THE UNIVERSITY of ADELAIDE

Examination in School of Mathematical Sciences

Semester 2, 2018

107352 APP MTH 3022 Optimal Functions and Nanomechanics III

Official Reading Time:	10 mins
Writing Time:	120 mins
Total Duration:	130 mins

NUMBER OF QUESTIONS: 5 TOTAL MARKS: 60

Instructions

- Attempt all questions.
- Begin each answer on a new page.
- Examination materials must not be removed from the examination room.

Materials

- 1 Blue book is provided.
- Formulae sheets are provided at the end.
- Only scientific calculators with basic capabilities are permitted. Graphics calculators are not permitted.

DO NOT COMMENCE WRITING UNTIL INSTRUCTED TO DO SO.

1. (a) Find the extremals of the functional

$$F\{y(x)\} = \int_{-1}^{0} \left(12xy - y'^2\right) dx,$$

with fixed end-points $y(-1) = 1$ and $y(0) = 0$.

(b) Find the extremals of the functional

$$G\{y(x), z(x)\} = \int_{0}^{\pi/2} (y'^2 + z'^2 + 2yz)\, dx,$$

subject to the boundary conditions

$$y(0) = 0, \quad y(\pi/2) = 1, \quad z(0) = 0, \quad z(\pi/2) = 1.$$

(c) Consider the functional

$$H\{y(x)\} = \int_{0}^{1} \left(x^2 yy' + xy^2\right)\, dx,$$

with fixed end-points $y(0) = 0$, $y(1) = 1$. What are the extrema for this functional? What value does $H\{y\}$ take for these extrema?

[16 marks]

2. (a) Using the definitions from the formula sheet provided, find an expression for the Complete elliptic integral of the second kind $E(k)$, in terms of hypergeometric functions.

(b) Consider an atom located at $P = (0, 0, \delta)$ on the z-axis and a circular ring molecule lying in the xy-plane, centred at the origin with radius r, and with uniform atomic line density η.

(i) Using the Lennard–Jones potential, write down an expression for the total van der Waals interaction between the atom at P and the ring molecule.

(ii) Evaluate the integral analytically to find a closed form expression for the interaction energy.

[12 marks]

3. Use the Calculus of Variations with an appropriate transversality condition to find the shortest distance in the plane from the point $A = (-1, 5)$ to the parabola $x = y^2$.

Hint: The cubic: $z^3 + 6z + 20$, has roots $z = -2, 1 \pm 3i$.

[10 marks]

Please turn over for page 3

4. Consider the problem of finding extremals of the functional

$$J\{x, y\} = \int_{t_0}^{t_1} (x\dot{y} - \dot{x}y)\, dt,$$

where x and y are functions of the independent variable t, and dots denote differentiation with respect to t. The extremals are subject to the fix end-point constraints

$$x(t_0) = x_0, \quad y(t_0) = y_0, \quad x(t_1) = x_1, \quad y(t_1) = y_1,$$

and the isoperimetric constraint

$$K\{x, y\} = \int_{t_0}^{t_1} \sqrt{\dot{x}^2 + \dot{y}^2}\, dt = L.$$

(a) Formulate a new functional that incorporates the isoperimetric constraint.

(b) Write the Euler-Lagrange equations that apply for this new functional.

(c) By solving the Euler–Lagrange equations, find a solution in the form $\phi(x, y) = 0$.

(d) If $x(t)$ and $y(t)$ denote the (x, y)-coordinates of a particle P at time t, what shape are the trajectories of P?

(e) Now assuming that x_1 and y_1 are not specified, derive the natural boundary conditions that would be used in place of the fixed end-point conditions at $t = t_1$.

[12 marks]

5. Consider a surface $\mathcal{S}$ in $\mathbb{R}^3$ parameterised by $\boldsymbol{x} = (X(u, v), Y(u, v), Z(u, v))$. The problem of determining curves of shortest distance lying in $\mathcal{S}$ is equivalent to finding extremals of the functional

$$L = \int ds = \int \sqrt{dx^2 + dy^2 + dz^2}.$$

(a) Show that this functional can be expressed in the form

$$L\{v(u)\} = \int_{u_0}^{u_1} f(u, v, v')\, du.$$

Using the chain rule, express $f(u, v, v')$ for this formulation in terms of u, v, v' and partial derivatives of $X(u, v)$, $Y(u, v)$, and $Z(u, v)$.

(b) Determine the Euler–Lagrange equation for your answer to part (a).
Do not attempt to solve this Euler–Lagrange equation.

(c) Assuming the specific surface $\mathcal{S}$, given by

$$\boldsymbol{x} = (\cosh u \cos v, \cosh u \sin v, \sinh u),$$

determine the Euler-Lagrange equation that applies for this choice of $\mathcal{S}$.
Do not attempt to solve this Euler–Lagrange equation.

