solution  $a_j \approx \frac{C}{(j/2)!}$ , for some constant  $C$ . At large  $\xi$ , this implies

$$H(\xi) \approx C \sum \frac{1}{(j/2)!} \xi^j \approx C \sum \frac{1}{j!} \xi^{2j} \approx C e^{\xi^2} \quad (24)$$

But if we put this solution for  $H(\xi)$  in  $\phi(\xi) = H(\xi)e^{-\xi^2/2}$  (Equation 16) we find that  $\phi \sim e^{+\xi^2/2}$  (for large  $\xi$ ). This is of course physically unacceptable.

The solution is therefore that **the power series must terminate**: namely, there is some “highest”  $j$  (we call it  $n$ ), such that  $a_{n+2} = 0$ . Here we must discriminate between “even” solutions (the even-numbered coefficients  $a_2, a_4, \dots \neq 0$ ) and “odd” solutions ( $a_1, a_3, \dots \neq 0$ ).

For even solutions we must require  $a_1 = 0$  (which means that all odd number coefficients will be zero as well, by the recursion). Similarly, for odd solutions we have  $a_0 = 0$ . The requirement of having some maximum number  $n$  above which all  $a_{n+2} = 0$  adds to these restrictions.

Using this physical constraint in Equation 21, one finds that for a physically acceptable solutions there must exist  $j = n$  such that

$$2n + 1 = \lambda \tag{25}$$

for some non-negative integer  $n$ . Since  $\lambda$  is the normalized energy (Equation 10,  $\lambda = 2E/\hbar\omega$ ), we therefore find that the energy spectrum of the SHO is given by

$$E_n = \left( n + \frac{1}{2} \right) \hbar\omega, \quad n = 0, 1, 2, \dots \tag{26}$$

This result is in sharp contrast to the classical mechanics result, in which the energy  $E$  of a SHO can have any value. In contrast, in QM the energy spectrum consists of infinite sequence of **discrete** energy levels. Even in its lowest energy state ( $n = 0$ ), the SHO has the energy  $\hbar\omega/2$ . This energy is called **zero point energy**, which is clearly a quantum phenomena, and is directly related to the uncertainty principle.

This result seem surprising: in principle, we could find a solution to the Schrödinger equation (9) for *any* value of  $E$ . The point is that the obtained wave functions will diverge at large  $\xi$  ( $=$  large  $x$ ), and therefore could not represent physical systems, unless the energy fulfills the condition set in Equation 26.

### 3.1. Hermite polynomials

Using the allowed values of  $\lambda = 2n + 1$ , the recursion formula (Equation 21) reads

$$a_{j+2} = \frac{-2(n-j)}{(j+1)(j+2)} a_j \tag{27}$$

If  $n = 0$ , there is only one term in the series:  $a_0$  (recall that: I.  $j \leq n$ , and so  $j = 0$ ; and II. We must pick  $a_1 = 0$  to kill the odd solutions). Equation 27 gives  $a_2 = a_4 = \dots = 0$ ,

namely

$$H_0(\xi) = a_0 \tag{28}$$

and therefore

$$\psi_0(\xi) = a_0 e^{-\xi^2/2}. \tag{29}$$

For  $n = 1$  we take  $a_0 = 0$  to kill the even solutions. Equation 27 with  $j = 1$  yields  $a_3 = a_5 = \dots = 0$ . Thus,

$$H_1(\xi) = a_1 \xi, \tag{30}$$

and

$$\phi_1(\xi) = a_1 \xi e^{-\xi^2/2}. \tag{31}$$

For  $n = 2$ , putting  $j = 0$  in Equation 27 gives  $a_2 = -2a_0$  and putting  $j = 2$  gives  $a_4 = 0$ . Thus,

$$H_2(\xi) = a_0(1 - 2\xi^2), \tag{32}$$

and

$$\phi_2(\xi) = a_0(1 - 2\xi^2)e^{-\xi^2/2}. \tag{33}$$

In general,  $H_n(\xi)$  is a polynomial of degree  $n$  in  $\xi$ , involving even powers only for even  $n$ , and odd powers only for odd  $n$ . Apart from the overall normalization factor ( $a_0$  or  $a_1$ ), these are called **Hermite polynomials**, honoring the French mathematician [Charles Hermite](#).

