



Mathematica Exercise: Tunneling Through a Barrier of Finite Width

Physical Chemistry I

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The expression for the tunneling probability for a particle of mass m having energy E through a square barrier of width a and height V is given by

$$P = \frac{1}{V^2 \sinh^2 \left(\frac{\sqrt{2m(V-E)}a}{\hbar} \right) + \frac{4E(V-E)}{4E(V-E)}}$$

where

$$\kappa = \sqrt{\frac{2m(V-E)a^2}{\hbar^2}}$$

P is sometimes written as

$$P = \frac{1}{1+G}$$

where

$$G = \frac{V^2 \sinh^2 \kappa}{4E(V-E)}$$

Sketch the potential function.

What parameters does the tunneling transmission probability depend on?

What is \sinh ? (Hint: Check Mathworld site at <http://mathworld.wolfram.com/>) What are the units on G ?

Consider an electron impinging on a barrier of 5.0 eV. The barrier has a width of 1 Angstrom (0.1 nm). What is the probability of the electron moving through the barrier when the energy of the electron is 10% of the barrier, 50% of the barrier and 90% of the barrier?

Consider the same question for a proton, deuteron, H₂ and CO. What effect does increasing the mass have on the tunnelling probability?

It has been proposed that precursors to amino acids have formed in comets by the tunnelling of H₂ and CO. Do you think this is reasonable?

What happens when you increase the length of the box? Decrease it? Does this make sense to you?

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