L-Università ta' Malta

Department of Chemistry
Faculty of Science

B.Sc. (Hons.) Year I

Sample Examination Paper I

CHE1215: Methods of Chemical Calculations — *n*th June 20XX, 08:30–11:35

Instructions

Read the following instructions carefully.

- Attempt only **TEN** questions.
- Each question carries **10** marks. The maximum mark is **100**.
- A list of mathematical formulae is provided on page 2.
- Only the use of non-programmable calculators is allowed.

MATHEMATICAL FORMULÆ

ALGEBRA

Factors

$$a^3 + b^3 = (a+b)(a^2 - ab + b^2)$$
$$a^3 - b^3 = (a-b)(a^2 + ab + b^2)$$

Quadratics

If $ax^2 + bx + c$ has roots α and β,

$$\Delta = b^2 - 4ac$$
$$\alpha + \beta = -\tfrac{b}{a} \qquad \alpha\beta = \tfrac{c}{a}$$

Finite Series

$$\sum_{k=1}^{n} 1 = n \qquad \sum_{k=1}^{n} k = \frac{n(n+1)}{2}$$
$$\sum_{k=1}^{n} k^2 = \frac{k(k+1)(2k+1)}{6}$$
$$(1+x)^n = \sum_{k=0}^{n} \binom{n}{k} x^n$$
$$= 1 + nx + \tfrac{n(n-1)}{2\cdot 1} x^2 + \cdots + x^n$$

GEOMETRY & TRIGONOMETRY

Distance Formula

If $A = (x_1, y_1)$ and $B = (x_2, y_2)$,

$$d(A,B) = \sqrt{(x_1 - x_2)^2 + (y_1 - y_2)^2}$$
$$= \sqrt{\Delta x^2 + \Delta y^2}$$

Pythagorean Identity

$$\cos^2\theta + \sin^2\theta = 1$$

General Solutions

$$\cos\theta = \cos\alpha \iff \theta = \pm\alpha + 2\pi\mathbb{Z}$$
$$\sin\theta = \sin\alpha \iff \theta = (-1)^n\alpha + \pi n,\ n \in \mathbb{Z}$$
$$\tan\theta = \tan\alpha \iff \theta = \alpha + \pi\mathbb{Z}$$

CALCULUS

Derivatives

$f(x)$	$f'(x)$
x^n	nx^{n-1}
$\sin x$	$\cos x$
$\cos x$	$-\sin x$
$\tan x$	$\sec^2 x$
$\cot x$	$-\operatorname{cosec}^2 x$
$\sec x$	$\sec x \tan x$
$\operatorname{cosec} x$	$-\operatorname{cosec} x \cot x$
e^x	e^x
$\log x$	$1/x$
uv	$u'v + uv'$
u/v	$(u'v - uv')/v^2$

Integrals

$f(x)$	$\int f(x)\,dx$
$x^n\ (n \neq -1)$	$\frac{x^{n+1}}{n+1}$
$\sin x$	$-\cos x$
$\cos x$	$\sin x$
$\tan x$	$\log(\sec x)$
$\cot x$	$\log(\sin x)$
$\sec x$	$\log(\sec x + \tan x)$
$\operatorname{cosec} x$	$\log(\tan \frac{x}{2})$
e^x	e^x
$1/x$	$\log x$
$\frac{1}{a^2+x^2}$	$\frac{1}{a}\tan^{-1}\left(\frac{x}{a}\right)$
$\frac{x}{\sqrt{a^2+x^2}}$	$\sin^{-1}\left(\frac{x}{a}\right)$

Homogeneous Linear Second Order ODEs

If the roots of $ak^2 + bk + c$ are k_1 and k_2, then the differential equation $ay'' + by' + cy = 0$ has general solution

$$y(x) = \begin{cases} c_1 e^{k_1 x} + c_2 e^{k_2 x} & \text{if } k_1 \neq k_2 \\ c_1 e^{kx} + c_2 x e^{kx} & \text{if } k = k_1 = k_2 \\ e^{\alpha x}(c_1 \cos\beta x + c_2 \sin\beta x) & \text{if } k = \alpha \pm \beta i \in \mathbb{C} \end{cases}$$

