1S Summer exam 2006 - Calculus Dr Paul May

1. Answer ***all*** parts (a) to (d). All parts carry equal marks.

   Determine the following:

   (a) dy/dx if $y = 27x^5$

   (b) du/dz if $u = 3.2z^2 + 6z – 5.7$

   (c) dβ/dθ if $\beta = 8\cos\theta$

   (d) d💣/d☠ if 💣 = 7 exp(–19☠)

   (4 marks)

2. Answer ***all*** parts (a) to (d). All parts carry equal marks.

   Differentiate the following functions with respect to x, and simplify the result where possible:

   (a) $y = (5 – 3x)(2 – 20x)$

   (b) $y = 2.8x^{56} \sin x$

   (c) $y = \dfrac{(2x^7 - 3x)}{(5x^3 - 3x + 1.67)}$

   (d) $y = 3 \ln(3x^2 – 6x^5)$

   (8 marks)

3. Answer ***all*** parts (a) to (d).

   The Lennard-Jones potential used to describe the van der Waals interaction energy between two neutral molecules is given by the following equation:

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

   where ε is the well depth and σ is the hard-sphere radius of the molecule. Measurements of V versus r are given in the table.

r / Å	1.8	1.9	2.0	2.1	2.2	2.3	2.4	2.5	2.6
V / (kJ mol^{-1})	66.4	19.6	0	-7.58	-9.83	-9.82	-8.91	-7.74	-6.57

   (a) Plot these data as a graph and estimate the co-ordinates (r_{min}, V_{min}) of the minimum of the curve

   (4 marks)

   (b) Differentiate the equation for the Lennard-Jones potential, and obtain an expression for r_{min} in terms of σ.

   (4 marks)

(c) Put this expression for r_{min} back into the original Lennard-Jones equation, and calculate an expression for V_{min} in terms of ε. Compare this to your estimate from (ii) and hence obtain a value for ε.

(2 marks)

(d) Using your estimate for r_{min} from (a) and your expression for r_{min} from (b), calculate a value for σ.

(2 marks)

Answers

1)

a) $dy/dx = 135x^4$

b) $du/dz = 6.4z + 6$

c) $d\beta/d\theta = -8\sin\theta$

d) d💣/d☠ = -133 exp(-19☠)

2)

a) Product Rule: $(5 - 3x).(-20) + (2 - 20x).(-3) \quad = \quad 120x - 106$

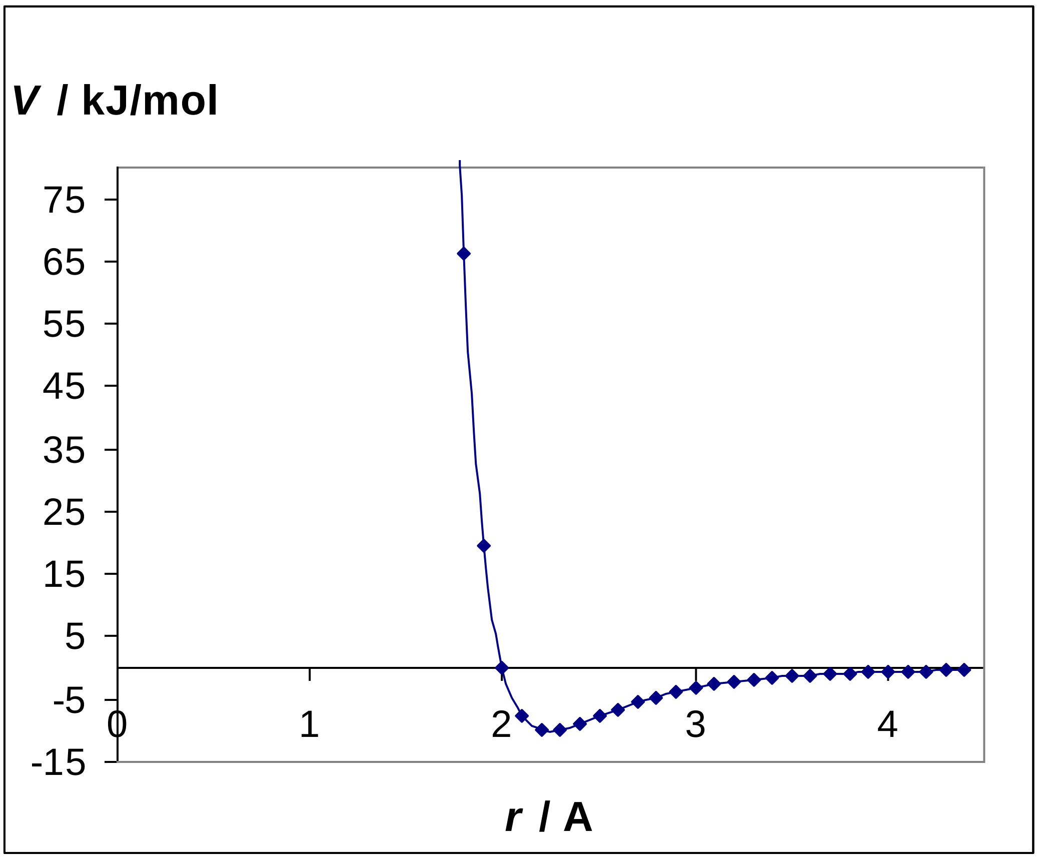
b) Product Rule: $2.8x^{56}(\cos x) + (\sin x)(156.8\, x^{55}) \quad = \quad 2.8x^{55}\,(x \cos x + 56\sin x)$

