Applications of A level Mathematics and Further Mathematics

Topics from A level Mathematics	-	Indices
	-	Calculus - differentiation of rational functions and finding stationary values

Chemistry degree – Interaction energy between atoms and molecules

Summary: The attractive and repulsive forces that act between atoms and molecules are modelled by a rational function.

Calculus can be used to find the equilibrium separation, where potential energy is a minimum..

The problem: The potential-energy from the interaction of two neutral atoms or molecules is modelled by the Lennard-Jones equation.

$$V_{LJ} = 4\varepsilon\left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right]$$

where ε is the depth of the potential well,

σ is the distance at which the inter-particle potential is zero,

r is the distance between the particles.

The r^{-12} term models the repulsive forces at short ranges and the r^{-6} term models the attractive long-range forces.

Questions:

1. Sketch how the potential energy varies as r increases from zero using graphing software.

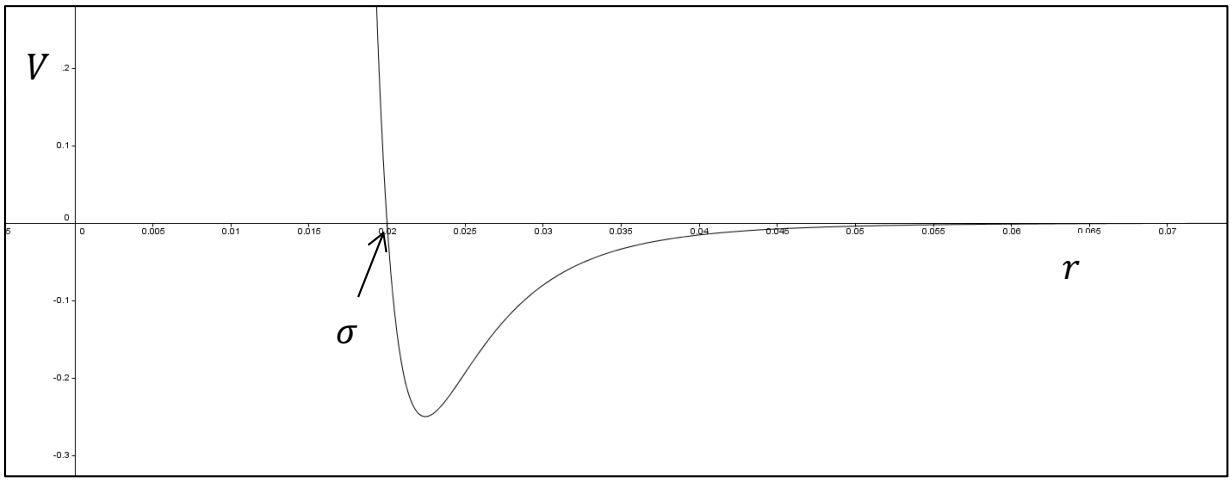
   By considering where the gradient of the function V_{LJ} is zero can you find that the potential energy has a minimum value.

2. By differentiating the function show that the minimum in the Lennard-Jones potential-energy function occurs at a separation of

$$r_e = 2^{\frac{1}{6}}\sigma$$

Solution

1. The graph of the potential energy function looks like the curve below



When $r = \sigma, V = 0.$

For $0 \leq r < \sigma$ the first term is dominant and $V \to +\infty$ as $r \to \sigma.$

For $r > \sigma$ the second term is more dominant and $V \to 0$ as $r \to \infty.$

2. Differentiating

$$\frac{dV}{dr} = 4\varepsilon[-12\sigma^{12}r^{-13} + 6\sigma^{6}r^{-7}]$$

When derivative is zero $-12\sigma^{12}r^{-13} + 6\sigma^{6}r^{-7} = 0$

$$(-2\sigma^{6}r^{-6} + 1)r^{-7} = 0$$

$r^{-7} = 0$ or $2\sigma^{6} = r^{6}$

Minimum value occurs at separation $r_e = 2^{\frac{1}{6}}\sigma$

(when $r = 0$ the potential energy is undefined.)