Infinite Series

$$e^x = \sum_{n=0}^{\infty} \frac{x^n}{n!} = 1 + x + \frac{x^2}{2} + \frac{x^3}{3!} + \frac{x^4}{4!} \cdots$$
$$\cos x = \sum_{\substack{n=0 \\ n \text{ even}}}^{\infty} \frac{(-1)^{\frac{n}{2}}}{n!} x^n = 1 - \frac{x^2}{2} + \frac{x^4}{4!} - \cdots$$
$$\sin x = \sum_{\substack{n=1 \\ n \text{ odd}}}^{\infty} \frac{(-1)^{\frac{n-1}{2}}}{n!} x^n = x - \frac{x^3}{3!} + \frac{x^5}{5!} - \cdots$$
$$\log(1+x) = \sum_{n=1}^{\infty} \frac{(-1)^{n+1}}{n} x^n = x - \frac{x^2}{2} + \frac{x^2}{3} - \cdots, \quad x \in (-1, 1]$$

⚠ Attempt only **TEN** questions.

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1. (a) Given that $\log x = 4$, $\log y = 2$ and $\log z = 5$, evaluate the following.

(i) $\log xyz$ (ii) $\log \frac{x}{zy}$ (iii) $4\log y\sqrt{x}$

(iv) $\log 4x - \log 3y$ (v) $(\log xy)^x$ (vi) $\log_x z$

(b) Solve for x:

$$4^x \times 3^{7-x} = 6^{2x-2} \times 2^{x-1}.$$

[6, 4 marks]

2. Consider the curve given by the equation

$$y = \frac{7e^{-x}}{4x^2+3}.$$

(a) Determine the coordinates of stationary points on the curve.

(b) Determine the nature of the stationary points, given that at their coordinates, we have $2x\frac{d^2y}{dx^2} + y\sin(\pi x) = 0$.

(c) Sketch the curve, labelling any turning points and intercepts with the x- and y-axes.

[4, 3, 3 marks]

3. (a) Consider the complex numbers

$$z_1 = 1 + i \qquad \text{and} \qquad z_2 = 3 + z_1^*.$$

Determine:

(i) $z_1 z_2$ (ii) z_1/z_2 (iii) $|z_1 + z_2|$

(b) Let ω be the complex number given by

$$4\omega = 1 + \sqrt{5} + \sqrt{10 - 2\sqrt{5}}\,i.$$

Given that $|\omega| = 1$ and $\arg\omega = \frac{\pi}{5}$, what is the value of ω^5?

[6, 4 marks]

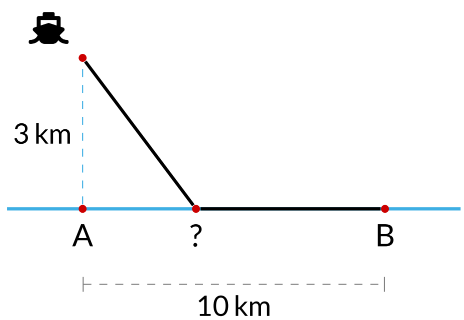
4. (a) Solve the equation $\operatorname{cosec}(2x) = 2$ for all x in the range $-\pi \leqslant x \leqslant \pi$.

(b) Show that the solutions to the equation $2\cos^2(2x) - 3\sin(2x) = 0$ are the same as the solutions to the equation in part (a).

(c) Sketch the curve $y = \sin 2x$ in the range $-\pi \leqslant x \leqslant \pi$, and indicate on it the solutions to the equations in (a) and (b).

