Harmonic Oscillator Eigenvalues and Eigenfunctions

The Quantum Mechanical Harmonic Oscillator

The quantum mechanical harmonic oscillator in one dimension is defined by a quadratic potential of the form

\[ V(x) = \frac{1}{2} k x^2, \quad (1) \]

where \( k \) is the force constant. The Hamiltonian operator therefore has the following form,

\[ \hat{H} = -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + \frac{1}{2} k x^2. \quad (2) \]

Solutions of the Schrödinger equation for the one-dimensional harmonic oscillator are discussed below.

Harmonic Oscillator Eigenvalues

The quantized energy eigenvalues of the harmonic oscillator are

\[ E_v = \hbar \nu_0 (v + \frac{1}{2}), \quad v = 0, 1, 2, \ldots. \quad (3) \]

The harmonic frequency \( \nu_0 \) is given by

\[ \nu_0 = \frac{1}{2\pi} \left( \frac{k}{m} \right)^{1/2}. \quad (4) \]

An important feature of the energy eigenvalues of the harmonic oscillator is that the energy levels are evenly spaced such that

\[ E_{v+1} - E_v = \hbar \nu_0. \quad (5) \]

The constant spacing arises because the eigenvalues depend linearly on the quantum number \( v \). This is in contrast with the particle in an infinite box where the eigenvalues depend quadratically on the quantum number, which leads to an increasing separation between levels as the energy increases. This is due to the fact that the confinement in the infinite well is abrupt – the potential jumps from 0 to \( \infty \) from one point to the next. This extreme confinement leads to the energy levels being pushed up higher and higher. On the other hand, in the harmonic oscillator the potential gradually goes to infinity over a large range in the coordinate. This lessens the confinement and allows the eigenvalues to increase at a slower rate.

The constant spacing at higher energy is unrealistic if the harmonic oscillator model is used to represent molecular vibrations. Because of the anharmonicity and dissociation limit of a diatomic molecule, as the energy increases, the spacing between allowed energy levels actually decreases in the real system.
Harmonic Oscillator Eigenfunctions

The eigenfunctions of the harmonic oscillator are

$$\psi_\nu(x) = N_\nu H_\nu(\sqrt{\alpha} x) e^{-\alpha x^2/2}.$$  \hspace{1cm} (6)

Here, the constant $\alpha$ is defined as

$$\alpha = \left(\frac{mk}{\hbar^2}\right)^{1/2}$$  \hspace{1cm} (7)

and $N_\nu$ is the normalization constant, which has the form

$$N_\nu = \left(\frac{\alpha}{\pi}\right)^{1/4} \left(\frac{1}{2^\nu \nu!}\right)^{1/2}.$$  \hspace{1cm} (8)

The functions $H_\nu(z)$ are called Hermite polynomials. The first several Hermite polynomials are tabulated below.

<table>
<thead>
<tr>
<th>$\nu$</th>
<th>$H_\nu(z)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>1</td>
</tr>
<tr>
<td>1</td>
<td>$2z$</td>
</tr>
<tr>
<td>2</td>
<td>$4z^2 - 2$</td>
</tr>
<tr>
<td>3</td>
<td>$8z^3 - 12z$</td>
</tr>
<tr>
<td>4</td>
<td>$16z^4 - 48z^2 + 12$</td>
</tr>
<tr>
<td>5</td>
<td>$32z^5 - 160z^3 + 120z$</td>
</tr>
</tbody>
</table>

The coefficients of the terms in each Hermite polynomial may be obtained from a recursion relation. Each polynomial has the form

$$H_\nu(z) = \sum_{n=0}^{\nu} a_n z^n.$$  \hspace{1cm} (9)

The two-term recursion formula for the coefficients $a_n$ is

$$a_{n+2} = \frac{2n + 1 - 2\varepsilon}{(n+1)(n+2)} a_n,$$  \hspace{1cm} (10)

where $\varepsilon$ corresponds to the dimensionless energy, $\varepsilon = E/\hbar \nu_0 = \nu + \frac{1}{2}$. 
As a result of the two-term recursion formula, only even terms or only odd terms are present in the summation in Eq. (12). In order to use the recursion formula, either the coefficient $a_0$ or $a_1$ must be supplied. For example, suppose we wish to determine the coefficients of the $v=3$ Hermite polynomial, $H_3(z)$. This polynomial has the form

$$H_3(z) = a_1 z^1 + a_3 z^3.$$ (11)

