Maths Preparation for CHEM203

For this course you will need to be able to differentiate and integrate, and you will also need to know something about complex numbers. All of you will have taken a maths course, but with the variety of courses available you may not have covered all the key principles required. You will want to fill in any gaps before the course starts.

Very good resources are 1st year engineering text books. The one available in the library is Engineering Mathematics: a Foundation for Electronic, Electrical, Communications and Systems Engineers, 4th edition or later, by Anthony Croft, Robert Davison, Martin Hargreaves and James Flint, Pearson, 2012.
Don't be put off by the title this is a good resource. There is an e-version available for the 5th edition!

Recommended reading from this textbook is as follows. If you are feeling good you can cover the whole chapter in each case (but you don't need it all), however if you are interested in the bare minimum, you should know the following:

- Chapter 9: Complex Numbers
  - read **9.1, 9.4, 9.5, 9.7** no exercises required
- Chapter 10 & 11: Differentiation
  - understanding and basics **10.1-10.7, exercises 10.7 (1)**
  - product rule, chain rule **11.1, 11.2, exercises 11.2(1)&(3)**
- Chapter 13 & 14: Integration
  - understanding and basics **13.1, 13.2 read 13.3, exercises 13.2(1)(2)&(3)**
  - by parts, and by substitution **14.1, 14.2, 14.3, exercises 14.2(1) and 14.3(1)**
- Chapter 19: Ordinary differential equations, specifically **section 19.5**
- Chapter 25: Functions of several variables, **specifically 15.1-25.3** covering partial derivatives

You can test yourself, you should feel able to differentiate the following:
basic:

$\frac{d}{dx}\sqrt{x}$ $\quad \frac{d}{dx}\frac{1}{x^5}$ $\quad \frac{d}{dx}2x^4 - 2x^3 - x^2 + 3x + 2$

the product rule:

$\frac{\partial}{\partial x}x^2 cosx$ $\quad \frac{\partial}{\partial x}x^2e^x$ $\quad \frac{\partial}{\partial x}e^{-x}(sin(x) + cos(x))$

the chain rule:

$\frac{d}{dx}(3x^3 + 2x^2 + 1)^5$ $\quad \frac{\partial}{\partial x}sin(2x + 3)$ $\quad \frac{\partial}{\partial x}3e^{-2x}$ $\quad \frac{\partial}{\partial x}cos^2(3x)$

You can test yourself, you should feel able to integrate the following:
basic:

$\int 3x^2dx$ $\quad \int (x^2 + 9)dx$ $\quad \int \frac{1}{x^2}dx$

linear operator:

$\int (cosx - x)dx$ $\quad \int e^{-3x}dx$ $\quad \int (3x^4 - \sqrt{x})dx$ $\quad \int 3sin(4x)dx$

trigonometric functions:

$\int cos^2(x)dx$ $\quad \int sin^2(x)dx$

definite integrals:

$\int_0^2 x^2dx$ $\quad \int_0^\pi sinxdx$ $\quad \int_{-1}^1 e^x dx$

integration by parts, integration by substitution:

$\int xsin(x)dx$ $\quad \int xe^x dx$ $\quad \int (3x + 1)^{2.7}dx$ $\quad \int (1 - x)^{\frac{1}{3}}dx$

Answers at the end of this document

Complex Numbers

- the square root of a negative number was discovered as a problem in the 16th century
  - as a result the square root of 1 was introduced as i= $\sqrt{-1}$
- complex numbers were developed to simplify equations
  - the complex value is written $z = x + iy$
  - where x and y are real numbers and z is a complex number
  - *x* is the "real" part and *iy* is the "imaginary" part
- complex numbers are represented on an *Argand* diagram
  - the y-axis is the imaginary axis and the x-axis is the real axis

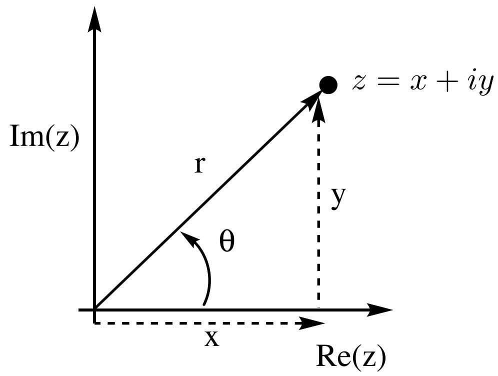

Figure 1 Argand diagram

- addition/subtraction

$$z_1 = x_1 + iy_1 \text{ and } z_2 = x_2 + iy_2$$
$$z_1 + z_2 = (x_1 + x_2) + i(y_1 + y_2)$$
$$z_1 - z_2 = (x_1 - x_2) + i(y_1 - y_2)$$