[4, 3, 3 marks]

5. A man rows 3 km out to sea from a starting point A. He wishes to get to a point B as fast as possible, 10 km away from A down the coast.



He can row 4 km an hour and run 5 km an hour. Assuming the coast is straight, how far from A should he land?

[10 marks]

6. The function f is defined by

$$f(x, y, z) = x^2y^3 + 2xy^2z^2 + 5x^4z.$$

(a) Find the partial derivatives $\frac{\partial f}{\partial x}$, $\frac{\partial f}{\partial y}$ $\frac{\partial f}{\partial z}$, $\frac{\partial^2 f}{\partial x \partial y}$ and $\frac{\partial^2 f}{\partial z^2}$.

(b) Find the total differential df.

(c) Use the total differential to show that, for inputs close to the point $(1, 2, -1)$, we have the approximation

$$f(x, y, z) \approx 4x + 20y - 11z - 44.$$

[5, 2, 3 marks]

7. (a) Find the derivatives of the following functions.

(i) $\sqrt{x}(\log 2x)^2$ (ii) $\log\left(\frac{\sqrt[3]{2x-1}}{x^{2/5}\sqrt{x-1}}\right)$ (iii) $\frac{x}{\sqrt{1+\cos^2 x}}$

(b) Verify that the function $y = \sqrt{x}e^{x^2}$ is a solution to the differential equation

$$4x^2\frac{d^2y}{dx^2} - 8x\frac{dy}{dx} + (5-16x^4)y = 0.$$

[6, 4 marks]

8. Determine the following integrals.

(a) $\int_1^2 \frac{\sqrt{x}(x+1)}{\sqrt[3]{x}}\,dx$ (b) $\int \sec^2(2x-1)\,dx$

(c) $\int \frac{x}{(x^2+1)(x+1)}\,dx$ (d) $\int_0^2 \frac{3x+1}{(x^2+3x+4)(x+3)}\,dx$

[2, 1, 3, 4 marks]

9. (a) Solve the equations:

(i) $x^2+4=15x$ (ii) $x^3+4=15x$

(b) Sketch the graph $y = x^3-15x+4$, and find the area bounded by the the curve, the x-axis and its two leftmost x-intercepts.

[5, 5 marks]

10. Solve the differential equation

$$(x^2+x-2)\frac{dy}{dx} = 3e^y,$$

given that $y=0$ when $x=0$. Give your solution in the form

$$y(x) = -\log\left(a+\log\left(\frac{2+x}{b(1-x)}\right)\right),$$

where a and b are constants. **[10 marks]**

11. Solve the differential equation

$$9\frac{d^2y}{dx^2} - 12\frac{dy}{dx} + 4y = 8x - 5e^{-x},$$

given that when $x = 0$, $y = \frac{14}{5}$ and $\frac{dy}{dx} = \frac{11}{5}$.

[*Hint*: When finding the particular integral, use $\mu x + \lambda + \eta e^{-x}$ as a trial solution.]

[10 marks]

12. Consider the quadratic expression $g(x) = 4x^2 + 4x - 15$.

(a) Express $g(x)$ in the form $a(x-p)^2 + q$ for appropriate values of a, p and q.

(b) Hence, sketch the graph of $y = g(x)$, clearly labelling any turning points and intercepts with the coordinate axes.

(c) Sketch on the same set of axes, the line $y = 8x - 7$, and label their points of intersection.

[3, 4, 3 marks]

13. Consider the matrix $\mathbf{A} = \begin{pmatrix} -1 & 3 \\ -2 & 7 \end{pmatrix}$.

(a) Find the matrix **B** such that **AB** = **I**. What is **B** called?

(b) Use part (a) to solve the simultaneous equations

$$\begin{cases} -x + 3y = 1 \\ -2x + 7y = 3. \end{cases}$$

(c) The matrix **C** represents a reflection in $y = -x$. Write down the matrix **C**, and say what $\mathbf{C}^8$ will be by reasoning geometrically.

