Theoretical Methods Problem Sheet 2: Spring Term

Series, Power Series Expansions and Thermodynamics

Power Series

The Maclaurin series expansion of a function f(x) was introduced in lecture 3.

$$f(x) = c_0 + c_1 x + c_2 x^2 + c_3 x^3 + \ldots + c_n x^n + \ldots$$

Where the coefficients can be computed from the derivatives of the target function;

$$c_0 = f(0)$$

$$c_1 = \left.\frac{df}{dx}\right|_{x=0}$$

$$c_2 = \left.\frac{1}{2!}\frac{d^2 f}{dx^2}\right|_{x=0}$$

$$c_3 = \left.\frac{1}{3!}\frac{d^2 f}{dx^2}\right|_{x=0}$$

$$\ldots$$

$$c_n = \left.\frac{1}{n!}\frac{d^n f}{dx^n}\right|_{x=0}$$

Reminder: 6! Simply means 6x5x4x3x2x1.

(i) Use the Maclaurin series to obtain the power series expansion of cos(x) and sin(x) up to n=7. Why does the cos(x) series contain only even powers of x and the sin(x) series contain only odd powers ?

Solutions:

(i)
$$\cos(x) = 1 - \frac{1}{2}x^2 + \frac{1}{24}x^4 - \frac{1}{720}x^6 + \ldots$$
$$\sin(x) = x - \frac{1}{6}x^3 + \frac{1}{120}x^5 + \frac{1}{5040}x^7 \ldots$$

cos(x) is an even function of x – that is, it is invariant under reflection in the origin cos(x)=cos(-x). Only polynomials with the same **symmetry** contribute to its expansion. That is even powers.

sin(x) is an odd function of x …..

Students may be interested in a discussion of expansions in general and their symmetry properties. Similar symmetry properties pertain when molecular orbitals are expanded in terms of atomic orbitals or when the time dependence of an IR spectrum is expanded in a Fourier series etc etc

(ii) How many terms of the series are required to obtain sin(π/3) and cos(π/3) to 3 decimal places.

Solutions:

(ii)
$$\cos(\pi/3) = 0.5$$
$$\sin(\pi/3) = 0.8660$$

The summation to n terms looks like:

	1	2	3	4	5
cos(π/3)	1	0.451689	0.501796	0.499965	0.50000
sin(π/3)	1.047198	0.855801	0.866295	0.866021	0.866025

So to get an accuracy of 3dp you need 4 terms from the cos(x) and sin(x) expansions.

In the vibrations of solids (phonons) and the electronic structure of semiconductors you will often come across periodic functions which can be written in terms of sin(x) and cos(x) but are more usually written in terms of the exponential function by using the famous Euler identity;

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

Reminder: *i* is the complex number and is defined so that $i^2=-1$

(iii) Make an Euler expansion of e^x to 6 terms and use it with your expansion of cos and sin from question (i) to prove the Euler identity.

(iii) Hoping that the students know that $\frac{de^x}{dx} = e^x$

So all the derivatives are trivial (1) and the expansion is;

$$e^x = 1 + x + \frac{1}{2}x^2 + \frac{1}{6}x^3 + \frac{1}{24}x^4 + \frac{1}{120}x^5 + \frac{1}{720}x^6 + \ldots$$

And so,

$$e^{ix} = 1 + ix - \frac{1}{2}x^2 - i\frac{1}{6}x^3 + \frac{1}{24}x^4 + i\frac{1}{120}x^5 + \frac{1}{720}x^6 + \ldots$$

Which is cos(x)+*i*sin(x)

With a bright student who's interested in the funny connections that formula's sometimes make you can now spend a day or two trying to understand how complex numbers (introduced as phase factors in the first year) and trigonometric functions (introduced as measures of angles in triangles when they were about 13) .. end up in the same equation together.