

Tutorial 7 - The Harmonic Oscillator

The Harmonic Oscillator

Perhaps the most important potential function is that of the harmonic oscillator, a motion that is governed by *Hooke's law*,

$$m \frac{d^2 x}{dt^2} = -kx \quad \rightarrow \quad x(t) = A \sin(\omega t) + B \cos(\omega t), \quad \text{where} \quad \omega \equiv \sqrt{\frac{k}{m}}.$$

The reason for this is that any potential $V(x)$ is *approximately* parabolic, in the neighborhood of a local minimum x_0 , as can be seen by expanding it in a *Taylor series*,

$$V(x) = \underbrace{V(x_0)}_{\text{constant}} + \underbrace{V'(x_0)}_{=0}(x-x_0) + \frac{1}{2}V''(x_0)(x-x_0)^2 + \dots \approx \frac{1}{2}V''(x_0)(x-x_0)^2.$$

The time-independent Schrödinger equation for the potential $V(x) = \frac{1}{2}m\omega^2 x^2$ is

$$-\frac{\hbar^2}{2m} \frac{d^2 \psi}{dx^2} + \frac{1}{2}m\omega^2 x^2 \psi = E\psi,$$

which can be written more simply in terms of $\xi \equiv \sqrt{\frac{m\omega}{\hbar}}x$, as

$$\left(\frac{d^2}{d\xi^2} - 2\xi \frac{d}{d\xi} + K - 1 \right) h(\xi) = 0,$$

where

$$\psi(\xi) = h(\xi) e^{-\xi^2/2}, \quad \text{and} \quad K \equiv \frac{2E}{\hbar\omega}.$$

The solutions to these equations are

$$\psi_n(x) = \left(\frac{m\omega}{\pi\hbar} \right)^{1/4} \frac{1}{\sqrt{2^n n!}} H_n \left(\sqrt{\frac{m\omega}{\hbar}} x \right) e^{-\frac{m\omega}{2\hbar} x^2}, \quad \text{with} \quad E_n = \hbar\omega \left(n + \frac{1}{2} \right) \quad n = 0, 1, 2, \dots$$

where H_n are the Hermite polynomials. Many times it is useful to use the parametrized form

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

Additional reading: David Griffiths, Introduction to Quantum Mechanics (3rd edition), Ch. 2.3.2, p.48-54.

Hermite Polynomials

The Hermite polynomials are defined through the derivatives of the Gaussian function

$$g(z) = e^{-z^2}.$$

The successive derivatives of a Gaussian are given by

$$\begin{aligned}g'(z) &= -2ze^{-z^2}, \\g''(z) &= (4z^2 - 2)e^{-z^2},\end{aligned}$$

then we would like to state that the n th-order derivative can be written as

$$g^{(n)}(z) = (-1)^n H_n(z) g(z),$$

where $H(z)$ is an n th-degree polynomial in z .

The Hermite polynomials can be generated using the *generating function* $F(z, \lambda)$ as follows:

$$F(z, \lambda) \equiv e^{-\lambda^2 + 2\lambda z} \quad \rightarrow \quad H_n(z) = \left\{ \frac{\partial^n}{\partial \lambda^n} F(z, \lambda) \right\}_{\lambda=0}.$$

Differentiating the generating function with respect to z or λ leads to recurrence relations of H_n :

$$\begin{aligned}\frac{d}{dz} H_n &= 2nH_{n-1}, \\H_n &= 2zH_{n-1} - 2(n-1)H_{n-2}.\end{aligned}$$

The differential equation for the Hermite polynomials is:

$$\left(\frac{d^2}{dz^2} - 2z \frac{d}{dz} + 2n \right) H_n(z) = 0,$$

which is precisely the differential equation for the quantum harmonic oscillator. Properties:

- The parity of H_n is $(-1)^n$.
- H_n has n real zeros, between which one finds those of H_{n-1} .

The first Hermite polynomials are:

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

Additional reading: Cohen Tannoudji, Quantum Mechanics (2nd edition), Ch. V Complement B_v, p.547-550.

Question 1:

Consider a particle with energy $E_n = \hbar\omega \left(n + \frac{1}{2}\right)$, moving under an harmonic potential of frequency ω .

1. For the ground state, calculate the probability of finding a particle outside the classically allowed region.
2. Repeat (1) for $n = 1$ and $n = 2$. Interpret the result.