[4, 3, 3 marks]

14. (a) Sketch the following graphs, labelling any x- and y-intercepts.

(i) $y = 3\log(x-2)$ (ii) $y = 2e^{-x}+1$ (iii) $y = \dfrac{x+1}{x+2}$

(b) A certain strain of E-coli bacteria doubles in number 30 minutes. If there are 100 E-coli bacteria that are allowed to grow under ideal conditions, how long will it take to reach 1 million bacteria?

[6, 4 marks]

15. (a) The rate law of the reaction A $\longrightarrow$ P following first order kinetics with respect to $[A]$ is given by

$$-\frac{d[A]}{dt} = k[A],$$

where $[A]$ is the concentration of A at time t after the commencement of the reaction, and k is the rate constant. If at $t = 0$, $[A] = [A]_0$, show that

$$[A] = [A]_0 \exp(-kt).$$

(b) The Schrödinger equation for a particle inside a one-dimensional box is given by

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} = E\psi,$$

where $\hbar$, m and E have their usual meaning and can be treated as constants for this question. Show that this has general solution

$$\psi(x) = c_1 \cos\left(\sqrt{\frac{2mE}{\hbar^2}}\,x\right) + c_2 \sin\left(\sqrt{\frac{2mE}{\hbar^2}}\,x\right).$$

[5, 5 marks]

Solutions

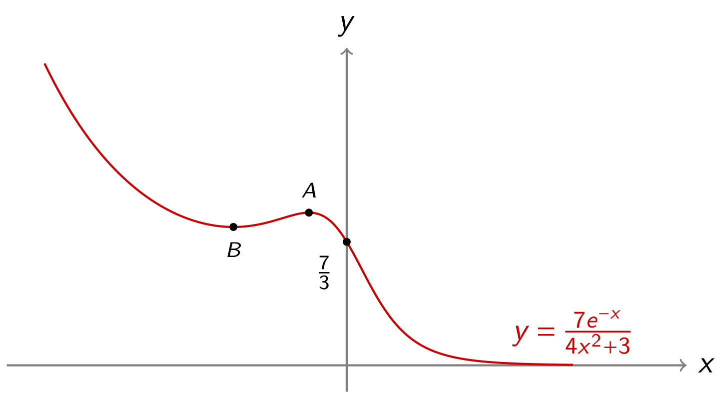
1. (a) (i) 11 (ii) -3 (iii) 16 (iv) $2+\log\frac{4}{3}$ (v) 6^{e^4} (vi) $\frac{5}{4}$

   (b) $x = 3$

2. (a) $A = \left(-\frac{1}{2}, \frac{7}{4}\sqrt{e}\right)$ and $B = \left(-\frac{3}{2}, \frac{7}{12}e^{3/2}\right)$

   (b) Instead of working out y'' (which involves a lot of working), the given fact allows us to deduce that when $x = -\frac{1}{2}$, $\frac{d^2y}{dx^2} = -\frac{7}{4}\sqrt{e} < 0$, and when $x = -\frac{3}{2}$, $\frac{d^2y}{dx^2} = \frac{7}{36}e^{3/2} > 0$. Thus by the second derivative test, A is a max, and B is a min.

   (c) Remember to find x- and y-intercepts, and to see what happens as $x \to \pm\infty$, they will help you with the sketch.