- multiplication

$$\begin{aligned} z_1 z_2 &= (x_1 + iy_1)(x_2 + iy_2) \\ &= x_1 x_2 + i(x_1 y_2 + y_1 x_2) + i^2 y_1 y_2 \\ i^2 &= -1 \\ &= (x_1 x_2 - y_1 y_2) + i(x_1 y_2 + y_1 x_2) \end{aligned}$$

  - division is more complicated and we won't be needing it
- we *define* z* as the *complex conjugate* of z

$$z = x + iy$$
$$z^* = x - iy$$

  - a nice relationship is

$$\begin{aligned} zz^* &= (x + iy)(x - iy) \\ &= (x^2 + y^2) + i(xy - yx) \\ &= x^2 + y^2 \end{aligned}$$

Practice Activity 1

- evaluate the following

$$(5 + i3)(2 - i) - (3 + j)$$

Answers at the end of this document

- we can write complex number in cylindrical coordinates
  - r is the absolute value (magnitude or distance) of z, r=|z|, ie without the direction
  - using the Argand diagram

$$sin\theta = \frac{y}{r} \qquad y = rsin\theta$$
$$cos\theta = \frac{x}{r} \qquad x = rcos\theta$$
$$z = x + iy = rcos\theta + irsin\theta$$
$$= r(cos\theta + isin\theta)$$

  - this gives us new way to form the product

$$z_1 = r_1(cos\theta_1 + isin\theta_1)$$
$$z_2 = r_2(cos\theta_2 + isin\theta_2)$$
$$z_1z_2 = (r_1cos\theta_1 + ir_1isin\theta_1)(r_2cos\theta_2 + ir_2isin\theta_2)$$
$$= r_1cos\theta_1r_2cos\theta_2 + ir_1cos\theta_1r_2sin\theta_2 + ir_1sin\theta_1r_2cos\theta_2 - r_1sin\theta_1r_2sin\theta_2$$
$$= r_1r_2\left[cos\theta_1cos\theta_2 - sin\theta_1sin\theta_2 + icos\theta_1sin\theta_2 + isin\theta_1cos\theta_2\right]$$
$$\text{using trig idenities}$$
$$sin(x+y) = sinxcosy + cosxsiny$$
$$\text{and } cos(x+y) = cosxcosy - sinxsiny$$
$$z_1z_2 = r_1r_2\left[cos(\theta_1+\theta_2) + isin(\theta_1+\theta_2)\right]$$

- very important for us is *Euler's formula*

$$e^{i\theta} = cos\theta + isin\theta$$

  - which allows us to write the complex number in an exponential form

$$z = r(cos\theta + isin\theta)$$
$$z = re^{i\theta}$$
$$z^* = re^{-i\theta}$$

  - the complex conjugate then becomes

<u>Practice Activity 2</u>

- rearrange $e^{i\theta} = cos\theta + isin\theta$ and $e^{-i\theta} = cos\theta - isin\theta$ to write an expression for cosθ and sinθ

Answers at the end of this document

The Gaussian and Odd functions

- a gaussian is a common function in QM

$$y = e^{-ax^2}$$

- the integral of a gaussian is non-trivial (look it up on the internet if you like!)

