School of Mathematical Sciences

Assignment Cover Sheet

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Assessment Title	**Assignment 5**
Due Date	Thursday, 24 October, 2019 @ 12:00 noon
Course / Program	APP MTH 3022–Optimal Functions & Nanomechanics
Date Submitted	24/10
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OFN Assignment 5

Andrew Martin

October 24, 2019

1. (a) Assume we are only considering the top surface of the substrate.
   i. Area of the solid-liquid interface, A_{sl}:

   $$A_{sl} = \pi r_0^2$$

   ii. Solid-gas interface, A_{sg}:
   This is the difference of the solid area and the solid liquid interface, that is:

   $$A_{sg} = A_s - A_{sl} = A_s - \pi r_0^2$$

   iii. Liquid-gas interface, A_{lg}:
   This is the surface area of the droplet above the solid. The surface area of the droplet is parameterised as

   $$\mathbf{r} = (r(z)\cos u, r(z)\sin u, z)$$

   This is nearly to the soap film in assignment 4, the surface area of this becomes

   $$\begin{aligned} S &= \int_0^{z_0} \int_{-\pi}^{\pi} r\sqrt{1+r'^2}dudz \\ &= 2\pi \int_0^{z_0} r\sqrt{1+r'^2}dz \end{aligned}$$

   Which is the liquid-gas interface

   $$A_{lg} = S - A_{sl} = S$$

   (b) Subbing all of the above into the total energy:

   $$\begin{aligned} E_{tot} &= \gamma_{sl}\left(\pi r_0^2\right) + \gamma_{sg}\left(A_s - \pi r_0^2\right) + \gamma_{lg} S \\ &= \gamma_{sl}\left(2\pi r_0\right) + \gamma_{sg}\left(A_s - \pi r_0^2\right) + \gamma_{lg}\left(2\pi \int_0^{z_0} r\sqrt{1+r'^2}dz\right) \end{aligned}$$

   (c) The volume of the droplet: cross sectional volume is just $dV = \pi r^2 dz$.

   $$V_l = \int_0^{z_0} \pi r^2 dz$$

That is the constraint is:

$$Constraint = -\pi\hat{\lambda}\int_0^{z_0} r^2 dz$$

And hence the functional (which is no longer explicitly the energy) is

$$F_1\{z\} = \gamma_{sl}\left(\pi r_0^2\right) + \gamma_{sg}\left(A_s - \pi r_0^2\right) + \gamma_{lg}\left(2\pi\left(\int_0^{z_0} r\sqrt{1+r'^2} - \lambda r^2 dz\right)\right)$$

Where $\lambda = \frac{\hat{\lambda}}{2\gamma_{lg}}$

(d)

$$\begin{aligned}
F_2\{z\} &= \gamma_{sl}\left(\pi r_0^2\right) + \gamma_{sg}\left(-\pi r_0^2\right) + \gamma_{lg}\left(2\pi\left(\int_0^{z_0} r\sqrt{1+r'^2} - \lambda r^2 dz\right)\right) \\
F\{z\} &= \frac{1}{2\gamma_{lg}}\gamma_{sl}\left(r_0\right) + \frac{1}{2\gamma_{lg}}\gamma_{sg}\left(-r_0\right) + \left(\int_0^{z_0} r\sqrt{1+r'^2} - \lambda r^2 dz\right) \\
&= \left(\frac{\gamma_{sl}-\gamma_{sg}}{2\gamma_{lg}} r_0^2\right) + \int_0^{z_0} r\sqrt{1+r'^2} - \lambda r^2 dz \\
&= \left[\left(\frac{\gamma_{sl}-\gamma_{sg}}{2\gamma_{lg}}\right) r^2\right]_{z=0} + \int_0^{z_0}\left(r\sqrt{1+r'^2} - \lambda r^2\right) dz
\end{aligned}$$

2. (a)

$$\begin{aligned}
p &= \frac{\partial f}{\partial r'} = \frac{rr'}{\sqrt{1+r'^2}} \\
H &= \frac{rr'^2}{\sqrt{1+r'^2}} - \left(r\sqrt{1+r'^2} - \lambda r^2\right)
\end{aligned}$$

(b) Since there is no explicit dependence on the independent variable z, this is autonomous, and so the Hamiltonian is constant