Hermite polynomials are unique, up to the normalization factors. Traditionally, these are chosen such that the multiplication of the highest power of  $\xi$  appears with the coefficient  $2^n$  in  $H_n(\xi)$ . This follows from an alternative definition of the Hermite polynomials, as solutions of the equation

$$H_n(\xi) = (-1)^n e^{\xi^2/2} \frac{d^{(n)} e^{-\xi^2/2}}{d\xi^n} \tag{34}$$

(this is known as “Rogrigue’s formula”).

The first few Hermite polynomials are

$$\begin{aligned} H_0(\xi) &= 1 \\ H_1(\xi) &= 2\xi \\ H_2(\xi) &= 4\xi^2 - 2 \\ H_3(\xi) &= 8\xi^3 - 12\xi \\ H_4(\xi) &= 16\xi^4 - 48\xi^2 + 12 \\ H_5(\xi) &= 32\xi^5 - 160\xi^3 + 120\xi. \end{aligned} \tag{35}$$

With this convention, the normalized wave functions, namely, the stationary states of the SHO are given by

$$\phi_n(x) = \left( \frac{\alpha}{\sqrt{\pi} 2^n n!} \right)^{1/2} e^{-\xi^2/2} H_n(\xi) = \left( \frac{m\omega}{\pi \hbar} \right)^{1/4} \frac{1}{\sqrt{2^n n!}} H_n(\alpha x) e^{-\alpha^2 x^2/2}. \quad (36)$$

where  $\alpha$  is given in Equations 12. These functions are normalized, namely

$$\int_{-\infty}^{\infty} \phi_n^*(x) \phi_m(x) dx = \delta_{nm} \quad (37)$$

In Figures 2 and 3 I show a few wavefunctions (left),  $\phi_n(\xi)$  for  $n = 0, 1, 2, 3$  and 20, and the corresponding probability density (right). On top of the probability density, I show the classical probability (given in Equation 7) for finding the particle at position  $\xi$ , in dashed red line. For a given  $n$ , the particle's energy is  $E_n = (n + 1/2)\hbar\omega$  (see Equation 26, and the classical maximum amplitude is  $X_0 = \sqrt{2E/m\omega^2} = \sqrt{(n + 1/2)\hbar/m\omega}$  (see Equation 6). Clearly, for large  $n$  (large particle energy), the probability of finding the particle at position  $x$  approaches the classical limit. However, for low energies, this probability is very different than the classical one. As is obvious from the figures, it is non-zero even for  $|x| > |X_0|$ .

#### 4. Quantum Mechanical treatment - II: Operators and Dirac's formalism

Let us look again at the SHO, now using the formalism developed by Dirac. This implies that we no longer need to rely on the position in space,  $\phi(x)$ , which is a particular representation.

We write the Hamiltonian (Equation 8) as

$$\hat{H} = -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + \frac{1}{2} kx^2 = \frac{p_x^2}{2m} + \frac{1}{2} m\omega^2 x^2, \quad (38)$$

where  $\omega = \sqrt{k/m}$ .

We now introduce two operators:  $a_+$  and  $a_-$ , defined via

$$a_{\pm} = \frac{1}{\sqrt{2}} \left[ \left( \frac{m\omega}{\hbar} \right)^{1/2} x \mp i \frac{p_x}{(m\hbar\omega)^{1/2}} \right]. \quad (39)$$

Since  $x$  and  $p_x$  are Hermitian operators,  $a_+$  and  $a_-$  are adjoint of each other, namely  $a_+ = a_-^\dagger$  and  $a_- = a_+^\dagger$ .



