School of Mathematical Sciences
Assignment Cover Sheet

Student Name	
Student ID	
Assessment Title	**Assignment 4**
Due Date	Thursday, 10 October, 2019 @ 12:00 noon
Course / Program	APP MTH 3022–Optimal Functions & Nanomechanics
Date Submitted	
OFFICE USE ONLY Date Received	

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OFN Assignment 4

Andrew Martin

October 10, 2019

1. (a) dA is obtained using the cross product of the tangent vectors of the parametrisation

$$\frac{\partial r}{\partial \theta} = (-b\sin\theta\sin\phi, b\cos\theta\sin\phi, 0)$$
$$\frac{\partial r}{\partial \phi} = (b\cos\theta\cos\phi, b\sin\theta\cos\phi, -c\sin\phi)$$

$$dA = \left|\frac{\partial r}{\partial \theta} \times \frac{\partial r}{\partial \phi}\right| d\theta d\phi$$

$$\frac{\partial r}{\partial \theta} \times \frac{\partial r}{\partial \phi} = \begin{vmatrix} \mathbf{i} & \mathbf{j} & \mathbf{k} \\ -b\sin\theta\sin\phi & b\cos\theta\sin\phi & 0 \\ b\cos\theta\cos\phi & b\sin\theta\cos\phi & -c\sin\phi \end{vmatrix}$$

$$\begin{aligned} \frac{\partial r}{\partial \theta} \times \frac{\partial r}{\partial \phi} &= \left(-bc\cos\theta\sin^2\phi, -bc\sin\theta\sin^2\phi, -b^2\sin^2\theta\sin\phi\cos\phi - b^2\cos\theta^2\sin\phi\cos\phi\right) \\ &= \left(-bc\cos\theta\sin^2\phi, -bc\sin\theta\sin^2\phi, -b^2\sin\phi\cos\phi\right) \\ &= b\sin\phi\det(-c\cos\theta\sin\phi, -c\sin\theta\sin\phi, -b\cos\phi) \end{aligned}$$

$$\begin{aligned} dA &= \left|\frac{\partial r}{\partial \theta} \times \frac{\partial r}{\partial \phi}\right| d\theta d\phi \\ &= b\sin\phi\sqrt{(-c\cos\theta\sin\phi)^2 + (-c\sin\theta\sin\phi)^2 + (-b\cos\phi)^2 d\theta d\phi} \\ &= b\sin\phi\sqrt{c^2\cos^2\theta\sin^2\phi + c^2\sin^2\theta\sin^2\phi + b^2\cos^2\phi d\theta d\phi} \\ &= b\sin\phi\sqrt{c^2\sin^2\phi + b^2\cos^2\phi d\theta d\phi} \\ &= b\sin\phi\sqrt{c^2\sin^2\phi + b^2(1-\sin^2\phi)d\theta d\phi} \\ &= b\sin\phi\sqrt{(c^2-b^2)\sin^2\phi + b^2 d\theta d\phi} \end{aligned}$$

(b) The surface area:

$$
\begin{aligned}
A &= \int_0^{\pi}\int_{-\pi}^{\pi} b\sin\phi\sqrt{(c^2-b^2)\sin^2\phi+b^2}d\theta d\phi \\
&= 2\pi b\int_0^{\pi}\sin\phi\sqrt{(c^2-b^2)\sin^2\phi+b^2}\ d\phi \\
&= 2\pi b\left(\int_0^{\pi/2}\sin\phi\sqrt{(c^2-b^2)\sin^2\phi+b^2}\ d\phi+\int_{\pi/2}^{\pi}\sin\phi\sqrt{(c^2-b^2)\sin^2\phi+b^2}\ d\phi\right) \\
&= 2\pi b\left(\int_0^{\pi/2}\sin\phi\sqrt{(c^2-b^2)\sin^2\phi+b^2}\ d\phi\right. \\
&\qquad\left.+\int_0^{\pi/2}\sin(\phi+\pi/2)\sqrt{(c^2-b^2)\sin^2(\phi+\pi/2)+b^2}\ d\phi\right) \\
&= 2\pi b\left(\int_0^{\pi/2}\sin\phi\sqrt{(c^2-b^2)\sin^2\phi+b^2}+\cos\phi\sqrt{(c^2-b^2)\cos^2\phi+b^2}\ d\phi\right)
\end{aligned}
$$