[10 marks]

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Formula Sheet, Special Functions

Gamma function, definition	$\Gamma(z) = \int_0^\infty t^{z-1} e^{-t}\, dt, \quad \text{for } \Re(z) > 0.$
Gamma function, duplication	$\Gamma(2z) = 2^{2z-1}\pi^{-1/2}\Gamma(z)\Gamma(z+1/2).$
Beta function, definition	$B(x,y) = \int_0^1 t^{x-1}(1-t)^{y-1}\, dt, \quad \text{for } \Re(x), \Re(y) > 0.$
Beta function, gamma relation	$B(x,y) = \dfrac{\Gamma(x)\Gamma(y)}{\Gamma(x+y)}.$
Pochhammer symbol, definition	$(a)_n = a(a+1)(a+2)\cdots(a+n-1) = \dfrac{\Gamma(a+n)}{\Gamma(a)}.$
Hypergeometric function, series	$F(a,b;c;z) = \sum_{n=0}^{\infty} \dfrac{(a)_n (b)_n}{(c)_n n!} z^n.$
Hypergeometric function, integral	$F(a,b;c;z) = \dfrac{\Gamma(c)}{\Gamma(b)\Gamma(c-b)} \times \int_0^1 t^{b-1}(1-t)^{c-b-1}(1-tz)^{-a}\, dt.$
Hypergeometric function, derivative	$\dfrac{d^n}{dz^n} F(a,b;c;z) = \dfrac{(a)_n (b)_n}{(c)_n} F(a+n, b+n; c+n; z).$
Elliptic integral, first kind	$F(\varphi, k) = \int_0^\varphi \dfrac{d\vartheta}{\sqrt{1-k^2\sin^2\vartheta}}.$
Elliptic integral, second kind	$E(\varphi, k) = \int_0^\varphi \sqrt{1-k^2\sin^2\vartheta}\, d\vartheta.$
Complete elliptic integrals	$K(k) = F\left(\dfrac{\pi}{2}, k\right), \quad E(k) = E\left(\dfrac{\pi}{2}, k\right).$
Lennard-Jones potential	$\Phi(\rho) = -\dfrac{A}{\rho^6} + \dfrac{B}{\rho^{12}}.$

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Formula Sheet, Variational

Theorem 2.2.1: Let $F : C^2[x_0, x_1] \to \mathbb{R}$ be a functional of the form

$$F\{y\} = \int_{x_0}^{x_1} f(x, y, y')\, dx,$$

where f has continuous partial derivatives of second order with respect to x, y, and y', and $x_0 < x_1$. Let

$$S = \{y \in C^2[x_0, x_1] \mid y(x_0) = y_0, y(x_1) = y_1\},$$

where y_0 and y_1 are real numbers. If $y \in S$ is an extremal for F, then for all $x \in [x_0, x_1]$

$$\boxed{\frac{d}{dx}\left(\frac{\partial f}{\partial y'}\right) - \frac{\partial f}{\partial y} = 0} \qquad \text{The Euler–Lagrange equation}$$

Theorem 2.3.1: Let J be a functional of the form

$$J\{y\} = \int_{x_1}^{x_2} f(y, y')dx$$

and define the function

$$H(y, y') = y'\frac{\partial f}{\partial y'} - f(y, y').$$

Then H is constant along any extremal of y.

Generalisation: Let $F : C^2[x_0, x_1] \to \mathbb{R}$ be a functional of the form

$$F\{y\} = \int_{x_0}^{x_1} f(x, y, y', \ldots, y^{(n)})\, dx,$$

where f has continuous partial derivatives of second order with respect to $x, y, y', \ldots, y^{(n)}$, and $x_0 < x_1$, and the values of $y, y', \ldots, y^{(n-1)}$ are fixed at the end-points, then the extremals satisfy the condition

$$\frac{\partial f}{\partial y} - \frac{d}{dx}\frac{\partial f}{\partial y'} + \frac{d^2}{dx^2}\frac{\partial f}{\partial y''} + \cdots + (-1)^n \frac{d^n}{dx^n}\frac{\partial f}{\partial y^{(n)}} = 0.$$

Natural boundary condition: When we extend the theory to allow a free x and y, we find the additional constraint

$$\Big[p\,\delta y - H\,\delta x\Big]_{x_0}^{x_1} = 0,$$

where $p = f_{y'}$ and $H = y'f_{y'} - f$.

Weierstrass–Erdman corner conditions: For a broken extremal

$$p\Big|_{x^{\star-}} = p\Big|_{x^{\star+}}, \quad H\Big|_{x^{\star-}} = H\Big|_{x^{\star+}},$$

must hold at any "corner".