



Tutorial 2; Physical Chemistry

- 1. For a quantum particle in a 1D box, the general expression for the wavefunction**

is $\Psi(x) = \sqrt{\frac{2}{L}} \sin \frac{n\pi x}{L}$. The terms have their usual meaning.

- (a) Find the general expression for the average position of the particle in the one-dimensional box with the length L .
- (b) Find the de Broglie wavelength of the electron in the ground state.

- 2. The general expression for the electron tunneling (transmission) probability across a barrier is expressed as**

$$T = \frac{|A|^2}{|A|^2} = \frac{1}{1 + \frac{(e^{\kappa L} - e^{-\kappa L})^2}{16\varepsilon(1-\varepsilon)}}$$

Find the transmission probability for high and wide barrier

- 3. Consider a scanning tunnelling microscope (STM). The tunnelling current is proportional to the tunnelling probability of electrons between the tip and the substrate surface. The separation between the tip and the substrate surface is 5Å . The wavefunction between the tip and the substrate surface can be assumed to be**

$\Psi = Be^{-\kappa x}$; where $\kappa = \frac{\{2m(V - E)\}^{1/2}}{\hbar}$. Consider $(V - E) = 2.0\text{ eV}$ and use

the formula for T derived for question 2. Find the factors by which the current would drop if the distances of separation were to be 6Å , 8Å and 10Å .