Solution:

1. Classically we have

$$x_c = A \cos \omega t, \quad \text{and} \quad p_c = -m\omega A \sin \omega t,$$

thus, the boundary position of the particle (i.e. the amplitude), in terms of energy, is

$$E = \frac{p^2}{2m} + \frac{1}{2}m\omega^2 x^2 = \frac{m\omega^2 A^2}{2} \quad \rightarrow \quad A_n = \sqrt{\frac{2E_n}{m\omega^2}} = \sqrt{\frac{\hbar(2n+1)}{m\omega}}.$$

Therefore, the probability for finding the particle outside the classical region is

$$\begin{aligned} P_n(|x| > A_n) &= 1 - P(|x| < A_n) \\ &= 1 - \int_{-A_n}^{A_n} \psi_n^*(x) \psi_n(x) dx \\ &= 1 - \sqrt{\frac{m\omega}{\pi\hbar}} \int_{-A_n}^{A_n} \frac{1}{2^n n!} H_n^2 \left(\sqrt{\frac{m\omega}{\hbar}} x \right) e^{-\frac{m\omega}{\hbar} x^2} dx \\ &= 1 - \frac{1}{2^n n! \sqrt{\pi}} \int_{-\sqrt{2n+1}}^{\sqrt{2n+1}} H_n^2(\xi) e^{-\xi^2} d\xi \end{aligned}$$

At the ground state ($n = 0$), $A_0 = \sqrt{\hbar/m\omega}$

$$P_0 = 1 - \frac{1}{\sqrt{\pi}} \int_{-1}^1 e^{-\xi^2} d\xi = 1 - \text{erf}(1) \approx 0.1578.$$

2. Plugging in $n = 1$ and $n = 2$ we get

$$\begin{aligned} P_1 &= 1 - \frac{1}{2\sqrt{\pi}} \int_{-\sqrt{3}}^{\sqrt{3}} 4\xi^2 e^{-\xi^2} d\xi \\ &= 1 - \frac{1}{\sqrt{\pi}} \int_{-\sqrt{3}}^{\sqrt{3}} \left[e^{-\xi^2} - \frac{d}{d\xi} (\xi e^{-\xi^2}) \right] d\xi \\ &= 1 - \frac{1}{\sqrt{\pi}} \left[\sqrt{\pi} \text{erf}(\sqrt{3}) - 2\sqrt{3}e^{-3} \right], \end{aligned}$$

and in the same manner

$$\begin{aligned} P_2 &= 1 - \frac{1}{8\sqrt{\pi}} \int_{-\sqrt{5}}^{\sqrt{5}} (4\xi^2 - 2)^2 e^{-\xi^2} d\xi \\ &= 1 - \frac{1}{2\sqrt{\pi}} \int_{-\sqrt{5}}^{\sqrt{5}} (4\xi^4 - 4\xi^2 + 1) e^{-\xi^2} d\xi \\ &= 1 - \frac{1}{2\sqrt{\pi}} \left[2\sqrt{\pi} \text{erf}(\sqrt{5}) - 22\sqrt{5}e^{-5} \right], \end{aligned}$$

thus

$$P_1 \approx 0.1116 \quad \text{and} \quad P_2 \approx 0.0951.$$

We see that the probability to find the particle in a classically forbidden region drops as its energy increases, i.e. more energetic particles behave more classically, as one would expect.

Question 2:

Use Heisenberg's uncertainty principle to estimate the ground state energy of a 1D harmonic oscillator. Is this estimate precise? If so, why?

Solution:

Starting from the expectation value of the Hamiltonian

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

Recalling that $\sigma_Q^2 = \langle Q^2 \rangle - \langle Q \rangle^2$, we see that if $\sigma_p^2 = \langle p^2 \rangle$ and $\sigma_x^2 = \langle x^2 \rangle$, then we can use $\sigma_x \sigma_p \sim \hbar/2$ to estimate $\langle H \rangle$. But in order to do that we first need to show that $\langle x \rangle = \langle p \rangle = 0$. Lets start with

$$\langle x \rangle_n = \int \psi_n^* x \psi_n dx = 0,$$

since $|\psi_n|$ is an even function. Next is

$$\frac{d}{dx} = \sqrt{\frac{m\omega}{\hbar}} \frac{d}{d\xi}$$

$$\begin{aligned} \langle p \rangle_n &= \int \psi_n^* \left(-i\hbar \frac{d}{dx} \right) \psi_n dx \\ &= -\frac{i m \omega}{2^n n! \sqrt{\pi}} \int H_n(\xi) e^{-\xi^2/2} \frac{d}{d\xi} \left(H_n(\xi) e^{-\xi^2/2} \right) dx \\ &= -\frac{i m \omega}{2^n n! \sqrt{\pi}} \int H_n(\xi) (H_n'(\xi) - \xi H_n(\xi)) e^{-\xi^2} dx \\ &= -\frac{i m \omega}{2^n n! \sqrt{\pi}} \int H_n(\xi) (2n H_{n-1}(\xi) - \xi H_n(\xi)) e^{-\xi^2} dx, \end{aligned}$$

but both terms are odd, since H_n^2 is even and $H_n H_{n-1}$ is odd, hence $\langle p \rangle_n = 0$. Therefore, we may write

$$\langle H \rangle_n = E_n = \frac{\sigma_p^2}{2m} + \frac{1}{2}m\omega^2 \sigma_x^2 \sim \frac{\hbar^2}{8m\sigma_x^2} + \frac{1}{2}m\omega^2 \sigma_x^2,$$

