L-Università ta' Malta

Department of Chemistry
Faculty of Science

B.Sc. (Hons.) Year I

Semester 2 Examination Session

CHE1215: Methods of Chemical Calculations — 8th June 2022, 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		Integrals	
$f(x)$	$f'(x)$	$f(x)$	$\int f(x)\,dx$
x^n	nx^{n-1}	$x^n\ (n \neq -1)$	$\frac{x^{n+1}}{n+1}$
$\sin x$	$\cos x$	$\sin x$	$-\cos x$
$\cos x$	$-\sin x$	$\cos x$	$\sin x$
$\tan x$	$\sec^2 x$	$\tan x$	$\log(\sec x)$
$\cot x$	$-\operatorname{cosec}^2 x$	$\cot x$	$\log(\sin x)$
$\sec x$	$\sec x \tan x$	$\sec x$	$\log(\sec x + \tan x)$
$\operatorname{cosec} x$	$-\operatorname{cosec} x \cot x$	$\operatorname{cosec} x$	$\log(\tan \frac{x}{2})$
e^x	e^x	e^x	e^x
$\log x$	$1/x$	$1/x$	$\log x$
uv	$u'v + uv'$	$\frac{1}{a^2+x^2}$	$\frac{1}{a}\tan^{-1}\left(\frac{x}{a}\right)$
u/v	$(u'v - uv')/v^2$	$\frac{x}{\sqrt{a^2+x^2}}$	$\sin^{-1}\left(\frac{x}{a}\right)$

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

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

⚠ Attempt only **TEN** questions.

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1. The function f is defined by

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

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

(b) Find $\frac{\partial^2 f}{\partial x^2}$ and $\frac{\partial^2 f}{\partial x \partial y}$.

(c) Find the total differential df.

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

$$f(x,y,z) \approx 24x + 7y + 9z - 32.$$

[3, 2, 2, 3 marks]

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

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

(b) Verify that the function $y = \sin(e^x)$ is a solution to the differential equation $\frac{d^2y}{dx^2} - \frac{dy}{dx} + e^{2x}y = 0$.

[7, 3 marks]

3. Consider the curve given by the equation

$$y = \frac{3+4x}{1+x^2}.$$

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

(b) Determine their nature.

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

[3, 4, 3 marks]

4. (a) Consider the complex numbers

$$z_1 = 2 + i \qquad \text{and} \qquad z_2 = 3 + 2i.$$

Determine:

(i) $5z_1 - 2z_2$ (ii) $z_1 z_2$ (iii) z_1/z_2

(iv) z_1^* (v) $|z_2|$ (vi) $\arg(z_2 - z_1)$

(b) Express $w = 3 + \sqrt{3}\,i$ in the form $Re^{i\theta}$. Hence, calculate w^{10}, writing your answer in both forms: $Re^{i\theta}$ and $a + bi$.

[6, 4 marks]

5. Determine the following integrals.

(a) $\displaystyle\int_0^1 x\sqrt{x}\,dx$ (b) $\displaystyle\int \sin(3\theta + \tfrac{\pi}{6})\,d\theta$

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

[2, 1, 3, 4 marks]

6. (a) Find the area bounded by the curves $y = x^2 + 1$ and $y = 3 - x^2$.

(b) Solve the equation $4x^3 + 6 = 13x$.

[*Hint*: use the rational roots theorem.]

[5, 5 marks]

7. Let $f(x) = (2x-1)(2x^2+5x-3)$.

(a) Sketch the graph $y = f(x)$, labelling any x- and y-intercept(s).

(b) On the same set of axes, sketch the line $y = x + 3$, and label their points of intersection.

(c) Find the total area of the region bounded by the curve and the line.

[3, 3, 4 marks]

8. (a) Sketch the function $y = \cos(3x - \frac{\pi}{6})$ for $0 \leqslant x \leqslant \pi$.

(b) Solve the equation $\cos(3x - \frac{\pi}{6}) = \frac{1}{2}$ for all x in the range $0 \leqslant x \leqslant \pi$.

(c) Indicate your solutions on your sketch from part (a), and also illustrate them on a sketch of the unit circle.