(c) The natural BC at $z = z_0$ since this is first order is:

$$\left[\frac{\partial f}{\partial r'}\right]_{z=z_0} = 0 \implies p|_{z=z_0} = 0$$

Since $[p\delta r - H\delta z]_{z_0} = 0$ This implies that $H\delta z\Big|_{z_0} = 0$ and for non-trivial solutions this implies that H is everywhere zero

(d) From b, c we obtain

$$\frac{rr'^2}{\sqrt{1+r'^2}} - \left(r\sqrt{1+r'^2} - \lambda r^2\right) = 0$$

(e) Solving the DE:

$$
\begin{aligned}
\frac{rr'^2}{\sqrt{1+r'^2}} - \left(r\sqrt{1+r'^2} - \lambda r^2\right) &= 0 \\
rr'^2 - r(1+r'^2) - \lambda r^2\sqrt{1+r'^2} &= 0 \\
-r + \lambda r^2\sqrt{1+r'^2} &= 0 \\
-1 + \lambda r\sqrt{1+r'^2} &= 0 \\
r\sqrt{1+r'^2} &= \frac{1}{\lambda} \\
r'^2 &= \frac{1}{\lambda^2 r^2} - 1 \\
r' &= \sqrt{\frac{1}{\lambda^2 r^2} - 1}
\end{aligned}
$$

$$
\int \frac{1}{\sqrt{\frac{1}{\lambda^2 r^2} - 1}} dr = \int dz
$$

The left integral:

$$
\begin{aligned}
\int \frac{1}{\sqrt{\frac{1}{\lambda^2 r^2} - 1}} dr &= \lambda \int \frac{1}{\sqrt{\frac{1}{r^2} - \lambda^2}} dr \\
&= \lambda \int \frac{r}{\sqrt{1-\lambda^2 r^2}} dr \\
&= \lambda \int \frac{\sqrt{1-\lambda^2 r^2}}{\lambda^2 r} \frac{r}{\sqrt{1-\lambda^2 r^2}} dv \\
&= \lambda \int \frac{r}{\sqrt{1-\lambda^2 r^2}} \frac{-\sqrt{1-\lambda^2 r^2}}{\lambda^2 r} dv \\
&= -\frac{1}{\lambda} \int dv \\
&= -\frac{\sqrt{1-\lambda^2 r^2}}{\lambda} + const
\end{aligned}
$$

Where I have used the substitution

$$
v = \sqrt{1-\lambda^2 r^2}, \quad dv = \frac{-\sqrt{1-\lambda^2 r^2}}{\lambda^2 r}
$$

Plugging this back in:

$$
\begin{aligned}
\int \frac{1}{\sqrt{\frac{1}{\lambda^2 r^2}-1}} dr &= \int dz \\
-\frac{\sqrt{1-\lambda^2 r^2}}{\lambda} &= z + c \\
1-\lambda^2 r^2 &= z^2\lambda^2 + c\lambda^2 z + c\lambda^2 \\
\lambda^2 r^2 &= 1 - z^2\lambda^2 - c\lambda^2 z - c\lambda^2 \\
r^2 &= \frac{1}{\lambda^2} - z^2 - cz - c \\
r^2 &= \frac{1}{\lambda^2} - (z-c)^2 \\
(z-c)^2 + r^2 &= \frac{1}{\lambda^2} \\
(z-c)^2 + r^2 &= R^2
\end{aligned}
$$

Where $R^2 = \frac{1}{\lambda^2}$

3. (a) The contact angle θ_c is defined as the angle inside the droplet tangential to its point of contact $(z, r) = (0, r_0)$. This is equivalent to the derivative of r at $z = 0$, i.e. $r'(z = 0)$.

Rewrite the solution for the droplet as

$$
r = \sqrt{R^2 - (z-c)^2}, \quad r' = -\frac{z-c}{R^2 - (z-c)^2}
$$

So that

$$
r_0 = \sqrt{R^2 - c^2}, \quad r'(z=0) = \theta_c = \frac{c}{r_0^2}
$$

$$
\begin{aligned}
\frac{p}{r} &= \frac{r'}{\sqrt{1+r'^2}} \\
&= \frac{-\frac{z-c}{R^2-(z-c)^2}}{\sqrt{1+\left(\frac{z-c}{R^2-(z-c)^2}\right)^2}} \\
\frac{p}{r}\Big|_{z=0} &= \frac{\frac{c}{R^2-c^2}}{\sqrt{1+\left(\frac{c}{R^2-c^2}\right)^2}} \\
&= \frac{c}{r_0\sqrt{1+c^2/r_0^2}} \\
&= \frac{c}{\sqrt{r_0^2+c^2}}
\end{aligned}
$$