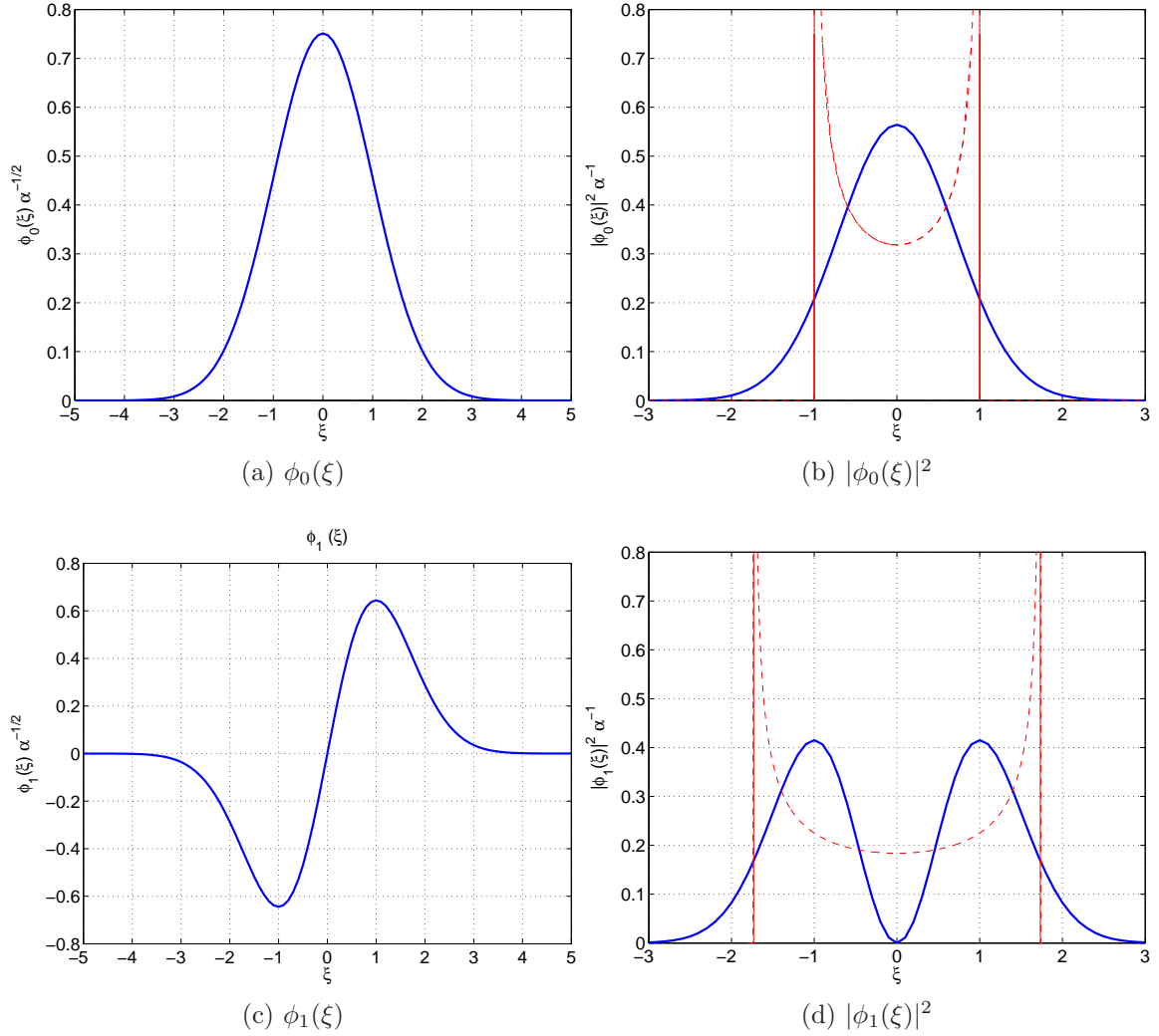


Fig. 2.— Left: the ground state and first excited state ( $\phi_0(\xi)$  and  $\phi_1(\xi)$ ) eigenfunctions of the SHO. Right: the corresponding probability densities,  $|\phi_n(\xi)|^2$  (solid curves), together with the probabilities obtained for the classical oscillator having energy  $E_n$  (dashed, red curves), calculated using Equation 7

Furthermore, Equation 39 can be inverted, to read

$$\begin{aligned} x &= \frac{1}{\sqrt{2}} \sqrt{\frac{\hbar}{m\omega}} (a_+ + a_-) \\ p_x &= \frac{i}{\sqrt{2}} \sqrt{\hbar m\omega} (a_+ - a_-) \end{aligned} \quad (40)$$