$$\int_{\infty}^{\infty} e^{-ax^2} dx = \sqrt{\frac{\pi}{a}}$$

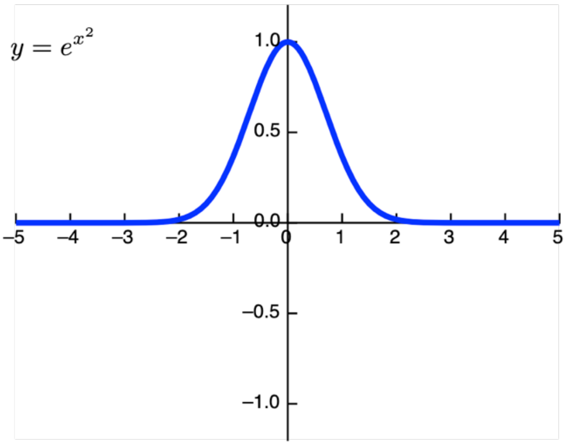

Figure 1: gaussian function

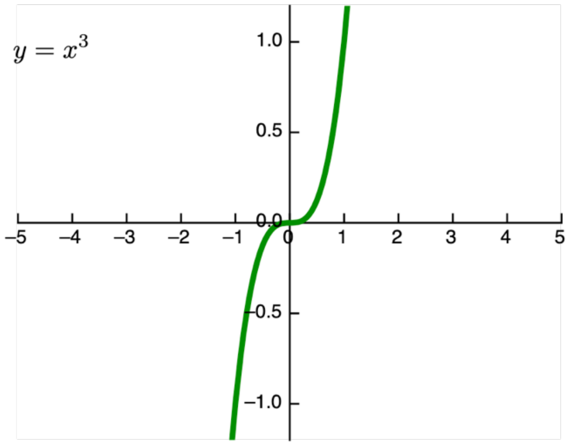

Figure 2: an odd function

- however in some cases there are easier ways to determine an integral using the "even" and "odd" nature of functions
- defining even and odd functions
  - an *even function* is symmetric with respect to reflection in the x-axis
  - f(x)=f(-x), the gaussian above is an even function
  - an *odd function* is symmetric with respect to rotation around the origin
  - -f(x)=f(-x), the function $y=x^3$ is odd
- integration
  - even functions will have a positive integral
  - odd functions always have zero integrals (on an even integration range) because the positive and negative parts cancel out
  - thus any even function multiplied by an odd function will integrate to zero!
  - below is shown the product of y=x and a gaussian, the positive and negative parts of the integral (area under the curve) cancel giving a zero integral

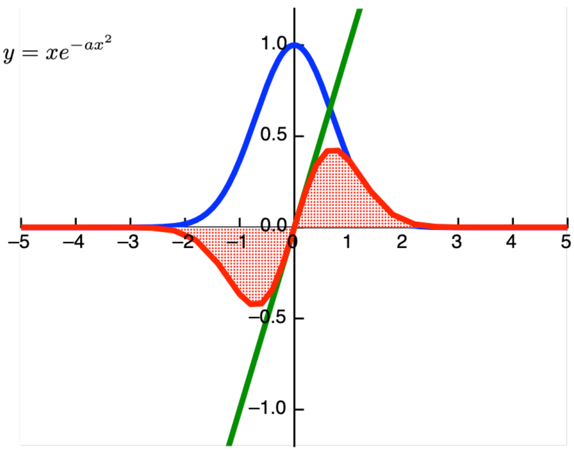

Figure 3: product of even and odd functions

Differential equations

- you are familiar with the equations for a line and for a quadratic

$$y = mx + c \qquad y = ax^2 + bx + c$$

- another group of equations can be written for *derivatives*

$$a\frac{\partial^2 f}{\partial x^2} + b\frac{\partial f}{\partial x} + cf = 0$$

  - f is a function of multiple variables (x,y,z)
  - the coefficients can be constants or functions
  - linear equations have no terms raised to a power or exponential/log components
  - this is a *linear partial differential* equation
- remember
  - for a 1D equation the total derivative is given by "d" df/dx
  - for a function dependent on more than one variable we use a partial derivative "∂" where df is the total derivative of f

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

- however the solutions to differential equations are *very different* to the solutions to algebraic equations (line or quadratic)
- starting with a simple example of an ordinary differential equation (just a straight derivative of an equation f(x) and not a partial derivative)

$$a\frac{d^2 f}{dx^2} + b\frac{df}{dx} = 0$$

  - in an algebraic equation we would *solve for x a variable*, in a differential equation we *solve for f a function*
  - solving differential equations can be difficult (there are whole math courses on just this topic)
  - however the general form of the solution for linear differential equations is known, this is normally expressed in terms of exponentials
  - in this course I will give you the solutions, however if you are interested to know more check out the various maths texts suggested earlier

differentials:

simple differentiation:

$\frac{d}{dx}x^a = ax^{a-1}$	$\frac{d}{dx}k = 0 \text{ and } x^0 = 1$
$\frac{d}{dx}cos(ax) = -asin(ax)$	$\frac{d}{dx}sin(ax) = acos(ax)$
$\frac{d}{dx}e^{ax} = ae^{ax}$	$\frac{d}{dx}lnx = \frac{1}{x}$

$$\frac{d}{dx}\sqrt{x} = \frac{d}{dx}x^{\frac{1}{2}} = \frac{1}{2}x^{-\frac{1}{2}} = \frac{1}{2\sqrt{x}}$$

$$\frac{d}{dx}\frac{1}{x^5} = \frac{d}{dx}x^{-5} = -5x^{-6} = \frac{-5}{x^6}$$

$$\frac{d}{dx}2x^4 - 2x^3 - x^2 + 3x + 2 = 2 \cdot 4x^3 - 2 \cdot 3x^2 - 2x^1 + 3x^0 + 0 = 8x^3 - 6x^2 - 2x + 3$$

product rule:	chain rule:
$\frac{d}{dx}(uv) = u\frac{dv}{dx} + \frac{du}{dx}v$ $(f \cdot g)' = f'g + fg'$	$\frac{d}{dx}f(g(x)) = f'(g(x)) \cdot g'(x)$

$$\text{evaluate } \frac{\partial}{\partial x}x^2cos(x)$$

$$u = x^2 \qquad \frac{\partial u}{\partial x} = 2x \text{ and } v = cos(x) \qquad \frac{\partial v}{\partial x} = -sin(x)$$

$$\frac{\partial}{\partial x}(uv) = u\frac{\partial v}{\partial x} + \frac{\partial u}{\partial x}v$$

$$\frac{\partial}{\partial x}x^2cosx = x^2 \cdot -sin(x) + 2x \cdot cos(x)$$

$$= -x^2sin(x) + 2xcos(x)$$

$$\text{evaluate } \frac{\partial}{\partial x}x^2e^x$$

$$u = x^2 \qquad \frac{\partial u}{\partial x} = 2x \text{ and } v = e^x \qquad \frac{\partial v}{\partial x} = e^x$$

$$\frac{\partial}{\partial x}(uv) = u\frac{\partial v}{\partial x} + \frac{\partial u}{\partial x}v$$

$$\frac{\partial}{\partial x}x^2e^x = x^2e^x + 2xe^x$$

$$= e^x(x^2 + 2x)$$

$$= e^xx(x + 2)$$

$$\text{evaluate } \frac{\partial}{\partial x}e^{-x}(sinx + cosx)$$

$$u = e^{-x} \qquad \frac{\partial u}{\partial x} = -e^{-x} \text{ and } v = sinx + cosx \qquad \frac{\partial v}{\partial x} = cosx - sinx$$

$$\frac{\partial}{\partial x}(uv) = u\frac{\partial v}{\partial x} + \frac{\partial u}{\partial x}v$$

$$\frac{\partial}{\partial x}e^{-x}(sinx + cosx) = e^{-x} \cdot (cosx - sinx) + -e^{-x} \cdot (sinx + cosx)$$

$$= \cancel{e^{-x}cosx} - e^{-x}sinx - e^{-x}sinx - \cancel{e^{-x}cosx}$$

$$= -2e^{-x}sinx$$

$$\text{evaluate } \frac{d}{dx}(3x^3 + 2x^2 + 1)^5$$

$$y = f(g(x)) \qquad \frac{dy}{dx} = f'(g(x)) \cdot g'(x)$$

$$g(x) = 3x^3 + 2x^2 + 1 \qquad g'(x) = 9x^2 + 4x$$

$$f = g(x)^5 \qquad f' = 5g(x)^4$$

$$\frac{dy}{dx} = 5(3x^3 + 2x^2 + 1)^4 \cdot (9x^2 + 4x)$$

$$\text{evaluate } \frac{\partial}{\partial x} sin(2x+3)$$
$$= cos(2x+3)\cdot 2$$
$$= 2cos(2x+3)$$

$$\text{evaluate } \frac{\partial}{\partial x} 3e^{-2x}$$
$$y = f(g(x)) \qquad \frac{dy}{dx} = f'(g(x))\cdot g'(x)$$
$$g(x) = -2x \qquad g'(x) = -2$$
$$f = e^{g(x)} \qquad f' = e^{g(x)}$$
$$\frac{dy}{dx} = 3e^{-2x}\cdot -2$$
$$= -6e^{-2x}$$