$$\begin{aligned}\left(\frac{\gamma_{sl}-\gamma_{sg}}{\gamma_{lg}}\right) r - p &= 0\\ \left(\frac{\gamma_{sl}-\gamma_{sg}}{\gamma_{lg}}\right) r - \frac{rr'}{\sqrt{1+r'^2}} &= 0\\ \left(\frac{\gamma_{sl}-\gamma_{sg}}{\gamma_{lg}}\right) - \frac{r'}{\sqrt{1+r'^2}} &= 0\end{aligned}$$

At $z=0$, use the derivative of r in terms of θ_c: If we use the parameterisation

$$\frac{\partial r}{\partial z} = \frac{\frac{\partial r}{\partial \theta}}{\frac{\partial z}{\partial \theta}} = -\frac{R\cos\theta}{R\sin\theta} = -\cot(\theta)$$

Then

$$\begin{aligned}r'|_{z=0} &= -\cot(\theta_c)\\ \frac{r'}{1+r'^2} &= \frac{-\cot(\theta_c)}{\sqrt{1+\cot^2(\theta_c)}}\\ &= \frac{-\cot(\theta_c)}{\operatorname{cosec}(\theta_c)}\\ &= \frac{-\cos(\theta_c)}{\sin(\theta_c)}\sin(\theta_c)\\ &= -\cos(\theta_c)\end{aligned}$$

$$\begin{aligned}\left(\frac{\gamma_{sl}-\gamma_{sg}}{\gamma_{lg}}\right) - \frac{r'}{\sqrt{1+r'^2}} &= 0\\ \left(\frac{\gamma_{sl}-\gamma_{sg}}{\gamma_{lg}}\right) - (-\cos(\theta_c)) &= 0\\ \gamma_{sl}-\gamma_{sg} &= -\gamma_{lg}\cos(\theta_c)\\ \gamma_{sg}-\gamma_{sl} &= \gamma_{lg}\cos(\theta_c)\end{aligned}$$

(b) Letting

$$z = c + R\cos\theta, \quad r = R\sin\theta$$

$$\begin{aligned}r' = -\cot\theta &= \frac{z-c}{r}\\ r'|_{z=0} = -\cot(\theta_c) &= \frac{-c}{r_0}\\ r_0 = c\tan(\theta_c)\end{aligned}$$

$$\begin{aligned}z=0 \implies c + R\cos\theta_c &= 0\\ c &= -R\cos\theta_c\end{aligned}$$

Which can simplify the previous expression:

$$
\begin{aligned}
-\frac{\cos\theta_c}{\sin\theta_c} &= \frac{R\cos\theta_c}{r_0} \\
-\frac{1}{\sin\theta_c} &= \frac{R}{r_0} \\
r_0 &= -R\sin\theta_c
\end{aligned}
$$

(c) The fixed volume constraint: We will have to convert $z = 0, z = z_0$ to theta points:

$$
\begin{aligned}
z = 0 \implies c - R\cos(\theta_0) &= 0 \\
\theta_0 &= \arccos\left(\frac{c}{R}\right) \\
&= \arccos\left(-R\cos\theta_c/R\right) \\
&= \arccos\left(-\cos\theta_c\right) \\
&= \pi - \arccos\left(\cos\theta_c\right) \\
\theta_0 &= \pi - \theta_c
\end{aligned}
$$

$$
z = z_0 \implies r = 0 \implies \theta_1 = n\pi = 0
$$

$$
\begin{aligned}
V_l &= \pi \int_0^{z_0} r^2 dz \\
&= \pi \int_{\theta_0}^{\theta_1} r^2 \frac{dz}{d\theta} d\theta \\
&= \pi \int_{\theta_0}^{0} R^2 \sin^2\theta(-R\sin\theta) d\theta \\
&= \pi \int_0^{\theta_0} R^3 \sin^3\theta d\theta \\
&= \pi R^3 \int_0^{\theta_0} \sin^3\theta d\theta \\
&= \pi R^3 \left[\frac{1}{3}\cos^3\theta - \cos\theta\right]_0^{\theta_0} \\
V_l &= \pi R^3 \left(-\frac{1}{3}\cos^3\theta_c + \cos\theta_c + \frac{2}{3}\right) \\
R^3 &= \frac{V_l}{\pi\left(-\frac{1}{3}\cos^3\theta_c + \cos\theta_c + \frac{2}{3}\right)} \\
R &= \left(\frac{V_l}{\pi\left(-\frac{1}{3}\cos^3\theta_c + \cos\theta_c + \frac{2}{3}\right)}\right)^{1/3}
\end{aligned}
$$