c) Quotient Rule: $$\frac{dy}{dx} = \frac{(5x^3 - 3x + 1.67)(14x^6 - 3) - (2x^7 - 3x)(15x^2 - 3)}{(5x^3 - 3x + 1.67)^2}$$

d) Funct. of a Funct.: $3\ln(3x^2 - 6x^5)$ $\quad dy/dx = \dfrac{dy}{dx} = \dfrac{3}{(3x^2 - 6x^5)} . \dfrac{(6x - 30x^4)}{} =$

$$\frac{dy}{dx} = \frac{(6 - 30x^3)}{(x - 2x^4)} \quad = \quad \frac{dy}{dx} = \frac{6(1 - 5x^3)}{x(1 - 2x^3)}$$

3) (a)



The graph shows that r_{min} should be between 2.2 and 2.3 Å, and V_{min} should be around -10 kJ mol^{-1}.

(b) Rewrite it as: $$V = 4\varepsilon\left[\sigma^{12} r^{-12} - \sigma^{6} r^{-6}\right]$$

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

At the minimum, $dV/dr = 0$, so $$0 = 4\varepsilon\left[-12\sigma^{12}r^{-13} + 6\sigma^{6}r^{-7}\right]$$

Dividing by 4ε, $$0 = -12\sigma^{12}r^{-13} + 6\sigma^{6}r^{-7}$$

$$12\sigma^{12}r^{-13} = 6\sigma^{6}r^{-7}$$

Dividing by 6, σ^6 and r^{-7} $$2\sigma^{6}r^{-6} = 1$$

or $$2\sigma^{6} = r^{6}$$

Sixth rooting: $$r_{\min} = \sigma\sqrt[6]{2}$$ i.e $\underline{\boldsymbol{r_{\min} = 1.122\sigma}}$

(c) Substituting back this value for $r_{\min}$ into the original LJ equation we get:

$$V_{\min} = 4\varepsilon\left[\left(\frac{\sigma}{\sigma\sqrt[6]{2}}\right)^{12} - \left(\frac{\sigma}{\sigma\sqrt[6]{2}}\right)^{6}\right]$$

Cancelling the σ's, we get:

$$V_{\min} = 4\varepsilon\left[\left(\frac{1}{2^2}\right) - \left(\frac{1}{2}\right)\right]$$

$$V_{\min} = 4\varepsilon\,[1/4 - 1/2]$$

So $\underline{V_{\min} = -\varepsilon}$, which should be around <u>–10 kJ mol</u>$^{-1}$ (which isn't surprising as ε is called the 'well depth', so should be the minimum of the curve!)

(d) Using $r_{\min} = 1.122\sigma$ and a value from the graph of $r_{\min} \sim 2.24$, we get $\underline{\sigma = 2\ \text{Å}}$ (which you could also get from the fact that when V=0 in the LJ equation, $r = \sigma$, so the graph crosses the axis at $r = \sigma$, which from the graph is 2 Å).