

Use de Broglie's equation, $p = mv = h/\lambda$, to show that the energy levels of a particle inside a one-dimensional box of length L and infinitely high sides are given by:

$$E_n = \frac{h^2 n^2}{8mL^2}$$

[4 marks]

The kinetic energy of a particle with mass m is $\frac{1}{2}mv^2$. As $p = mv$:

$$E = \frac{1}{2}mv^2 = \frac{p^2}{2m}$$

Using the de Broglie equation, $p = h/\lambda$ so:

$$\frac{p^2}{2m} = \frac{(h/\lambda)^2}{2m} = \frac{h^2}{2m\lambda^2}$$

As the walls are infinitely high, the probability of finding the particle at the wall must be zero. For a particle in a box, only wavelengths which are zero at the edges of the box are allowed. Only waves which have wavelengths given by the general formula below are then allowed:

$$\lambda = 2L/n \quad \text{where } n = 1, 2, 3, 4 \dots$$

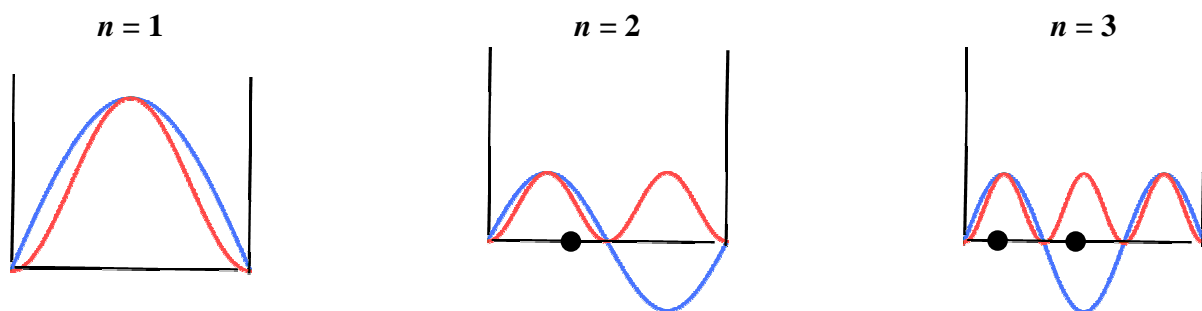
Hence:

$$E_n = \frac{h^2}{2m\lambda^2} = \frac{h^2}{2m(2L/n)^2} = \frac{h^2 n^2}{8mL^2}$$

Draw the corresponding wavefunctions and probability densities for $n = 1 - 3$. Mark the positions of the nodes for each function.

[3 marks]

The wavefunctions (in blue) and the probability densities (in red) are shown below with the nodes labelled with a black dot.



Explain why (a) the energy levels of a particle in a box are quantized but the energy levels of a free particle are not and (b) the lowest possible energy for a particle in a box is not zero.

[4 marks]

For a free particle, any wavelength is possible. There are no restrictions on its value. As λ can have any value, so can the energy. The longest wavelength possible is infinite for a completely free particle, and this corresponds to $E = 0$.

Placing the particle in a box restricts the possible wavelengths as only waves which are zero at the walls are allowed. This leads to quantization of the wavelength and this, in turn, restricts the possible energy that the particle can have.

The longest wavelength now corresponds to the wave shown above for $n = 1$. The wavelength is equal to twice the length of the box and this gives the minimum energy to be:

$$E_1 = \frac{h^2}{2m(2L/1)^2} = \frac{h^2}{8mL^2}$$

By considering the effect of large n and L for a particle in a box, discuss how the classical and quantum mechanical pictures can be reconciled.

[3 marks]

If the mass of the particle is very large:

$$E_1 \rightarrow 0$$

The zero point energy is so close to zero that it appears that a 'heavy' object can have zero kinetic energy.

If the mass of the particle is very large, the separation between the energy levels also tends to zero. It appears that the energy levels of a 'heavy' object are not quantized.

If the length of the box, L , is large, the zero point energy also tends to zero as does the separation between energy levels.

As mL^2 becomes large compared to \hbar^2 , the predictions of the quantum mechanical expressions are the same as those of the classical expressions.