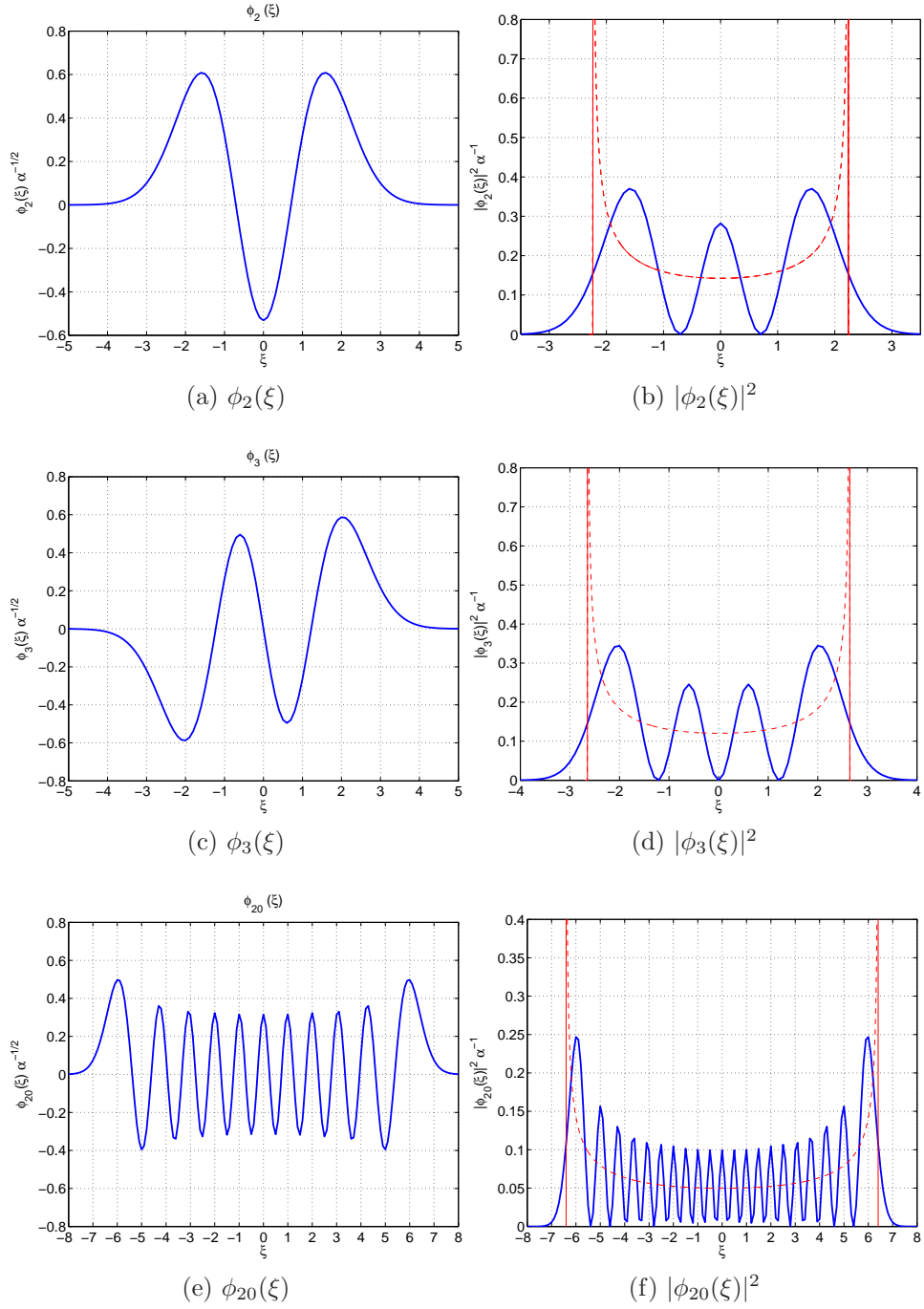


Fig. 3.— Same as in Figure 2, for  $\phi_2(\xi)$ ,  $\phi_3(\xi)$  and  $\phi_{20}(\xi)$ . For large  $n$ , the quantum mechanical result approaches the classical result, as is to be expected.