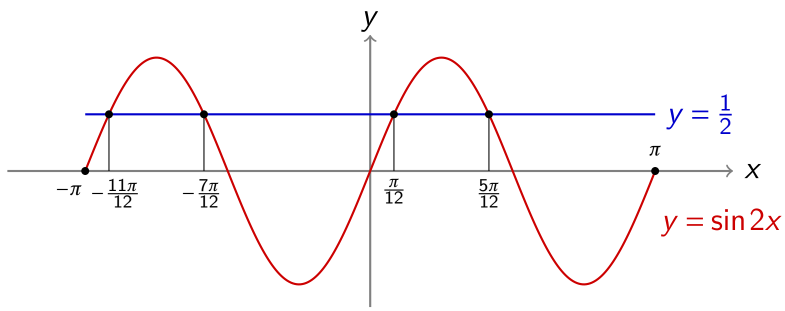
3. (a) (i) $5+3i$ (ii) $\frac{3}{17}+\frac{5}{17}i$ (iii) 5

   (b) Since we know $|\omega|$ and $\arg\omega$, then $\omega = e^{i\pi/5}$, and we don't need to use the given complicated form for ω. Then $(e^{i\pi/5})^5 = e^{i\frac{\pi}{5}\cdot 5} = e^{i\pi} = \cos(\pi) + i\sin(\pi) = -1$.

4. (a) $x = -\frac{11\pi}{12}, -\frac{7\pi}{12}, \frac{\pi}{12}, \frac{5\pi}{12}$

   (b) By using the Pythagorean identity $\cos^2(2x) + \sin^2(2x) = 1$, we can replace the term $\cos^2 2x$ in the given equation to get the quadratic $(\sin 2x + 2)(2\sin 2x - 1) = 0$. The first factor corresponds to the equation $\sin 2x = -2$, which is impossible; thus any solutions must come from the second factor, which corresponds to $\sin 2x = \frac{1}{2}$. This is the same as the equation from (a).

(c) Sketch:



5. Assuming he lands x km away from A, the time he takes to arrive at B is $T(x)=\frac{1}{4}\sqrt{9+x^2}+\frac{1}{5}(10-x)$. By differentiation, this is minimised when $T'(x)=0$, which has solution $x=4$, i.e., he should land 4 km from A.

6. (a) $\frac{\partial f}{\partial x}=20x^3z+2xy^3+2y^2z^2$ $\quad$ $\frac{\partial f}{\partial y}=3x^2y^2+4xyz^2$

$\frac{\partial f}{\partial z}=5x^4+4xy^2z$ $\quad$ $\frac{\partial^2 f}{\partial x\partial y}=6xy^2+4yz^2$

$\frac{\partial^2 f}{\partial z^2}=4xy^2$

(b) $df=\frac{\partial f}{\partial x}dx+\frac{\partial f}{\partial y}dy+\frac{\partial f}{\partial z}dz$
$=(20x^3z+2xy^3+2y^2z^2)\,dx+(3x^2y^2+4xyz^2)\,dy+(5x^4+4xy^2z)\,dz$

(c) Near $(1,2,-1)$,

$$\begin{aligned} f(x,y,z) &\approx f(1,2,-1)+df(1,2,-1)\\ &=11+4dx+20dy-11dz\\ &=11+4(x-1)+20(y-2)-11(z+1)\\ &=4x+20y-11z-44 \end{aligned}$$

7. (a) (i) $\frac{\log(2x)}{2\sqrt{x}}(4+\log(2x))$ $\quad$ (ii) $\frac{2}{3(2x-1)}-\frac{2}{5x}-\frac{1}{2(x-1)}$

(iii) $\frac{\cos^2 x+x\cos x\sin x+1}{(1+\cos^2 x)^{3/2}}$

(b) $y=\sqrt{x}e^{x^2}$

$\frac{dy}{dx}=\frac{e^{x^2}}{2\sqrt{x}}(4x^2+1)$ $\quad$ $\frac{d^2y}{dx^2}=\frac{e^{x^2}}{4x^{3/2}}(16x^4+16x^2-1)$,

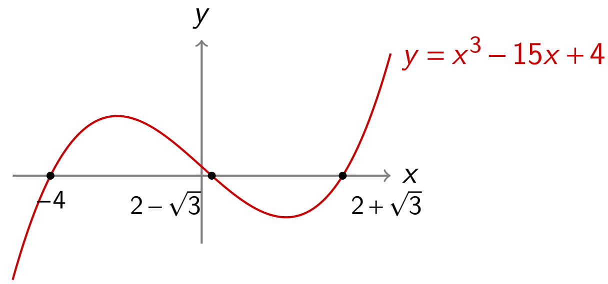
plug them into the LHS and it should simplify to zero.