[4, 4, 2 marks]

9. Consider the matrices

$$\mathbf{A} = \begin{pmatrix} 1 & 1 & 1 \\ 1 & 2 & 2 \\ 1 & 2 & 3 \end{pmatrix} \qquad \text{and} \qquad \mathbf{B} = \begin{pmatrix} 2 & -1 & 0 \\ -1 & 2 & -1 \\ 0 & -1 & 1 \end{pmatrix}.$$

(a) Find the matrix product **AB**, and deduce the relationship between **A** and **B**.

(b) Hence or otherwise, solve the simultaneous equations

$$\begin{cases} x + \;\; y + \;\; z = 2 \\ x + 2y + 2z = 3 \\ x + 2y + 3z = 6. \end{cases}$$

(c) The matrix **P** represents a reflection in the x-axis, and the matrix **Q** represents a rotation by 90° (anticlockwise).

(i) Write down the matrices **P** and **Q**.

(ii) Find the matrix which represents doing **P** followed by **Q**.

(iii) Is there a simpler way to describe what this matrix is doing, geometrically?

[3, 3, 4 marks]

10. Solve the differential equation $(x+1)(x+2)\frac{dy}{dx} = \cos^2 y$, given that $y = 0$ when $x = 0$. Give your solution in the form

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

where a is a constant to be determined.

[10 marks]

11. Solve the differential equation

$$\frac{d^2y}{dx^2} - 3\frac{dy}{dx} + 2y = 4x^2,$$

given that when $x = 0$, y and $\frac{dy}{dx}$ are both 1.

[10 marks]

12. (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 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]

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

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

(b) Solve the equation

$$10^{3x} \times 36^{2x-1} \times 14^{x} = 2^{5x+1} \times 35^{x} \times 15^{x+1}.$$

[6, 4 marks]

14. (a) Given that $\log x = 2$, $\log y = 3$ and $\log z = 4$, evaluate the following.

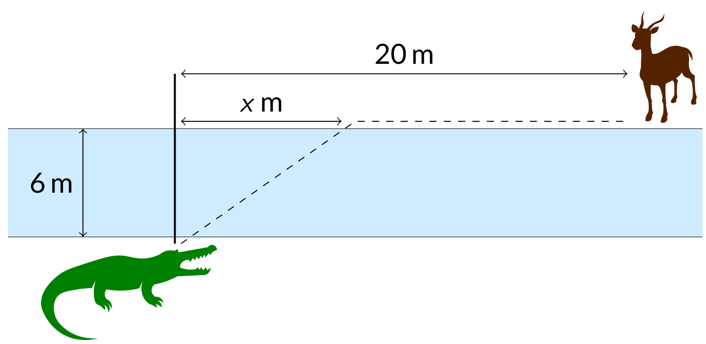
(i) $\log xy^2z^3$ (ii) $\log \frac{x}{z^2y}$ (iii) $4\log y\sqrt[3]{x}$

(iv) $\log x - \sqrt{\log\sqrt{x}}$ (v) $\log_x z$ (vi) x^y

(b) The pH value of a fruit juice is 2.8. Determine the hydronium ion concentration, $[H_3O^+]$, using the definition $\mathrm{pH} = -\log_{10}[H_3O^+]$.

[6, 4 marks]

15. A crocodile is stalking a gazelle that is 20 m upstream on the opposite side of a river. In water, crocodiles travel at 4 m/s, whereas on land, they travel at 5 m/s. Suppose the crocodile swims to a point that is x m upstream on the opposite bank of the river, and runs on land the rest of the way, as depicted below.



(a) Show that the time taken for the crocodile to reach the gazelle is given by $T(x) = \frac{1}{4}\sqrt{36 + x^2} + \frac{1}{5}(20 - x)$.

(b) What is the time taken if the crocodile does not travel on land?

(c) What is the time taken if it swims the shortest distance possible?

(d) What should x be if it gets to the gazelle as fast as possible?