Let $t=\sin^2\phi$, $d\phi=2\cos\phi\sin\phi dt=2\sqrt{t}\sqrt{1-t}d\theta$

$$
\begin{aligned}
A &= 2\pi b\left(\int_0^{\pi/2}\sin\phi\sqrt{(c^2-b^2)\sin^2\phi+b^2}+\cos\phi\sqrt{(c^2-b^2)\cos^2\phi+b^2}\ d\phi\right) \\
&= 2\pi b\left(\int_0^1\frac{1}{2\sqrt{t}\sqrt{1-t}}\sqrt{t}\sqrt{(c^2-b^2)t+b^2}+\frac{1}{2\sqrt{t}\sqrt{1-t}}\sqrt{1-t}\sqrt{(c^2-b^2)(1-t)+b^2}\ dt\right) \\
&= \pi b\left(\int_0^1\frac{1}{\sqrt{1-t}}\sqrt{(c^2-b^2)t+b^2}+\frac{1}{\sqrt{t}}\sqrt{(c^2-b^2)(1-t)+b^2}\ dt\right) \\
&= \pi b\left(b\int_0^1\frac{1}{\sqrt{1-t}}\sqrt{1+(\frac{c^2}{b^2}-1)t}+\frac{c}{\sqrt{t}}\sqrt{(1-\frac{b^2}{c^2})(1-t)+\frac{b^2}{c^2}}\ dt\right) \\
&= \pi b\left(b\int_0^1\frac{1}{\sqrt{1-t}}\sqrt{1+(\frac{c^2}{b^2}-1)t}+\frac{c}{\sqrt{t}}\sqrt{1-(1-\frac{b^2}{c^2})t}\ dt\right) \\
&= \pi b\left(b\int_0^1\frac{1}{\sqrt{1-t}}\sqrt{1-(1-\frac{c^2}{b^2})t}dt+c\int_0^1\frac{1}{\sqrt{t}}\sqrt{1-(1-\frac{b^2}{c^2})t}\ dt\right)
\end{aligned}
$$

The Euler form of the hypergeometric function is:

$$F(a,b;c;z)=\frac{\Gamma(c)}{\Gamma(b)\Gamma(c-b)}\int_0^1 x^{b-1}(1-x)^{c-b-1}(1-zx)^{-a}dx$$

The first integral is hypergeometric with

$$a_f=-1/2,\quad b_f=1,\quad c_f=3/2,\quad \text{and}\quad z_f=1-\frac{c^2}{b^2}$$

And the second with

$$a_{f2}=-1/2,\quad b_{f2}=1/2,\quad c_{f2}=3/2,\quad \text{and}\quad z_{f2}=1-\frac{b^2}{c^2}$$

Hence it can be written as

$$
\begin{aligned}
A &= 4\pi b \left(b\frac{\Gamma(1)\Gamma(1/2)}{\Gamma(3/2)} F\left(-1/2, 1, 3/2, 1 - \frac{c^2}{b^2}\right) + c\frac{\Gamma(1/2)\Gamma(1)}{\Gamma(3/2)} F\left(-1/2, 1/2, 3/2, 1 - \frac{b^2}{c^2}\right)\right) \\
&= \pi b \frac{\sqrt{\pi}}{\sqrt{\pi}/2} \left(bF\left(-1/2, 1, 3/2, 1 - \frac{c^2}{b^2}\right) + cF\left(-1/2, 1/2, 3/2, 1 - \frac{b^2}{c^2}\right)\right) \\
A &= 2\pi b \left(bF\left(-1/2, 1, 3/2, 1 - \frac{c^2}{b^2}\right) + cF\left(-1/2, 1/2, 3/2, 1 - \frac{b^2}{c^2}\right)\right)
\end{aligned}
$$

