PHYS2024 Quantum Physics of Matter

Some Useful Mathematical Tools

This course is basically statistical mechanics so we're going to use a lot of maths, so we'll begin by understanding some tools that will help us throughout this course

Gamma Function

The gamma function is defined as:

$$\boxed{\Gamma(z) = \int_0^\infty x^{z-1} e^{-x}\, dx}$$

where z is a real number.
& $z = n$ where n is a positive integer:

$\Gamma(n) = (n-1)!$ which implies:

$$\boxed{n! = \int_0^\infty x^n e^{-x}\, dx}$$

This is very useful in calculating factorials but can get tricky for large n. For large n, we instead use Stirling's formula.

Stirling's Formula

Stirling's approximation is:

$$\boxed{n! \approx \sqrt{2\pi n} \left(\frac{n}{e}\right)^n}$$

which can be written in logaritmic form as:

$$\boxed{\ln(n!) \approx n\ln(n) - n}$$

This is very useful and we will use it a lot on this course

In stat mech, we are usually dealing with $n \sim 10^{23}$ particles hence the need for this approximation.

The Gaussian Integral

A common integral we will be using is:

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

we will use this particularly with gaussian functions, hence the name.

Taylor Expansion

The taylor expansion of a function $f(x)$ about a point $x=a$ is:

$$\boxed{f(x) = f(a) + (x-a)\left(\frac{df}{da}\right)_{x=a} + \frac{1}{2}(x-a)^2\left(\frac{d^2f}{dx^2}\right)_{x=a} + O\left[(x-a)^3\right]}$$

You will normally only need the first 2 terms.

Exact Differentials

consider a function $f(x,y)$ dependent on variables x and y

$\Rightarrow df = \frac{\partial f}{\partial x}dx + \frac{\partial f}{\partial y}dy$ The df here is called an <u>exact</u> differential.

An important property of an exact differential is that when integrated between 2 points A and B, the result does not depend on the path taken.

$$\int_{f(A)}^{f(B)} df = f(B) - f(A) = \underbrace{\int_C \frac{\partial f}{\partial x}dx + \frac{\partial f}{\partial y}dy}_{\text{line integral along path C}}$$

so for a closed loop $A \to B \to A$ $\quad \oint df = 0$

Exact differentials are important because thermodynamic functions of state like P, V, S have exact differential forms.

we can represent the exact differential form a bit neater with:

$$\delta g = g_x(x,y)\,dx + g_y(x,y)\,dy \quad \text{where} \quad g_x = \frac{\partial f}{\partial x} \quad g_y = \frac{\partial f}{\partial y}$$

so if δg is an exact differential, there must be a function f where $g_x = \frac{\partial f}{\partial x}$ and $g_y = \frac{\partial f}{\partial y}$ is true.

we can find this by considering the second differential

$$\frac{\partial^2 f}{\partial x \partial y} = \frac{\partial^2 f}{\partial y \partial x} \quad \text{so} \quad \boxed{\frac{\partial g_x}{\partial y} = \frac{\partial g_y}{\partial x}}$$

so if this is true, then δg is an exact differential df.

if $\frac{\partial g_x}{\partial y} \neq \frac{\partial g_y}{\partial x}$, we call δg an inexact differential. $đf$

we can use this to see if a function has an exact diff. form

example:

$$\delta z = 6y\,dx + (10y + 6x)\,dy$$

$$\frac{\partial}{\partial y}(6y) = \underline{6} \quad \frac{\partial}{\partial x}(10y + 6x) = \underline{6}$$

so this is an <u>exact differential</u>

example:

$$\delta z = (2yx + y^2)\,dx + (3y^2 + 4yx)\,dy$$

$$\frac{\partial}{\partial y}(2yx + y^2) = \underline{2x + 2y} \quad \frac{\partial}{\partial x}(3y^2 + 4yx) = \underline{4y}$$

so this is an <u>inexact</u> differential