[4, 1, 1, 4 marks]

Solutions

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

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

   (b) $\frac{\partial^2 f}{\partial x^2} = 2y^3 + 60x^2z$ $\quad\frac{\partial^2 f}{\partial x \partial y} = 6xy^2 + 4yz^2$

   (c) $df = \frac{\partial f}{\partial x}dx + \frac{\partial f}{\partial y}dy + \frac{\partial f}{\partial z}dz$

   $= (2xy^3+2y^2z^2+20x^3z)\,dx + (3x^2y^2+4xyz^2)\,dy + (4xy^2z+5x^4)\,dz$

   (d) Near $(1,1,1)$,

$$\begin{aligned} f(x,y,z) &\approx f(1,1,1) + df(1,1,1) \\ &= 8 + 24dx + 7dy + 9dz \\ &= 8 + 24(x-1) + 7(y-1) + 9(z-1) \\ &= 24x + 7y + 9z - 32 \end{aligned}$$

2. (a) (i) $2x(\cos(2x) - x\sin(2x))$ $\quad$ (ii) $\dfrac{xe^{x^2}}{\sqrt{1+e^{x^2}}}$

   (iii) $\dfrac{1}{3(2+x)} - \dfrac{2}{x} - \dfrac{1}{2(1+x)}$

   (b) $y = \sin(e^x)$ $\quad \frac{dy}{dx} = e^x\cos(e^x)$ $\quad \frac{d^2y}{dx^2} = e^x(\cos(e^x) - e^x\sin(e^x))$

   Plugging in to the LHS, thing should simplify to zero.

3. (a) The first derivative is $\frac{dy}{dx} = -\frac{2(2-3x-2x^2)}{(1+x^2)^2}$. Solving $\frac{dy}{dx} = 0$, we get $x = -2$ and $x = \frac{1}{2}$. Finding the corresponding y-coordinates, we get the coordinates $(-2,-1)$ and $\left(\frac{1}{2}, 4\right)$.

   (b) The second derivative is $\frac{d^2y}{dx^2} = \frac{4x^3+9x^2-12x-3}{(1+x^2)^3}$.

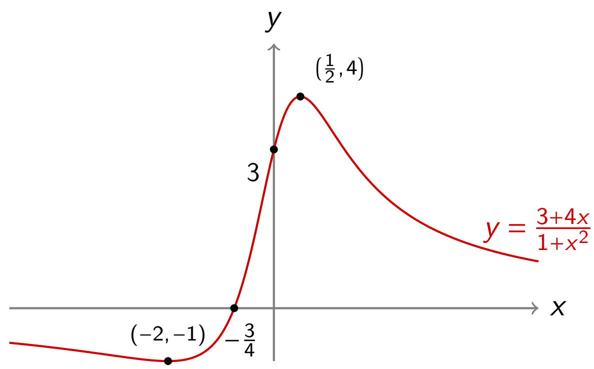
   When $x = -2$, we have $\frac{d^2y}{dx^2} = \frac{1}{5} > 0$, so $(-2,-1)$ is a minimum t.p.

   When $x = \frac{1}{2}$, we have $\frac{d^2y}{dx^2} = -\frac{16}{5} < 0$, so $\left(\frac{1}{2}, 4\right)$ is a maximum t.p.

   (c) For intercepts: when $x = 0$, we get $y = 3$. When $x = 0$, $y = -\frac{3}{4}$.

   Also, as $x \to \infty$, $y \to 0^+$, as $x \to -\infty$, $y \to 0^-$.

Final sketch:



4. (a) (i) $4+i$ (ii) $4+7i$ (iii) $\frac{8}{13} - \frac{1}{13}i$ (iv) $2-i$ (v) $\sqrt{13}$ (vi) $\frac{\pi}{4}$

   (b) $w = 2\sqrt{3}e^{i\pi/6}$, so $w^{10} = (2\sqrt{3}e^{i\pi/6})^{10} = 2^{10}\cdot 3^5 \cdot e^{10i\pi/6} = 248\,832 e^{-i\pi/3}$.

   Thus, $w^{10} = 248\,832(\cos\frac{\pi}{3} - i\sin\frac{\pi}{3}) = 124\,416 - 124\,416\sqrt{3}\,i$.

5. (a) Primitive: $\frac{2}{5}x^{5/2}$, integral: $\frac{2}{5}$.