(c) Mean atomic surface density is the number of atoms divided by the surface area of the molecule. For a C_{70} fullerene the surface density is given by

$$\eta = \frac{70}{A}$$

This is solved numerically in the code, giving:

```
eta =

    0.1948
```

2. Minimising the surface area of the soap film.

(a) Parameterise the position on the surface as

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

$$
\begin{aligned}
\frac{\partial \mathbf{r}}{\partial u} &= (-r\sin u, r\cos u, 0) \\
\frac{\partial \mathbf{r}}{\partial z} &= (r'\cos u, r'\sin u, 1) \\
\frac{\partial \mathbf{r}}{\partial u} \times \frac{\partial \mathbf{r}}{\partial z} &= \left(r\cos u, r\sin u, -rr'\sin^2 u - rr'\cos^2 u\right) \\
&= r(\cos u, \sin u, -r')
\end{aligned}
$$

The delta surface area:

$$
\begin{aligned}
dA &= \left|\frac{\partial \mathbf{r}}{\partial u} \times \frac{\partial \mathbf{r}}{\partial z}\right| dudz \\
&= r\sqrt{\cos^2 u + \sin^2 u + r'^2} dudz \\
&= r\sqrt{1 + r'^2} dudz
\end{aligned}
$$

So the surface area, for $r_0 = 9$ and $r_1 = 10$, is:

$$
\begin{aligned}
S &= \int_{z_0}^{z_1} \int_{-\pi}^{\pi} r\sqrt{1 + r'^2} dudz \\
&= 2\pi \int_{z_0}^{z_1} r\sqrt{1 + r'^2} dz \\
\implies S &= 2\pi \int_{z_0}^{z_1} r\sqrt{1 + r'^2} dz = \int_{z_0}^{z_1} s(r, r') dz
\end{aligned}
$$

We want to minimise S, and so the E-L equation is (since it doesn't explicitly contain z):

$$\frac{\partial s}{\partial r} - \frac{d}{dz}\left(\frac{\partial s}{\partial r'}\right) = 0$$
$$H = r'\frac{\partial s}{\partial r'} - s = c$$

$$\begin{aligned}
r'\frac{rr'}{\sqrt{1+r'^2}} - r\sqrt{1+r'^2} &= c\\
rr'^2 - r - rr'^2 &= c\sqrt{1+r'^2}\\
-r &= c\sqrt{1+r'^2}\\
r^2 &= c(1+r'^2)\\
c^2r'^2 &= r^2 - c^2\\
r' &= \pm\frac{1}{c}\sqrt{r^2-c^2}
\end{aligned}$$

Separable DE:

$$\begin{aligned}
\int \frac{1}{\sqrt{r^2-c^2}}dr &= \pm\int\frac{1}{c}dz\\
\int \frac{1}{\sqrt{u^2-1}}du &= \pm\int\frac{1}{c}dz, \quad \left(u = \frac{r}{c}\right)
\end{aligned}$$

As in lectures, let $u = \cosh(v)$ and $du = \sinh(v)dv$

$$\begin{aligned}
\int \frac{\sinh v}{\sqrt{\cosh^2 v - 1}}du &= \pm\frac{1}{c}\int dz\\
\int \frac{\sinh v}{\sqrt{\sinh^2 v}}dv &= \pm\frac{1}{c}\int dz\\
\int 1dv &= \pm\frac{1}{c}\int dz\\
v &= \pm\frac{z}{c} + b\\
\text{arcosh}(\frac{r}{c}) &= \pm\frac{z}{c} + b\\
\frac{r}{c} &= \cosh\left(\pm\frac{z}{c}+b\right)\\
r &= c\cosh\left(\pm\frac{z}{c}+b\right)
\end{aligned}$$

Since cosh is even, and b is an arbitrary constant, the $\pm$ can be ignored.

$$r = c\cosh\left(\frac{z+b}{c}\right)$$

BCs:

$$r(0) = 9 = c\cosh\left(\frac{b}{c}\right)$$
$$r(1) = 10 = c\cosh\left(\frac{10+b}{c}\right)$$

Solving in matlab gives to 4sf:

$$b = -4.272, \quad c = 7.801$$

(b) Plotted in figure 1.