The operators  $a_{\pm}$  satisfy the commutation relations:

$$[a_-, a_+] = \frac{i}{2\hbar}[p_x, x] - \frac{i}{2\hbar}[x, p_x] = \frac{1}{2} + \frac{1}{2} = 1 \quad (41)$$

where we used  $[x, p_x] = i\hbar$ .

Using Equation 40, we can write the Hamiltonian as

$$\hat{H} = \frac{p_x^2}{2m} + \frac{1}{2}m\omega^2 x^2 = -\frac{1}{2}\frac{\hbar m\omega}{2m}(a_+ - a_-)^2 + \frac{1}{2}m\omega^2 \frac{\hbar}{2m\omega}(a_+ + a_-)^2 = \frac{\hbar\omega}{2}[a_+a_- + a_-a_+] \quad (42)$$

Using the commutation relation (Equation 41), this can be written as

$$\hat{H} = \hbar\omega \left( a_-a_+ - \frac{1}{2} \right) = \hbar\omega \left( a_+a_- + \frac{1}{2} \right) \equiv \hbar\omega \left( N + \frac{1}{2} \right) \quad (43)$$

where we have defined the operator

$$N \equiv a_+a_-. \quad (44)$$

This operator is known as the **number operator**. Equation 43 implies that **eigenvectors of  $\hat{H}$  are eigenvectors of  $N$ , and vice versa**.

Using Equations 41 and 43, we have

$$[H, a_{\pm}] = \pm\hbar\omega a_{\pm}. \quad (45)$$

Assume now that  $|E\rangle$  is an eigenket of  $\hat{H}$ , with corresponding eigenvalue  $E$ :  $\hat{H}|E\rangle = E|E\rangle$ . From Equation 45, we have:

$$\hat{H}a_{\pm}|E\rangle = (a_{\pm}\hat{H} \pm \hbar\omega a_{\pm})|E\rangle = (E \pm \hbar\omega)a_{\pm}|E\rangle \quad (46)$$

This means that the kets  $a_{\pm}|E\rangle$  are also eigenkets of  $\hat{H}$ , with corresponding eigenvalues  $E \pm \hbar\omega$ . Thus,  $a_+$  raises the energy  $E$  and  $a_-$  lowers it; hence their names **raising** and **lowering operators**, respectively.

#### 4.1. Determining the spectrum of $\hat{H}$

Since  $\hat{H}$  only contains the square of the operators  $p_x$  and  $x$ , the expectation value of  $\hat{H}$  in any state cannot be negative. Thus, **the eigenvalues of  $\hat{H}$  must be non-negative**. Let us denote the smallest non-negative eigenvalue of  $\hat{H}$  by  $E_0$ , and the corresponding eigenket by  $|E_0\rangle$ . Then, from Equation 46, we must have

$$a_-|E_0\rangle = 0. \quad (47)$$

Otherwise,  $a_-|E_0\rangle$  would be an eigenket of  $\hat{H}$  with corresponding eigenvalue  $E_0 - \hbar\omega$ , contrary to the hypothesis that  $E_0$  is the lowest eigenvalue. (This can also be understood as follows: from Equation 46, we know that

$$\hat{H}(a_-|E\rangle) = (E - \hbar\omega)(a_-|E\rangle)$$

from which we deduce that  $a_-|E\rangle$  is an eigenket of  $\hat{H}$  with eigenvalue  $(E - \hbar\omega)$ . However, by definition, the state  $|E - \hbar\omega\rangle$  is also an eigenket of  $\hat{H}$  with the same eigenvalue, since  $\hat{H}|E - \hbar\omega\rangle = (E - \hbar\omega)|E - \hbar\omega\rangle$ . We must therefore conclude that the state  $|E - \hbar\omega\rangle$  is similar to the state  $a_-|E\rangle$ , up to some constant. For  $E_0$  be the smallest non-negative eigenvalue of  $\hat{H}$ , Equation 47 must therefore be fulfilled.)