   (b) $-\frac{1}{3}\cos\left(3\theta + \frac{\pi}{6}\right) + c$.

   (c) Partial fractions: $\frac{1}{2}\left(\frac{x+1}{x^2+1} - \frac{1}{x+1}\right)$,

   Primitive: $\frac{1}{2}\tan^{-1}x + \log\left(\frac{\sqrt[4]{x^2+1}}{\sqrt{x+1}}\right) + c$.

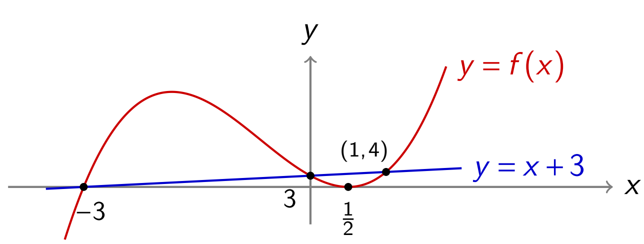
   (d) Partial fractions: $\frac{2x+3}{x^2+3x+4} - \frac{2}{x+3}$,

   Primitive: $\log(x^2+3x+4) - 2\log(x+3)$, integral: $\log\left(\frac{63}{50}\right)$.

6. (a) $\int_{-1}^{1}[(3-x^2)-(x^2+1)]\,dx = \frac{8}{3}$.

   (b) Using the rational roots theorem, the equation can be factorised as $(x+2)(2x-3)(2x-1) = 0$, so its solutions are $x = -2, \frac{1}{2}$ and $\frac{3}{2}$.

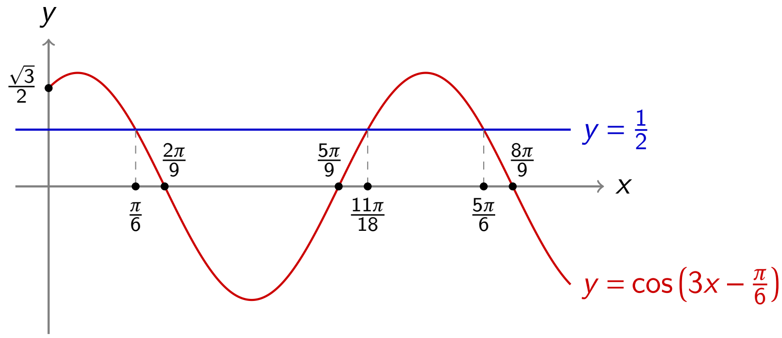
7. (a) When $y = 0$, $x = -3$ or $\frac{1}{2}$ (twice). When $y = 0$, $x = 3$. Sketch:



(b) They intersect at $(-3,0)$, $(0,3)$ and $(1,4)$.

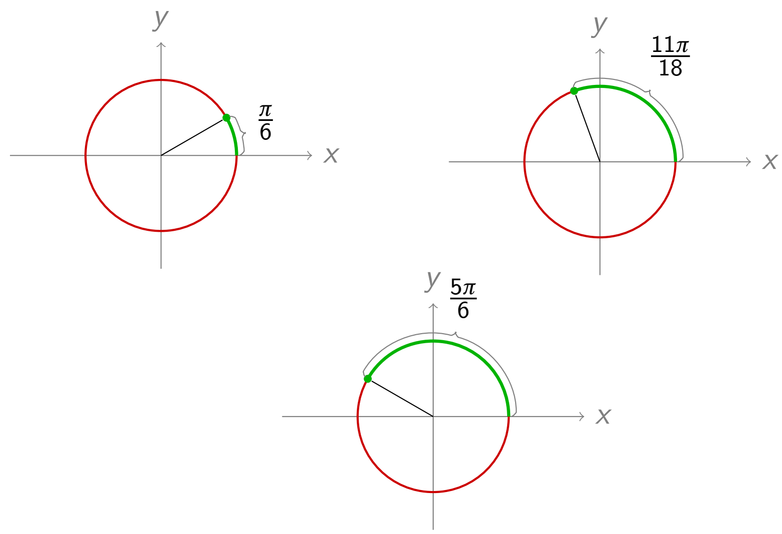
(c) The area is $\int_{-3}^{0}[f(x)-(x+3)]\,dx+\int_{0}^{1}[(x+3)-f(x)]\,dx=\frac{142}{3}$.