8. (a) $\frac{12}{91}(27\sqrt[6]{2}-10)$ (b) $\frac{1}{2}\tan(2x-1)+c$

(c) $\frac{1}{2}\tan^{-1}x+\log\left(\frac{\sqrt[4]{1+x^2}}{\sqrt{1+x}}\right)+c$ (d) $\log\left(\frac{63}{50}\right)$

9. (a) (i) $x=\frac{1}{2}(15\pm\sqrt{209})$ (ii) $x=-4, 2\pm\sqrt{3}$

(b)



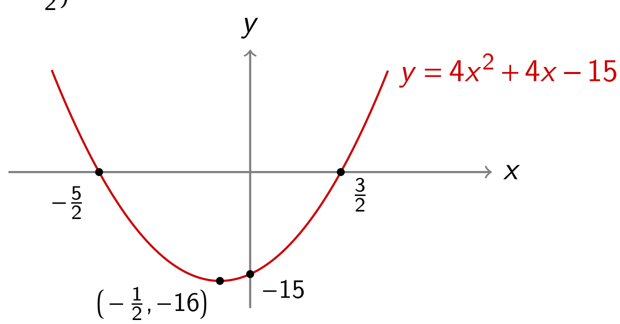
$$\text{Area}=\int_{-4}^{2-\sqrt{3}}(x^3-15x+4)\,dx=\frac{207}{4}+12\sqrt{3}.$$

10. $a=1$, $b=2$.

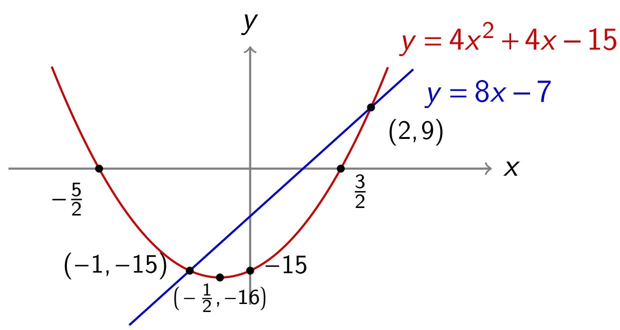
11. $y(x)=2(x+3)+2e^{2x/3}(2x-3)-\frac{1}{5}e^{-x}$.

12. (a) $g(x)=4\left(x+\frac{1}{2}\right)^2-16$

(b)



(c)



13. (a) $\mathbf{B} = \begin{pmatrix} -7 & 3 \\ -2 & 1 \end{pmatrix}$. **B** is the **inverse** of **A**.

(b) The system is $\mathbf{A}\boldsymbol{x} = \boldsymbol{b}$, where $\boldsymbol{x} = (x, y)$ and $\boldsymbol{b} = (1, 3)$.

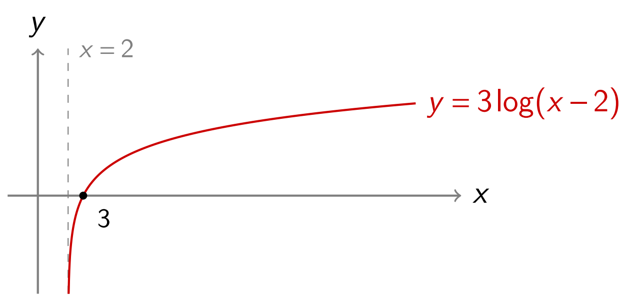
Thus $\boldsymbol{x} = \mathbf{A}^{-1}\boldsymbol{b} = \mathbf{B}\boldsymbol{b} = \begin{pmatrix} -7 & 3 \\ -2 & 1 \end{pmatrix}\begin{pmatrix} 1 \\ 3 \end{pmatrix} = \begin{pmatrix} 2 \\ 1 \end{pmatrix}$,

i.e., $x = 2$ and $y = 1$.

