Physical Chemistry
Lecture 14
The 1-D Harmonic Oscillator

The 1-D harmonic oscillator

Hamiltonian

\[ H = \frac{p^2}{2m} + \frac{k}{2} (x - x_0)^2 \]

Particle (mass m) attached to a spring of force constant, k

Potential energy depends on position as a Hooke's-law spring

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

Classical solution of the 1-D harmonic oscillator

\[ x(t) = \frac{2E}{m \omega_0^2} \cos \omega_0 t \]

\[ p(t) = -\sqrt{2mE} \sin \omega_0 t \]

\[ \omega_0 = \sqrt{\frac{k}{m}} \]

\[ x_{\text{max}} = \pm \frac{2E}{m \omega_0^2} \]

Oscillatory motion

Maximum displacements are classical turning points

\[ E = V(x_{\text{max}}) \]

Quantum 1-D harmonic oscillator

Schroedinger's equation

\[ \hat{H} \psi(x) = E \psi(x) \]

Convenient to make dimensionless equation

\[ \frac{\hbar^2}{2m} \frac{d^2 \psi}{dx^2} + \frac{k}{2} x^2 \psi = E \psi \]

Hermite's associated differential equation

1-D harmonic-oscillator wave functions and energies

Wavefunctions

\[ \psi_{\nu}(x) = A_{\nu} H_{\nu}(\sqrt{x/m}) \exp \left( -\frac{x^2}{2a^2} \right) \quad \nu = 0, 1, 2, 3, \ldots \]

Energy eigenvalues

\[ E_{\nu} = \left( \nu + \frac{1}{2} \right) \hbar \omega_0 = \left( \nu + \frac{1}{2} \right) \hbar \nu_0 \]

Energy levels

The 1-D harmonic oscillator has equally spaced energy states

Energy spacing depends on the fundamental frequency

Energy levels are nondegenerate

One state per level
Harmonic-oscillator wave functions

- Harmonic-oscillator wave functions are related to the Hermite polynomials.
- Hermite polynomials are well-known sets of functions.

<table>
<thead>
<tr>
<th>$\nu$</th>
<th>$H_\nu(y)$</th>
<th>Symmetry</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>1</td>
<td>Even</td>
</tr>
<tr>
<td>1</td>
<td>$2y$</td>
<td>Odd</td>
</tr>
<tr>
<td>2</td>
<td>$4y^2 - 2$</td>
<td>Even</td>
</tr>
<tr>
<td>3</td>
<td>$8y^3 - 12y$</td>
<td>Odd</td>
</tr>
</tbody>
</table>

Wave functions

- Hermite polynomials multiplied by a Gaussian function.
- Note alternation in symmetry about $x = 0$.
  - Even
  - Odd

Probability Functions

- The square of the wave function gives the probability density at each position.
- Finite possibility the particle is outside of the classical turning points.

Summary

- Harmonic oscillator is easily identified as Hermite's differential equation.
- Nondegenerate levels.
- Symmetry about $x = 0$ alternates with quantum number.
- Equally spaced energy levels.
- Finite probability of finding the particle in the classically forbidden region (where the potential energy is greater than the total energy).