and find the minimum value with respect to σ_x

$$\frac{dE_n}{d\sigma_x} = -\frac{\hbar^2}{4m\sigma_x^3} + m\omega^2 \sigma_x = 0 \quad \rightarrow \quad \sigma_x^2 = \frac{\hbar}{2m\omega},$$

$$\left. \frac{d^2 E_n}{d\sigma_x^2} \right|_{\sigma_x^2 = \frac{\hbar}{2m\omega}} = \frac{3\hbar^2}{4m\sigma_x^4} + m\omega^2 > 0 \quad \rightarrow \quad \text{minimum,}$$

which corresponds to

$$\boxed{(E_n)_{\min} \sim \frac{\hbar\omega}{2}}.$$

In this case the results are accurate since the ground state is a Gaussian, but in case of non-Gaussian ground state we would get $E_n \gtrsim \hbar/2$.

Question 3:

Consider an isotropic two-dimensional harmonic oscillator.

1. Perform separation of variables and find the eigenstates of the system.
2. Find the eigenvalues of the Hamiltonian and determine the degeneracy of each level.

Solution:

1. The time-independent Schrödinger equation reads

$$\hat{H}\psi(x, y) = \left[\frac{1}{2m} (\hat{p}_x^2 + \hat{p}_y^2) + \frac{1}{2}m\omega^2 (x^2 + y^2) \right] \psi(x, y) = E\psi(x, y),$$

which can be separated into $\hat{H} = \hat{H}_x + \hat{H}_y$ that acts on the wave function

$$\psi(x, y) = \chi(x) \eta(y),$$

so that

$$\begin{aligned} (\hat{H}_x + \hat{H}_y) \chi(x) \eta(y) &= \eta(y) \hat{H}_x \chi(x) + \chi(x) \hat{H}_y \eta(y) \\ &= \eta(y) E_n^x \chi(x) + \chi(x) E_m^y \eta(y) \\ &= (E_n^x + E_m^y) \chi_n(x) \eta_m(y) \\ &= E_{n,m} \psi_{n,m}(x, y). \end{aligned}$$

So that the eigenstates are just a multiplication of two copies of one-dimensional harmonic oscillator,

$$\psi_{n,m}(x, y) = \left(\frac{m\omega}{\pi\hbar} \right)^{1/2} \frac{1}{\sqrt{2^{n+m} n! m!}} H_n(\xi_x) H_m(\xi_y) e^{-(\xi_x^2 + \xi_y^2)/2}.$$

2. The energy levels are

$$E_{n,m} = \hbar\omega (n + m + 1),$$

with degeneracies at

$$(n, m) = \left\{ (0, 0), \begin{pmatrix} (0, 1) \\ (1, 0) \end{pmatrix}, \begin{pmatrix} (0, 2) \\ (1, 1) \\ (2, 0) \end{pmatrix}, \begin{pmatrix} (0, 3) \\ (1, 2) \\ (2, 1) \\ (3, 0) \end{pmatrix}, \dots \right\},$$

or in general

$$g_n = n + 1.$$

Question 4:

Consider a particle of mass m that is moving in a one dimensional potential $V(x)$. Assume that in a certain region of space the potential is a constant i.e. $V(x) = V_0$. In that region, find a general solution for the time independent Schrödinger equation, for each of the following cases:

1. $E > V_0$.
2. $E < V_0$.
3. $E = V_0$.

Where E is the energy of the particle.

Solution:

The Schrödinger equation in the region with a finite potential $V = V_0$ reads

$$-\frac{\hbar^2}{2m} \frac{d^2\psi}{dx^2} + V_0\psi = E\psi.$$

1. In the case of $E > V_0$ we may write the Schrödinger equation as

$$\frac{d^2\psi}{dx^2} = -k^2\psi^2, \quad \text{where} \quad k = \frac{\sqrt{2m(E - V_0)}}{\hbar} \quad \text{is real,}$$

which is just the equation for the harmonic oscillator, which has the general solution

$$\boxed{\psi(x) = Ae^{ikx} + Be^{-ikx}}.$$

This solution is not-normalizable and is referred to as the *free particle* solution.

2. In the case of $E < V_0$, we may write the Schrödinger equation as

$$\frac{d^2\psi}{dx^2} = \kappa^2\psi^2, \quad \text{where} \quad \kappa = \frac{\sqrt{2m(V_0 - E)}}{\hbar} \quad \text{is real,}$$

for which the general solution is

$$\boxed{\psi(x) = Ae^{\kappa x} + B^{-\kappa x}}.$$

This solution is normalizable if $A = 0, B \neq 0$ at $x > 0$ and $B = 0, A \neq 0$ at $x < 0$, and is referred to as *bound particle* solution.

3. In the case of $E = V_0$, the Schrödinger equation reduces to

$$\frac{d^2\psi}{dx^2} = 0,$$

in which case the solution is simply

$$\boxed{\psi(x) = Ax + B}.$$