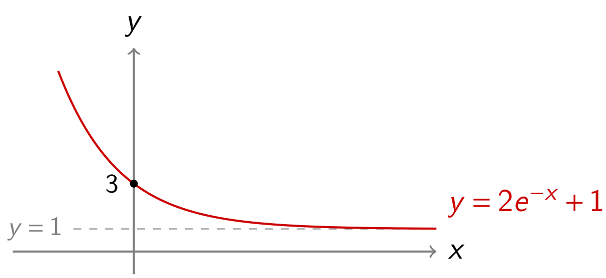
(c) $\mathbf{C} = \begin{pmatrix} 0 & -1 \\ -1 & 0 \end{pmatrix}$.

$\mathbf{C}^8$ represents the matrix which carries out the transformation **C** 8 times. But doing **C** 8 times (i.e., reflecting in $y = -x$ 8 times) will leave vectors unchanged, thus $\mathbf{C}^8 = \mathbf{I}$.

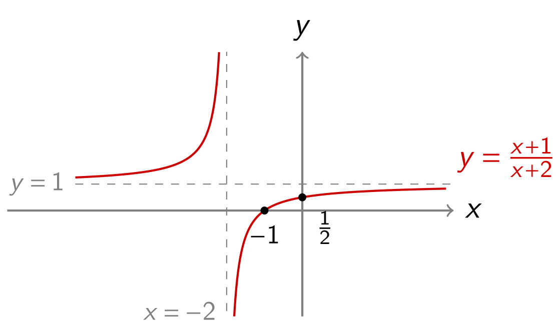
14. (a) (i)



(ii)



(iii)



(b) Since the number of bacteria doubles every 30 minutes, the total number of them after t minutes is $100 \times 2^{t/30}$. So we solve the equation $100 \times 2^{t/30} = 10^6$ for t, which gives the solution $t \approx 398.63$, i.e., 6 hours and 39 minutes (to the nearest minute).

15. (a) This is a separable first order ordinary differential equation. Indeed, we can separate the variables:

$$
\begin{aligned}
& & -\frac{d[A]}{dt} &= k[A] \\
\Longrightarrow & & \frac{d[A]}{[A]} &= -k\,dt \\
\Longrightarrow & & \int \frac{d[A]}{[A]} &= -k \int dt \\
\Longrightarrow & & \log[A] &= -kt + \log c \\
\Longrightarrow & & [A] &= \exp(-kt + \log c) \\
\therefore & \text{Gen. sol.:} & [A] &= c\exp(-kt).
\end{aligned}
$$

Since we are given that when $t = 0$, $[A] = [A]_0$, we have that

$$[A]_0 = c\exp(-k \cdot 0) \Longrightarrow [A]_0 = c,$$

and thus we have the particular solution

$$[A] = [A]_0 \exp(-kt),$$

as required. □

(b) This is a homogeneous second order linear ordinary differential equation with constant coefficients. The first step is to rearrange it into the form

$$\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + E\psi = 0,$$

so we have the auxiliary equation

$$\frac{\hbar^2}{2m}k^2 + E = 0$$

$$\implies \qquad k^2 = -\frac{2mE}{\hbar^2}$$

$$\implies \qquad k = \pm\sqrt{\frac{2mE}{\hbar^2}}\, i,$$

and so the general solution is that of the case of complex roots, i.e.,

$$\psi(x) = c_1 \cos\left(\sqrt{\frac{2mE}{\hbar^2}}\, x\right) + c_2 \sin\left(\sqrt{\frac{2mE}{\hbar^2}}\, x\right),$$

as required. □