(d) So using the conditions:

$$R = \left(\frac{V_l}{\pi\left(-\frac{1}{3}\cos^3\theta_c + \cos\theta_c + \frac{2}{3}\right)}\right)^{1/3}$$
$$r_0 = -R\sin\theta_c$$
$$c = -R\cos\theta_c$$

Figure 1 shows the plots of these solutions. They either indicate that no solutions exist in this region (unlikely) or that there is an error in previous working.

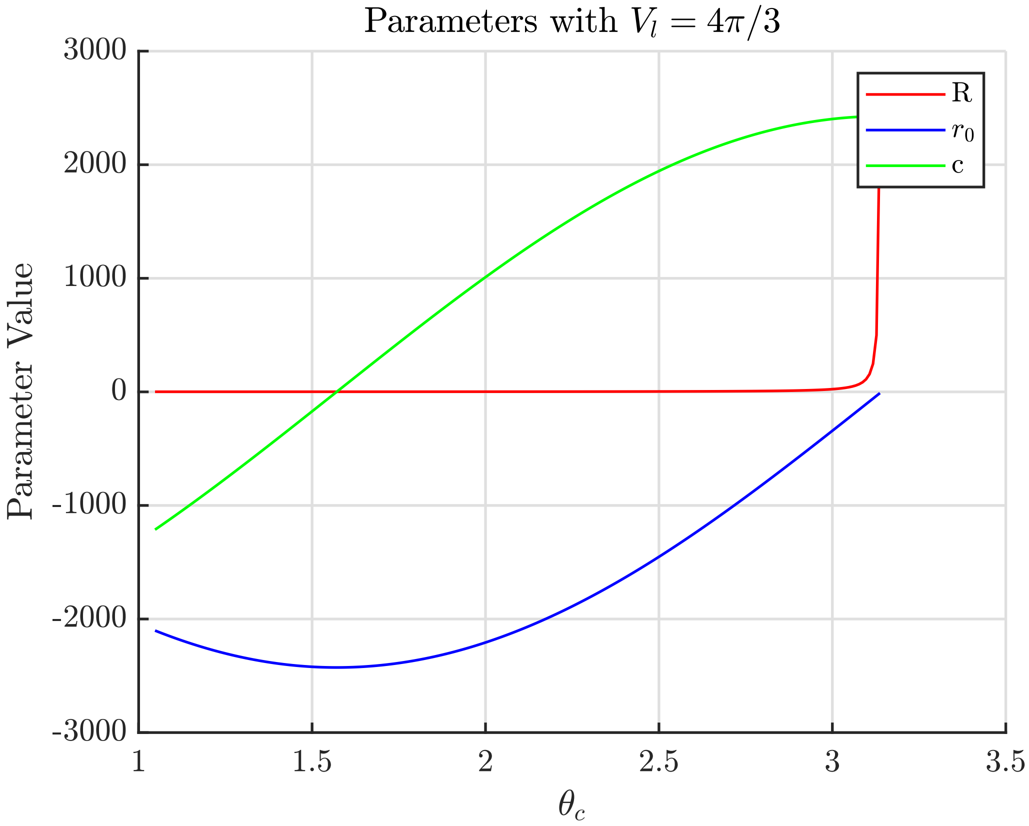


Figure 1: Plot of the parameters against θ_c.