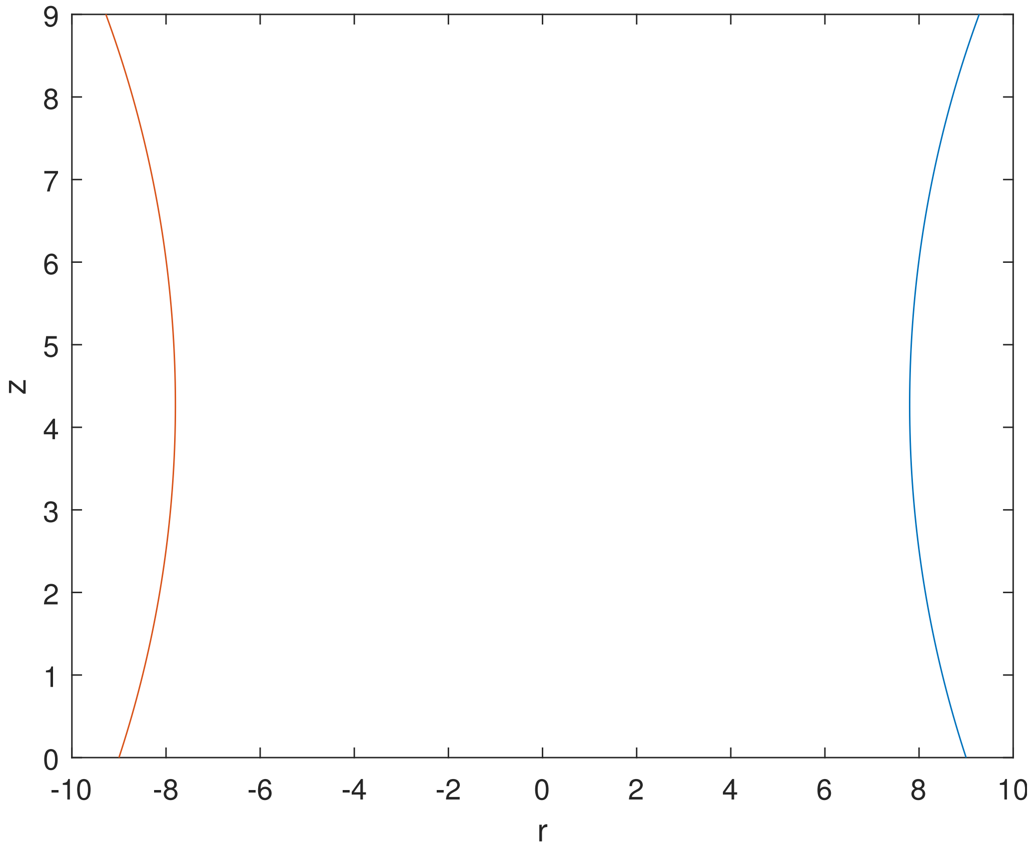


Figure 1: Profile of the soap film. Both the r and $-r$ profiles are shown.

3. Extremal calculation using Ritz' method

$$\begin{aligned}\bar{y} &= c_1\phi_1(x) + c_2\phi_2(x)\\ &= c_1(1-x^2) + c_2(1-x^4)\end{aligned}$$

$$\begin{aligned}\bar{y}' &= c_1\phi_1'(x) + c_2\phi_2'(x)\\ &= c_1(-2x) + c_2(-4x^3)\end{aligned}$$

$$\begin{aligned}\bar{y}^2 &= (c_1(1-x^2) + c_2(1-x^4))^2\\ &= c_1^2(1-2x^2+x^4) + 2c_1c_2(1-x^2)(1-x^4) + c_2^2(1-2x^4+x^8)\\ &= c_1^2(1-2x^2+x^4) + 2c_1c_2(1-x^2-x^4+x^6) + c_2^2(1-2x^4+x^8)\end{aligned}$$

$$\begin{aligned}\bar{y}'^2 &= (c_1(-2x) + c_2(-4x^3))^2 \\ &= 4c_1^2x^2 + 16c_1c_2x^4 + 16c_2x^6\end{aligned}$$