We can now operate on Equation 47 with the operator  $\hbar\omega a_+$ , using Equations 43 and 44 to get:

$$\hbar\omega a_+ a_- |E_0\rangle = \hbar\omega N |E_0\rangle = \left( \hat{H} - \frac{1}{2}\hbar\omega \right) |E_0\rangle = 0 \quad (48)$$

We can write Equation 48 as  $\hat{H}|E_0\rangle = \frac{1}{2}\hbar\omega|E_0\rangle$ , from which we deduce that the lowest eigenvalue  $E_0$  is given by

$$E_0 = \frac{1}{2}\hbar\omega \quad (49)$$

Using Equation 46, we see that by operating repeatedly with  $a_+$  on the eigenket  $|E_0\rangle$ , we obtain a sequence of (unnormalized) eigenkets:

$$|E_0\rangle, a_+|E_0\rangle, a_+^2|E_0\rangle, \dots, a_+^n|E_0\rangle \dots \quad (50)$$

The eigenvalue corresponding to the eigenket  $a_+^n|E_0\rangle$  is

$$E_n = \left( n + \frac{1}{2} \right) \hbar\omega, \quad n = 0, 1, 2, \dots \quad (51)$$

(compare to Equation 26).

#### 4.1.1. Normalization of the eigenkets

Let us assume that  $|E_n\rangle$  is a normalized eigenket of  $\hat{H}$ , with corresponding eigenvalue  $E_n$ . Be  $|E_{n+1}\rangle$  the normalized eigenket whose corresponding eigenvalue is  $E_{n+1}$ . We have, from Equation 50:

$$|E_{n+1}\rangle = C_{n+1} a_+ |E_n\rangle \quad (52)$$

where  $C_{n+1}$  is the normalization coefficient that we would like to determine. By assumption,  $\langle E_{n+1}|E_{n+1}\rangle = 1$ , and using  $a_- = a_+^\dagger$ , we have

$$|C_{n+1}|^2 \langle E_n | a_- a_+ | E_n \rangle = 1. \quad (53)$$

We know that  $a_-a_+ = (\hat{H}/\hbar\omega) + 1/2$  (see Equation 43). Furthermore,  $\hat{H}|E_n\rangle = E_n|E_n\rangle$  with  $E_n = (n + 1/2)\hbar\omega$ , and by assumption,  $\langle E_n|E_n\rangle = 1$ . Combined together, we have

$$|C_{n+1}|^2(n+1) = 1, \quad (54)$$

or

$$C_{n+1} = (n+1)^{-1/2} \quad (55)$$

Putting this in Equation 52, we find that

$$a_+|E_n\rangle = (n+1)^{1/2}|E_{n+1}\rangle \quad (56)$$

We can now begin with  $n = 0$  and use the relation 56 repeatedly to obtain all the eigenvectors  $|E_n\rangle$  once  $|E_0\rangle$  is known:

$$|E_n\rangle = \frac{1}{\sqrt{n!}} a_+^n |E_0\rangle \quad (57)$$

We can play a similar game with  $a_-$ . Let  $|E_{n-1}\rangle$  be the normalized eigenket corresponding to the eigenvalue  $E_{n-1}$ . From Equations 52 and 55 we have

$$|E_n\rangle = C_n a_+ |E_{n-1}\rangle, \quad (58)$$

with  $C_n = n^{-1/2}$ . Operating on both sides of Equation 58 with  $a_-$ , we find that

$$a_-|E_n\rangle = n^{-1/2} a_- a_+ |E_{n-1}\rangle.. \quad (59)$$

Using again  $a_-a_+ = (\hat{H}/\hbar\omega) + 1/2$  and  $\hat{H}|E_{n-1}\rangle = (n - 1/2)\hbar\omega|E_{n-1}\rangle$  one finds

$$a_-|E_n\rangle = n^{1/2}|E_{n-1}\rangle. \quad (60)$$

**Examples.** The operators  $a_+$  and  $a_-$  can be used to calculate any property of the system. Let us, as an example, evaluate the expectation value of  $x^4$  in the ground state,  $|E_0\rangle$  of the SHO. We do that by using Equation 40,