Code

```
close all
%Make plots less repulsive
set(groot, 'DefaultLineLineWidth', 1, ...
     'DefaultAxesLineWidth', 1, ...
     'DefaultAxesFontSize', 12, ...
     'DefaultTextFontSize', 12, ...
     'DefaultTextInterpreter', 'latex', ...
     'DefaultLegendInterpreter', 'latex', ...
     'DefaultColorbarTickLabelInterpreter', 'latex', ...
     'DefaultAxesTickLabelInterpreter','latex');
Vl = 4*pi/3;
R = [];
```

```
r0 = [];
c = [];
figure
hold on
syms Rsym r0sym
assume(Rsym,'real')

thetacarr = pi/3:0.01:pi;
R = zeros(size(thetacarr));
c = zeros(size(thetacarr));
r0 = zeros(size(thetacarr));
%i could vectorise this but its not worth it
for i= 1:length(thetacarr)
    thetac = thetacarr(i);
    R(i) = (Vl/(pi *(-cos(thetac)^3/3 + cos(thetac) + 2/3)))^(1/3);

    c(i) = -Rsol*cos(thetac);

    r0(i) = -Rsol*sin(thetac);

end
    plot(thetacarr,R,'r')
    plot(thetacarr,r0,'b')
    plot(thetacarr,c,'g')
    legend(["R","$r_0$","c"])
    xlabel("$\theta_c$")
    ylabel("Parameter Value")
    title("Parameters with $V_l = 4\pi/3$")
    grid on

    saveas(gcf,'A5q3d.eps','epsc')
```

School of Mathematical Sciences

APP MTH 3022/7106 - Optimal Functions and Nanomechanics

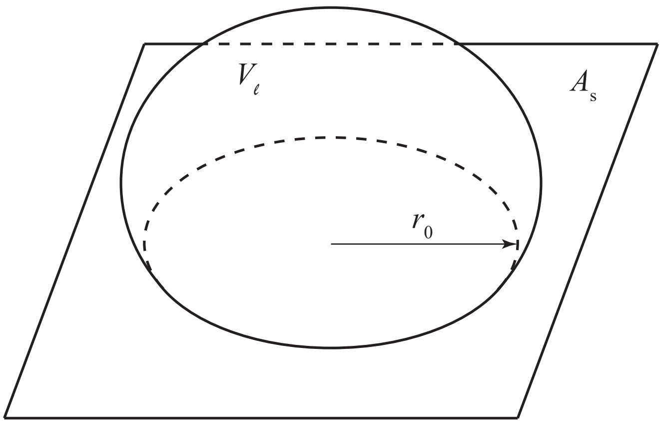
Assignment 5 question sheet

Due: Thursday, 24 October, at 12 noon (in the hand-in box on level 6)

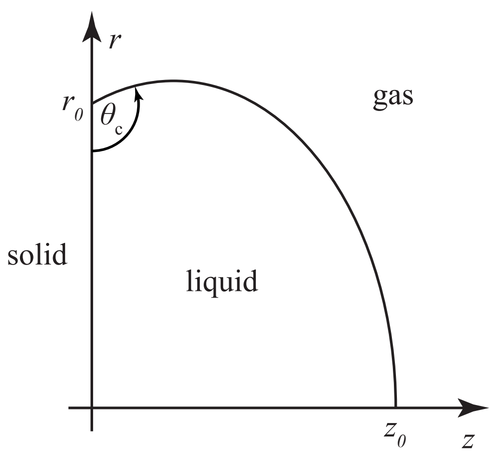
When presenting your solutions to the assignment, please include some explanation in words to accompany your calculations. It is not necessary to write a lengthy description, just a few sentences to link the steps in your calculation. Messy, illegible or inadequately explained solutions may be penalised. The marks awarded for each part are indicated in brackets.

All students are to attempt Questions 1–3.

For the whole assignment we will consider the problem of a liquid metal droplet sitting on a solid substrate. The substrate has a fixed Area A_s, the droplet has a circular contact interface on the substrate of radius r_0 and a fixed volume of liquid V_ℓ as pictured below.



We assume that the drop has rotational symmetry, which in a cylindrical coordinate system (r, ϕ, z), leads to all derivatives with respect to ϕ vanishing and the problem become one of finding a curve $r(z)$ in the plane. We define the contact angle θ_c as the angle between the curve $r(z)$ and negative direction of the r-axis at the point of contact $(z, r) = (0, r_0)$.



1. If the droplet is small (nanoscaled) then the surface energy dominates over gravity, which can be neglected, and the droplet shape is that which minimises the total surface energy. Surface energy is an interface cost per unit area and are specified for the solid-gas interface γ_{sg}, the solid-liquid interface $\gamma_{\mathrm{s}\ell}$ and the liquid gas interface $\gamma_{\ell\mathrm{g}}$. We wish to find the profile shape $z(r)$, including the values of the contact angle θ_{c} and the solid-liquid interface radius r_0.