$$\begin{aligned}F\{\bar{y}\} &= \int_0^1 x(\bar{y}'^2 - \lambda\bar{y}^2)dx \\ &= \int_0^1 x((-2c_1x - 4c_2x^3)^2 - \lambda(c_1(1-x^2) + c_2(1-x^4)^2)dx \\ &= \int_0^1 x((2c_1x + 4c_2x^3)^2 - \lambda(c_1^2(1-x^2)^2 + 2c_1c_2(1-x^2)(1-x^4) + c_2^2(1-x^4)^2))dx \\ &= \int_0^1 x(4c_1^2x^2 + 16c_1c_2x^4 + 16c_2^2x^6 \\ &- \lambda(c_1^2(1-2x^2+x^4) + 2c_1c_2(1-x^2-x^4+x^6) + c_2^2(1-2x^4+x^8)))dx \\ &= \int_0^1 4c_1^2x^3 + 16c_1c_2x^5 + 16c_2^2x^7 \\ &- \lambda(c_1^2(x-2x^3+x^5) + 2c_1c_2(1-x^3-x^5+x^7) + c_2^2(x-2x^5+x^9))dx \\ &= \Big[c_1^2x^4 + \frac{16}{6}c_1c_2x^6 + 2c_2^2x^8 \\ &-\lambda(c_1^2(\frac{1}{2}x^2 - \frac{1}{2}x^4 + \frac{1}{6}x^6) + 2c_1c_2(\frac{1}{2}x^2 - \frac{1}{4}x^4 - \frac{1}{6}x^6 + \frac{1}{8}x^8) + c_2^2(\frac{1}{2}x^2 - \frac{1}{3}x^6 + \frac{1}{10}x^{10}))\Big]_0^1\end{aligned}$$

$$\begin{aligned}F\{\bar{y}\} &= c_1^2 + \frac{16}{6}c_1c_2 + 2c_2^2 - \lambda(c_1^2(\frac{1}{2} - \frac{1}{2} + \frac{1}{6}) + 2c_1c_2(\frac{1}{2} - \frac{1}{4} - \frac{1}{6} + \frac{1}{8}) + c_2^2(\frac{1}{2} - \frac{1}{3} + \frac{1}{10})) \\ F &= {c_1}^2 + \frac{8c_1c_2}{3} + 2{c_2}^2 - \lambda\left(\frac{{c_1}^2}{6} + \frac{5c_1c_2}{12} + \frac{4{c_2}^2}{15}\right) \\ &= c_1^2\left(1 - \frac{\lambda}{6}\right) + c_1c_2\left(\frac{8}{3} - \frac{5\lambda}{12}\right) + c_2^2\left(2 - \frac{4\lambda}{15}\right)\end{aligned}$$

$$\begin{aligned}\frac{\partial F}{\partial c_1} &= 2c_1\left(1 - \frac{\lambda}{6}\right) + c_2\left(\frac{8}{3} - \frac{5\lambda}{12}\right) = 0 \\ \frac{\partial F}{\partial c_2} &= c_1\left(\frac{8}{3} - \frac{5\lambda}{12}\right) + 2c_2\left(2 - \frac{4\lambda}{15}\right) = 0\end{aligned}$$

Linear system in (c_1, c_2). Non trivial solutions if the determinant is zero, i.e.

$$\begin{vmatrix} 2\left(1-\frac{\lambda}{6}\right) & \left(\frac{8}{3} - \frac{5\lambda}{12}\right) \\ \left(\frac{8}{3} - \frac{5\lambda}{12}\right) & 2\left(2 - \frac{4\lambda}{15}\right)\end{vmatrix} = 0$$

$$\begin{aligned}2\left(1 - \frac{\lambda}{6}\right)2\left(2 - \frac{4\lambda}{15}\right) - \left(\frac{8}{3} - \frac{5\lambda}{12}\right)\left(\frac{8}{3} - \frac{5\lambda}{12}\right) &= 0 \\ \lambda^2/240 - (8\lambda)/45 + 8/9 &= 0 \\ \lambda &= \frac{\frac{8}{45} \pm \sqrt{\frac{64}{2025} - \frac{4*8}{240*9}}}{\frac{2}{240}}\end{aligned}$$

The smallest lambda has value (to 4 sf):

$$\lambda_{-} = 5.784$$

I verify this arithmetic in the code.