$$x = \frac{1}{\sqrt{2}} \sqrt{\frac{\hbar}{m\omega}} (a_+ + a_-).$$

In calculating the expectation value of  $x^4$ , we must expand  $(a_+ + a_-)^4$ , to obtain 16 different terms. However, many of these terms will end up as 0, since  $a_-|E_0\rangle = 0$ , and also  $\langle E_0|a_+ = \langle E_0|a_-^\dagger = \langle a_-E_0| = 0$ . Thus, after removing all the zero terms, we are left with

$$\langle E_0|x^4|E_0\rangle = \frac{\hbar^2}{4m^2\omega^2} \langle E_0|a_-a_+^3 + a_-a_+a_-a_+ + a_-^2a_+^2 + a_-^3a_+|E_0\rangle \quad (61)$$

Furthermore, terms in which the number of  $a_-$  is not equal to the number of  $a_+$  operators will have zero contribution as well, as we are only evaluating diagonal matrix elements. We are thus left with

$$\langle E_0|x^4|E_0\rangle = \frac{\hbar^2}{4m^2\omega^2}\langle E_0|a_-a_+a_-a_+ + a_-^2a_+^2|E_0\rangle \quad (62)$$

We can now evaluate:

$$a_-a_+a_-a_+|E_0\rangle = a_-a_+a_-|E_1\rangle = a_-a_+|E_0\rangle = a_-|E_1\rangle = |E_0\rangle \quad (63)$$

Similarly,

$$a_-^2a_+^2|E_0\rangle = a_-^2a_+|E_1\rangle = \sqrt{2}a_-^2|E_2\rangle = 2a_-|E_1\rangle = 2|E_0\rangle \quad (64)$$

Thus,

$$\langle E_0|x^4|E_0\rangle = \frac{3\hbar^2}{4m^2\omega^2} \quad (65)$$

#### 4.2. Matrix representation in the $\{|E_n\rangle\}$ basis

We saw (“Fundamentals”, sec. 6.3.3) that in a given basis, every operator can be represented by a matrix. The set  $\{|E_n\rangle\}$  ( $n = 0, 1, 2, \dots$ ) form an orthonormal set of basis eigenkets of the Hamiltonian, since, by definition (see below Equation 45),  $\hat{H}|E_n\rangle = E_n|E_n\rangle$ , where  $E_n = (n + 1/2)\hbar\omega$  (Equation 51) and furthermore  $\langle E_m|E_n\rangle = \delta_{mn}$ .

Furthermore, we saw that the eigenkets of  $\hat{H}$  are also eigenkets of  $N$  (see Equation 44), with eigenvalues  $n$  (that follows equations 56 and 60). This implies that both operators  $\hat{H}$  and  $N$  can be written as a diagonal matrices,

$$\hat{H} = \hbar\omega \begin{pmatrix} \frac{1}{2} & 0 & 0 & 0 & \dots \\ 0 & \frac{3}{2} & 0 & 0 & \dots \\ 0 & 0 & \frac{5}{2} & 0 & \dots \\ 0 & 0 & 0 & \frac{7}{2} & \dots \\ \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix}; \quad N = \begin{pmatrix} 0 & 0 & 0 & 0 & \dots \\ 0 & 1 & 0 & 0 & \dots \\ 0 & 0 & 2 & 0 & \dots \\ 0 & 0 & 0 & 3 & \dots \\ \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix}. \quad (66)$$

We can further use the orthogonality condition to calculate the matrix representation of the operators  $a_+$  and  $a_-$ . We have:

$$\langle E_k|E_{n+1}\rangle = C_{n+1}\langle E_k|a_+|E_n\rangle = \delta_{k,n+1} \quad (67)$$

This implies that the matrix element of  $a_+$  in the  $\{|E_n\rangle\}$  representation are

$$(a_+)_{kn} = C_{n+1}^{-1/2}\delta_{k,n+1} = (n + 1)^{1/2}\delta_{k,n+1} \quad (68)$$