   (a) Find expressions for

      i. The area of the solid-liquid interface $A_{\mathrm{s}\ell}$.

      ii. The area of the solid-gas interface A_{sg}.

      iii. The area of the liquid-gas interface $A_{\ell\mathrm{g}}$.

   (b) The total surface energy cost will be given by

   $$E_{\mathrm{tot}} = \gamma_{\mathrm{s}\ell}A_{\mathrm{s}\ell} + \gamma_{\mathrm{sg}}A_{\mathrm{sg}} + \gamma_{\ell\mathrm{g}}A_{\ell\mathrm{g}}.$$

   Substitute your expressions from part (a) into the energy equation to derive the unconstrained functional for this problem.

   (c) Next derive an expression encapsulating the constraint that the liquid volume V_ℓ is fixed, and incorporate this into your unconstrained functional from part (b) using a Lagrange multiplier to derive a constrained functional.

   (d) Finally take your expression from part (c) and simplify it by taking $\gamma_{\mathrm{sg}}A_s$ as the datum energy and scaling the remaining expression by dividing by $2\pi\gamma_{\ell\mathrm{g}}$.

[7 marks]

2. In the previous question we derived the functional

$$F\{z\} = \left[\left(\frac{\gamma_{\mathrm{s}\ell} - \gamma_{\mathrm{sg}}}{2\gamma_{\ell\mathrm{g}}}\right) r^2\right]_{z=0} + \int_0^{z_0} \left(r\sqrt{1+r'^2} - \lambda r^2\right) dz.$$

   We also have natural boundary conditions applying for r at $z = 0$ and for z at $z = z_0$.

   (a) Derive expressions for the quantities

   $$p = \frac{\partial f}{\partial r'}, \quad \text{and} \quad H = r'\frac{\partial f}{\partial r'} - f,$$

   where as usual f is the integrand of the integral part of F.

   (b) Classify the functional to determine a quantity that extremals of this functional must conserve.

   (c) Use the natural boundary condition at $z = z_0$ to determine what value this conserved quantity must take.

   (d) Using your answers from the previous three parts derive a differential equation for $r(z)$ that extremals of F must satisfy.

   Hint: We do not appeal to the Euler-Lagrange equation to solve this problem.

   (e) Solve the differential equation from part (d) to determine the shape of the profile.

[8 marks]

3. In the previous question we derived a solution given by the arc of a circle centred somewhere on the z-axis like

$$(z - c)^2 + r^2 = R^2,$$

where we have defined $R = 1/\lambda$, and c is a constant of integration. Thus we have have two unknown constants still to determine: R and c.

(a) When determining the natural boundary condition at $z = 0$ we must also consider the term outside the integral. When taking the first variation of F we find

$$\delta F = \left[\left(\frac{\gamma_{s\ell} - \gamma_{sg}}{2\gamma_{\ell g}} \right) \frac{\partial}{\partial r}(r^2)\, \delta r \right]_{z=0} + [p\, \delta r - H\, \delta z]_{z=0}^{z_0} + \int_0^{z_0} \cdots dz.$$

This means that the natural boundary condition that applies at $z = 0$ is

$$\left(\frac{\gamma_{s\ell} - \gamma_{sg}}{\gamma_{\ell g}} \right) r - p = 0.$$

Using this condition and the definition of the contact angle θ_c given in Question 1, derive Young's equation

$$\gamma_{sg} - \gamma_{s\ell} = \gamma_{\ell g} \cos\theta_c.$$

(b) Adopting the parameterisation

$$z = c + R\cos\theta, \quad \text{and} \quad r = R\sin\theta,$$

give expressions for r_0 and c in terms of R and θ_c.

(c) Employ the fixed volume constraint from Question 1, part (c) to find an expression for R in terms of V_ℓ and θ_c

Hint: Recall that

$$\int \sin^3\theta\, d\theta = \frac{1}{3}\cos^3\theta - \cos\theta + \text{constant}.$$

(d) Using a fixed value of $V_\ell = 4\pi/3$ units^3 and on the same set of axes, use a computer package like MATLAB to plot R, r_0 and c for contact-angles in the range $\pi/3 < \theta_c < \pi$.

[9 marks]