8. (a)



(b) $x=\frac{\pi}{6},\frac{11\pi}{18},\frac{5\pi}{6}$.

(c)



9. (a) $\mathbf{AB}=\mathbf{I}$, $\mathbf{A}$ and $\mathbf{B}$ are mutual inverses.

(b) $\mathbf{A}\boldsymbol{x}=\boldsymbol{b}\implies\boldsymbol{x}=\mathbf{A}^{-1}\boldsymbol{b}=\mathbf{B}\boldsymbol{b}=(1,-2,3)$.

(c) (i) $\mathbf{P}=\begin{pmatrix}1&0\\0&-1\end{pmatrix}$, $\mathbf{Q}=\begin{pmatrix}0&-1\\1&0\end{pmatrix}$

(ii) $\mathbf{QP}=\begin{pmatrix}0&1\\1&0\end{pmatrix}$

(iii) Reflection in the line $y=x$.

10. $a = 2$.

11. Trial sol: $\lambda x^2 + \mu x + \eta$, particular sol: $y(x) = 2x^2 + 6x + 7 + e^{2x} - 7e^x$.

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

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

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

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

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

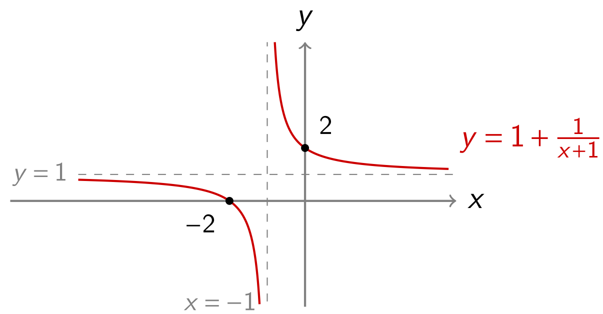
$$
\begin{aligned}
& & \frac{\hbar^2}{2m}k^2 + E &= 0 \\
&\implies & k^2 &= -\frac{2mE}{\hbar^2} \\
&\implies & k &= \pm\sqrt{\frac{2mE}{\hbar^2}}\,i,
\end{aligned}
$$

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

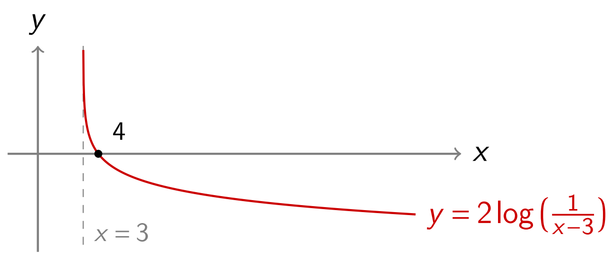
$$\psi(x) = c_1 \cos\left(\sqrt{\frac{2mE}{\hbar^2}}\, x\right) + c_2 \sin\left(\sqrt{\frac{2mE}{\hbar^2}}\, x\right),$$

as required. □

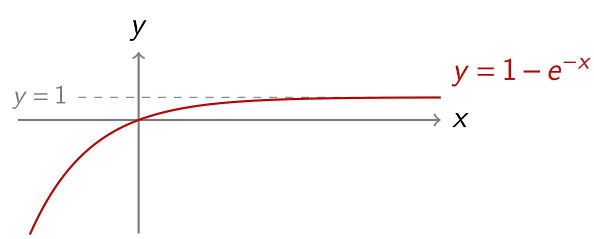
13. (a) (i)



(ii)



(iii)



(b) $x = 1$

14. (a) (i) 20 (ii) -9 (iii) $\frac{44}{3}$ (iv) 1 (v) 2 (vi) e^{2e^3}.

(b) $[H_3O^+] = 0.001585$.

15. (a) *Hint:* Pythagoras' theorem.

(b) $T(20) = 5.22$ seconds.

(c) $T(0) = 5.5$ seconds.

(d) $T'(x) = 0 \implies x = 8$.