This means that  $a_+$  is represented by a real matrix whose only non-zero elements are those of the diagonal immediately **below** the main diagonal:

$$a_+ = \begin{pmatrix} 0 & 0 & 0 & 0 & \dots \\ \sqrt{1} & 0 & 0 & 0 & \dots \\ 0 & \sqrt{2} & 0 & 0 & \dots \\ 0 & 0 & \sqrt{3} & 0 & \dots \\ \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix}. \quad (69)$$

We can use the fact that  $a_- = a_+^\dagger$ , and  $a_+$  is a real matrix, to deduce the matrix elements of  $a_-$ :

$$(a_-)_{kn} = (k+1)^{1/2} \delta_{k+1,n}, \quad (70)$$

namely  $a_-$  is a real matrix whose only non-zero components lie on the diagonal immediately **above** the main diagonal:

$$a_- = \begin{pmatrix} 0 & \sqrt{1} & 0 & 0 & \dots \\ 0 & 0 & \sqrt{2} & 0 & \dots \\ 0 & 0 & 0 & \sqrt{3} & \dots \\ 0 & 0 & 0 & 0 & \dots \\ \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix}. \quad (71)$$

By use of Equation 40, one can find the matrix elements of the operators  $x$  and  $p_x$ .

### 4.3. Obtaining the wave functions: transition from the $\{|E_n\rangle\}$ to the position representation

I stated that one of the advantages of Dirac's notation is that it enables us to generalize the discussion. Indeed, so far the discussion was general. If we want to retrieve back the SHO eigenfunctions as a function of position (as we did in Section 3), we need to specify the **position representation** of the operators  $a_+$  and  $a_-$ .

Recall that in this representation, the operator  $x$  is represented by an ordinary multiplication by  $x$ , and the operator  $p_x$  is represented by  $-i\hbar(\partial/\partial x)$ , where in the 1-d case, we have  $\partial/\partial x = d/dx$ .

In this case, we can write the operators  $a_\pm$  introduced in Equation 39 as

$$a_\pm = \frac{1}{\sqrt{2}} \left[ \left( \frac{m\omega}{\hbar} \right)^{1/2} x \mp \left( \frac{\hbar}{m\omega} \right)^{1/2} \frac{d}{dx} \right]. \quad (72)$$

In terms of the normalized variable  $\xi = (m\omega/\hbar)x = \alpha x$  (see Equations 11, 12) this is equal to

$$a_{\pm} = \frac{1}{\sqrt{2}} \left( \xi \mp \frac{d}{d\xi} \right) \quad (73)$$

We proceed along the same lines as before: we write the equation  $a_-|E_0\rangle = 0$  as

$$\left( \xi + \frac{d}{d\xi} \right) \psi_0(\xi) = 0 \quad (74)$$

The solution to this equation is

$$\psi_0(\xi) = N_0 e^{-\xi^2/2} \rightarrow \psi_0(x) = N_0 e^{-\alpha^2 x^2/2} \quad (75)$$

where  $N_0$  is a constant, which we choose to be real, and such that  $\psi_0(x)$  is normalized to unity; thus,

$$N_0 = \left( \frac{\alpha}{\sqrt{\pi}} \right)^{1/2}. \quad (76)$$

All other eigenfunctions can be found by repeated use of  $a_+$  (see Equation 57), which becomes:

$$\psi_n(\xi) = \frac{1}{\sqrt{n!}} \left[ \frac{1}{\sqrt{2}} \left( \xi - \frac{d}{d\xi} \right) \right]^n \psi_0(\xi) \quad (77)$$

Using the definitions of the Hermite polynomials, we obtain the solution

$$\psi_n(\xi) = \left( \frac{\alpha}{\sqrt{\pi} 2^n n!} \right)^{1/2} e^{-\xi^2/2} H_n(\xi). \quad (78)$$

This is of course identical to the results derived in section 3 (see Equation 36).

## REFERENCES

- [1] B.H. Bransden & C.J. Joachain, *Quantum Mechanics* (Second edition), Chapter 5.
- [2] C. Cohen-Tannoudji, B. Diu & F. Laloe, *Quantum Mechanics*, Vol. 1., Chapter 5.
- [3] D. Griffiths, *Introduction to Quantum Mechanics*, Chapter 2.