Next Up Previous Contents
Next: The Same Problem with **Up:** Eigenfunctions, Eigenvalues and Vector **Previous:** Eigenfunctions and Vector Space **Contents**

The Particle in a 1D Box

As a simple example, we will solve the 1D **Particle in a Box** problem. That is a particle confined to a region $0 < x < a$. We can do this with the (unphysical) potential which is zero with in those limits and $+\infty$ outside the limits.

$$V(x) = \begin{cases} 0 & 0 < x < a \\ \infty & \text{elsewhere} \end{cases}$$

Because of the infinite potential, this problem has very **unusual boundary conditions**. (Normally we will require continuity of the wave function and its first derivative.) The wave function must be zero at $x = 0$ and $x = a$ since it must be continuous and it is zero in the region of infinite potential. The first derivative does not need to be continuous at the boundary (unlike other problems), because of the infinite discontinuity in the potential.

The time independent **Schrödinger equation** (also called the energy eigenvalue equation) is

$$Hu_j = E_j u_j$$

with the Hamiltonian (inside the box)

$$H = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2}$$

Our solutions will have

$$u_j = 0$$

outside the box.

The **solution inside the box** could be written as

$$u_j = e^{ikx}$$

where k can be positive or negative. We do **need to choose linear combinations that satisfy the boundary condition** that $u_j(x=0) = u_j(x=a) = 0$.

We can do this easily by **choosing**

$$u_j = C\sin(kx)$$

which automatically satisfies the BC at 0. To satisfy the BC at $x = a$ we need the argument of sine to be $n\pi$ there.

$$u_n = C\sin\left(\frac{n\pi x}{a}\right)$$

Plugging this back into the Schrödinger equation, we get

$$\frac{-\hbar^2}{2m}\left(-\frac{n^2\pi^2}{a^2}\right)C\sin(kx) = EC\sin(kx).$$

There will only be a solution which satisfies the BC for a **quantized set of energies**.

$$E_n = \frac{n^2\pi^2\hbar^2}{2ma^2}$$

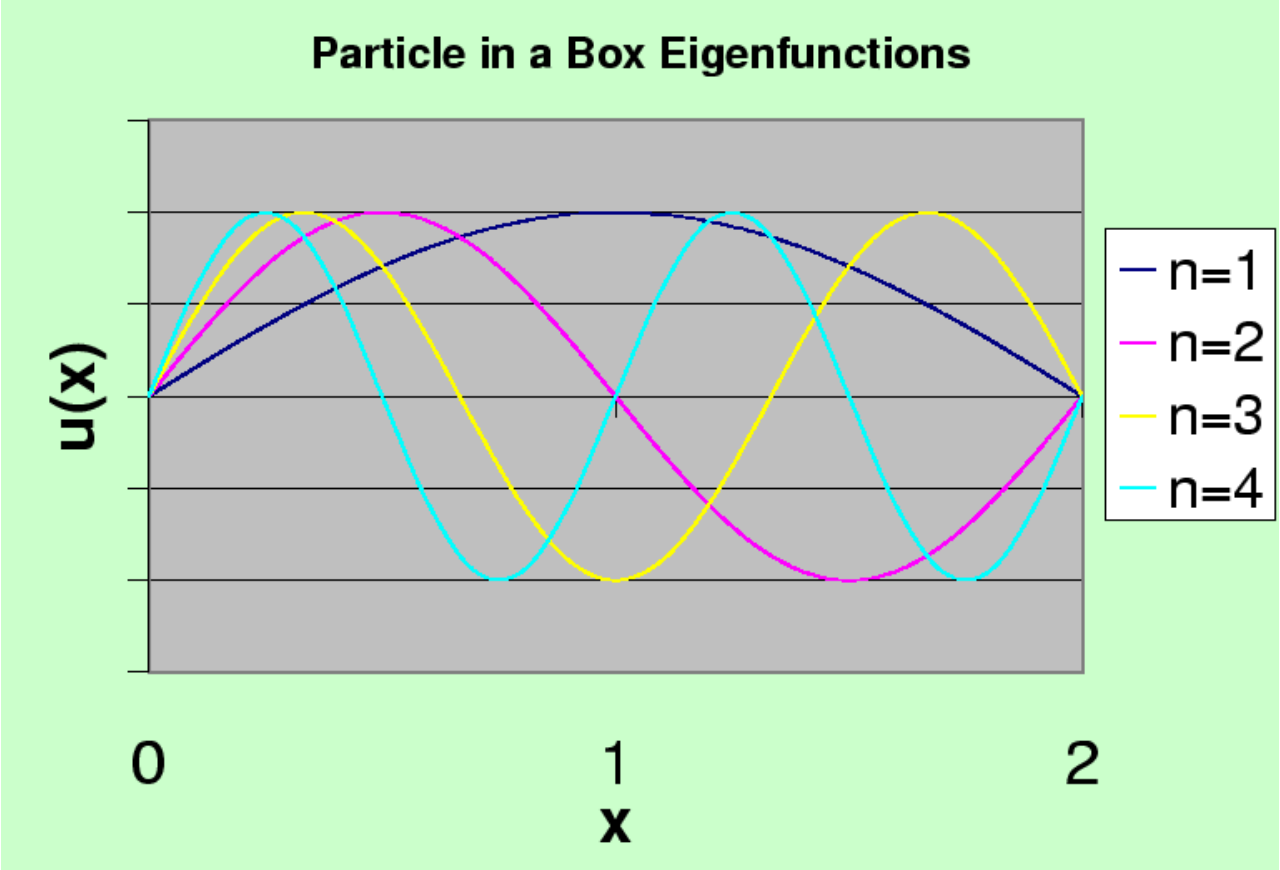
We have solutions to the Schrödinger equation that satisfy the boundary conditions. Now we need to set the constant C to **normalize** them to 1.

$$\langle u_n|u_n\rangle = |C|^2\int_0^a \sin^2\left(\frac{n\pi x}{a}\right)dx = |C|^2\frac{a}{2}$$

Remember that the average value of $\sin^2$ is one half (over half periods). So we set C giving us the eigenfunctions

$$u_n = \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi x}{a}\right)$$

The first four eigenfunctions are graphed below. The ground state has the least curvature and the fewest zeros of the wavefunction.



Note that these states would have a definite parity if $x = 0$ were at the center of the box.

The **expansion** of an arbitrary wave function in these eigenfunctions is essentially our **original Fourier Series**. This is a good example of the energy eigenfunctions being orthogonal and covering the space.

Subsections

- The Same Problem with Parity Symmetry

Next Up Previous Contents

Next: The Same Problem with **Up:** Eigenfunctions, Eigenvalues and Vector **Previous:** Eigenfunctions and Vector Space **Contents**

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