Code

```
%Q1c
b = 3.59
c = 4.17
a1 = b* hypergeom([-1/2,1],3/2,1 - c^2/b^2);
a2 = c* hypergeom([-1/2,1/2],3/2,1 - b^2/c^2);
A = 2*pi*b * gamma(1)*gamma(1/2)/gamma(3/2) * (a1 + a2)
eta = 70./A
%%
%Q2
%solve the BCs symbolically
syms r(z) c b
r(z) = c*cosh((z + b)/c);
cond = [r(0) == 9; r(10) == 10];
sol = solve(cond);
%only labelling these so that they print out
B = sol.b
C = sol.c

r(z) = subs(r,b,sol.b);
r(z) = subs(r,c,sol.c);


rfunc = matlabFunction(r);
z = linspace(0,10);
close all
plot(rfunc(z),z);
hold on
plot(-rfunc(z),z);
%plot3()
axis([-10,10,0,9])
xlabel("r")
ylabel("z")
saveas(gcf,'A4Plot.ep','epsc')
%%
%q3 verification
syms lambda
mat = [2*(1-lambda/6), 8/3 - 5*lambda/12 ; 8/3 - 5*lambda/12 ,
    2*(2-4*lambda/15)]
lambda = double(solve(det(mat)==0))
```

School of Mathematical Sciences

APP MTH 3022/7106 - Optimal Functions and Nanomechanics

Assignment 4 question sheet

Due: Thursday, 10 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.

1. A spheroidal surface $\mathcal{P}$ is given parametrically by the position vector $\boldsymbol{r}(\theta, \phi)$ as

$$\boldsymbol{r}(\theta, \phi) = (b\cos\theta\sin\phi, b\sin\theta\sin\phi, c\cos\phi),$$

where $-\pi < \theta \leqslant \pi$, and $0 \leqslant \phi \leqslant \pi$ and the constant b is the minor semi-axis length and c is the major semi-axis length.

   (a) Derive an expression for the scalar surface element $\mathrm{d}A$ for $\mathcal{P}$.

   (b) Integrate your answer from part (a) to find the surface area of $\mathcal{P}$ as a function of b and c.
   Hint: it is easiest to express this in terms of the usual hypergeometric function.

   (c) One isomer of the C_{70} fullerene may be modelled as a spheroid with a minor semi-axis length of $b = 3.59$ Å and major semi-axis length of $c = 4.17$ Å. Use your answer from part (b) to derive a reasonable approximation (to four decimal places) of the mean surface density of carbon atoms for this molecule.

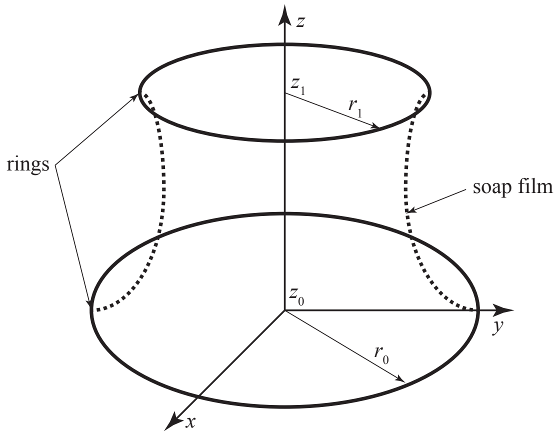
[8 marks]

2. Consider a soap film suspended between two parallel concentric, but displaced rings of radius r_0 and r_1 at an offset in the z-direction of z_0 and z_1 (see the figure for a clearer view). Ignoring gravity and other external forces, the shape of the soap film will minimise the surface area.

   (a) Use the Calculus of Variations to determine the profile that the soap film will adopt.

   (b) Plot the resulting profile for $(z_0, r_0) = (0, 9)$ and $(z_1, r_1) = (10, 10)$.

[8 marks]



3. Consider the problem of finding the extremal of the functional

$$F\{y\} = \int_0^1 x(y'^2 - \lambda y^2)\, dx,$$

subject to $y(0)$ being finite and $y(1) = 0$. Assuming that the extremal will be an even function of x, we may choose as basis functions

$$\phi_n(x) = 1 - x^{2n},$$

and propose an approximate series solution of the form

$$y(x) \approx \bar{y}(x) = c_1\phi_1(x) + c_2\phi_2(x) + \cdots .$$

Use Ritz's method with $\bar{y}(x) = c_1\phi_1(x) + c_2\phi_2(x)$, to derive a constraint on λ that must be satisfied for a non-trivial solution to exist. Give the numerical value (to four significant digits) of the smallest λ that satisfies the constraint.

[8 marks]