From the recursion relation, we have

$$a_3 = \frac{2 \cdot 1 + 1 - 2 \left(3 + \frac{1}{2}\right)}{(1+1)(1+2)} a_1,$$

or

$$a_3 = -\frac{2}{3} a_1.$$ (12)

Here the relation $v = v + \frac{1}{2}$ with $v=3$ has been used. If we are then given that $a_1 = -12$ in this case, we can determine $a_3$,

$$a_3 = -\frac{2}{3} (-12) = 8.$$ (13)

Thus, the Hermite polynomial $H_3(z)$ is therefore

$$H_3(z) = -12 z + 8 z^3.$$ (14)

The specific choice of the value of $a_0$ or $a_1$ for each even or odd Hermite polynomial is arbitrary. However, by convention $a_0$ or $a_1$ is chosen so that the highest coefficient $a_v$ in the Hermite polynomial $H_v(z)$ is $2^v$.

An alternate method for determining Hermite polynomials is to use a recurrence relation. Once $H_0(z)$ and $H_1(z)$ are determined, the other Hermite polynomials may be determined using a recurrence relation for the Hermite polynomials,

$$H_{n+1}(z) = 2z H_n(z) - 2n H_{n-1}(z).$$ (15)

For example, to obtain the $v=6$ Hermite polynomial, $H_6(z)$, the recurrence relation is

$$H_6(z) = 2z H_5(z) - 2 \cdot 5 \cdot H_4(z),$$ (16)

where $n=5$ has been substituted. If $H_5(z)$ and $H_4(z)$ are already known, then this relation yields

$$H_6(z) = 2z H_5(z) - 10 H_4(z)$$

$$= 2z \left(32z^5 - 160z^3 + 120z\right) - 10 \left(16z^4 - 48z^2 + 12\right)$$

$$H_6(z) = 64z^6 - 480z^4 + 720z^2 - 120.$$ (17)
Plots of the first several eigenfunctions of the harmonic oscillator are shown in the figures below. These wavefunctions are computed for $\alpha = 1.0$. 

$v=0$ 

$v=1$ 

$v=2$ 

$v=3$ 

$v=4$ 

$v=5$
**Tunneling in the Harmonic Oscillator**

The harmonic oscillator wavefunctions do exhibit tunneling. The wavefunctions extend into the classically forbidden region. For the classical harmonic oscillator, the turning points $x_t$ for a classical particle with an energy equal to the ground state eigenvalue are

$$x_t = \pm \frac{1}{\sqrt{\alpha}}.$$  \hspace{1cm} (18)

The tunneling of the ground state wavefunction is shown below. The classical turning points are indicated by the dashed vertical lines.

Likewise, for the $v$th level, the classical turning points are given by

$$x_t = \pm \sqrt{\frac{2v+1}{\alpha}}.$$  \hspace{1cm} (19)

The tunneling of the $v=5$ wavefunction is shown in the figure below.

As you can qualitatively see from this figure, the tunneling does not substantially increase as the energy increases. This is because there is not a finite barrier, but rather the potential increases gradually as the energy increases.
**The Correspondence Principle**

The harmonic oscillator exhibits a trait common to many quantum mechanical systems. As the energy increases, the properties of the system approach the classical values. This is known as the correspondence principle.

As an example, let us consider the probability density. For the first four harmonic oscillator wavefunctions, the probability density for each is shown below. Note that these wavefunctions are computed for $\alpha=1$. The dashed vertical lines indicate the classical turning points.

The classical and quantum systems are the least similar for the ground state. For the ground state, the most probable location of the quantum system is $x=0$. In the classical system, $x=0$ is the least likely position since at $x=0$ the classical particle has the highest velocity. In the classical system, the most probable locations are the turning points since at those points the velocity is zero and therefore the particle spends the most time near the turning points.

As the energy of the quantum system increases, the most probable location moves away from $x=0$ and toward the classical turning points. In addition, a greater proportion of the probability is concentrated in the outer regions of the probability distribution as the energy of the system increases.
By the time that the quantum system is in the $v=10$ level, the correspondence with the classical result has become even more apparent, as is evident in the figure below.