$$\text{evaluate } \frac{\partial}{\partial x} cos^2(3x)$$
$$cos^2(3x) = (cos(3x))^2$$
$$y = f(g(x)) \qquad \frac{dy}{dx} = f'(g(x))\cdot g'(x)$$
$$g(x) = cos(3x) \qquad g'(x) = -3sin(3x)$$
$$f = g(x)^2 \qquad f' = 2g(x)$$
$$\frac{dy}{dx} = -3sin(3x)\cdot 2cos(3x)$$
$$= -6sin(3x)cos(3x)$$

integrals:

simple integration:

$\int x^n dx = \frac{1}{n+1}x^{n+1} + C \quad n \neq 1$	$\int k dx = kx + C$
$\int cos(ax)dx = \frac{1}{a}sin(ax) + C$	$\int sin(ax)dx = -\frac{1}{a}cos(ax) + C$
$\int e^{ax}dx = \frac{1}{a}e^{x} + C$	$\int \frac{1}{x}dx = ln\|x\| + C$

$$\int 3x^2 dx = \frac{3}{3}x^3 + C$$

$$\int (x^2+9)dx = \frac{1}{3}x^3 + 9x + C$$

$$\int \frac{1}{x^2}dx = \int x^{-2}dx = \frac{1}{-1}x^{-1} = -\frac{1}{x}$$

$$\int (cosx - x)dx = \int cosx dx - \int x dx = (sinx + C) - (\frac{x^2}{2} + C') = sinx - \frac{x^2}{2} + C\text{''}$$

$$\int e^{-3x}dx = \frac{1}{3}e^{-3x} + C$$

$$\int (3x^4 - \sqrt{x})dx = \int 3x^4 dx - \int x^{\frac{1}{2}}dx = \frac{3}{5}x^5 - \frac{2}{3}x^{\frac{3}{2}} + C$$

$$\int 3sin(4x)dx = -\frac{3}{4}cos(4x) + C$$

$$\text{check your answer by differentiating: } \frac{d}{dx}(-\frac{3}{4}cos(4x)) = -\frac{3}{4} \cdot -sin(4x) \cdot 4 = 3sin(4x)$$

useful trigonometric identities:

$cos^2x + sin^2x = 1$	$cos(2x) = 2cos^2x - 1$
	$cos(2x) = 1 - 2sin^2x$

$$\text{evaluate } \int cos^2(x)dx$$

$$cos(2x) = 2cos^2x - 1 \text{ therefor } cos^2x = \frac{1}{2}(cos(2x) + 1)$$

$$\int cos^2(x)dx = \int \frac{1}{2}dx + \int \frac{1}{2}cos(2x)dx$$

$$= \frac{1}{2}x + \frac{1}{2} \cdot \frac{1}{2} \cdot sin(2x) + C$$

$$= \frac{1}{2}x + \frac{1}{4}sin(2x) + C$$

$$\text{evaluate } \int sin^2(x)dx$$

$$cos(2x) = 1 - 2sin^2(x) \text{ therefor } 2sin^2(x) = 1 - cos(2x)$$

$$\text{and } sin^2(x) = \frac{1}{2} - \frac{1}{2}cos(2x)$$

$$\int sin^2(x)dx = \int \frac{1}{2}dx - \int \frac{1}{2}cos(2x)dx$$

$$= \frac{1}{2}x - \frac{1}{2} \cdot \frac{1}{2} \cdot sin(2x) + C$$

$$= \frac{1}{2}x - \frac{1}{4}sin(2x) + C$$

definite integrals evaluated between limits

$$\int_0^2 x^2dx = \left[\frac{1}{3}x^3 + C\right]_1^2 = \frac{1}{3}2^3 - \frac{1}{3}1^3 = \frac{8}{3} - \frac{1}{3} = \frac{7}{3}$$

$$\int_0^\pi sin(x)dx = [-cos(x) + C]_0^\pi = -cos(\pi) - -cos(0) = -(-1) - -(+1) = - + 1 + 1 = 2$$

$$\int_{-1}^1 e^x dx = [e^x + C]_{-1}^1 = e^1 - e^{-1} = 2.7183 - 0.3679 = 2.3504$$

integration by parts

$$\boxed{\int u(\frac{dv}{dx})dx = uv - \int v(\frac{du}{dx})dx}$$

$$\text{evaluate } \int xsin(x)dx$$

$$u = x \qquad \frac{du}{dx} = 1$$

$$\frac{dv}{dx} = sin(x) \text{ therefore } v = \int \frac{dv}{dx}dx = \int sin(x)dx$$

$$v = \int sin(x)dx = -cos(x) + C$$

$$\int xsin(x)dx = uv - \int v\frac{du}{dx}dx$$

$$= x(-cos(x)) - \int (-cos(x)) \cdot 1dx$$

$$= -xcos(x) + sin(x) + C$$

$$\text{evaluate } \int xe^x dx$$

$$u = x \qquad \frac{du}{dx} = 1$$

$$\frac{dv}{dx} = e^x \text{ therefore } v = \int e^x dx = e^x + C$$

$$\int xe^x dx = uv - \int v\frac{du}{dx}dx$$

$$= x(e^x) - \int (e^x) \cdot 1dx$$

$$= -xe^x - e^x + C$$

$$= e^x(x-1)$$

integration using the chain rule/ or by substitution

$$\text{evaluate } \int (3x+1)^{2.7}dx$$

$$\text{let } z = 3x+1 \qquad \frac{dz}{dx} = 3 \text{ therefore } dx = \frac{1}{3}dz$$

$$\int (3x+1)^{2.7}dx = \int z^{2.7}\frac{1}{3}dz$$

$$= \frac{1}{3}(\frac{1}{3.7}z^{3.7}) + C$$

$$= \frac{1}{11.1}(3x+1)^{3.7} + C$$

$$\text{evaluate } \int (1-x)^{\frac{1}{3}} dx$$

$$\text{let } z = 1-x \qquad \frac{dz}{dx} = -1 \text{ therefore } dx = -dz$$

$$= -\int (z)^{\frac{1}{3}} dz$$

$$= -\frac{3}{4} z^{\frac{4}{3}} + C$$

$$= -\frac{3}{4}(1-x)^{\frac{4}{3}} + C$$

<u>Complex numbers Practice Activity 1</u>

- evaluate the following

$$(5+i3)(2-i)-(3+j)$$

$$(5+i3)(2-i)-(3+i)$$

$$= (10-5i+6i+3)-(3+i)$$

$$= (13+i)-(3+i)$$

$$= 10$$

<u>Complex numbers Practice Activity 2</u>

- write an expression for cosθ and sinθ using the exponential form of complex numbers

$$e^{i\theta} = cos\theta + isin\theta$$

$$\text{rearrange to get } cos\theta$$

$$cos\theta = e^{i\theta} - isin\theta$$

$$\text{now rearrange } e^{-i\theta} \text{ to get } -isin\theta$$

$$e^{-i\theta} = cos\theta - isin\theta$$

$$-isin\theta = e^{-i\theta} + cos\theta$$

$$\text{substitute into } cos\theta = e^{i\theta} - isin\theta$$

$$cos\theta = e^{i\theta} + (e^{-i\theta} + cos\theta)$$

$$\text{pull } cos\theta \text{ terms together}$$

$$2cos\theta = e^{i\theta} + e^{-i\theta}$$

$$\text{push the 2 back}$$

$$cos\theta = \frac{e^{i\theta} + e^{-i\theta}}{2}$$

$$e^{i\theta} = cos\theta + isin\theta$$

$$\text{rearrange to get } isin\theta$$

$$isin\theta = e^{i\theta} - cos\theta$$

$$\text{now rearrange } e^{-i\theta} \text{ to get } cos\theta$$

$$e^{-i\theta} = cos\theta - isin\theta$$

$$cos\theta = e^{-i\theta} + isin\theta$$

$$\text{substitute into } isin\theta = e^{i\theta} - cos\theta$$

$$isin\theta = e^{i\theta} - (e^{-i\theta} + isin\theta)$$

$$\text{pull } isin\theta \text{ terms together}$$

$$2isin\theta = e^{i\theta} - e^{-i\theta}$$

$$\text{push the 2i back}$$

$$sin\theta = \frac{e^{i\theta} - e^{-i\theta}}{2i}$$