Statistical Physics Computer Lab. #1
Tutorial, Gamma Function, and the Stirling Approximation

We start by learning how to do simple computations with MathCad.

(1) Type: 4*6= The answer is: 24.

$$4\cdot 6 = 24$$

(2) Type 42-53= The answer is -11. ▪

$$42 - 53 = -11$$

(3) Type: \5= (this is square root of 3). The answer is 2.24.

$$\sqrt{5} = 2.23607$$

(4) Type 3.2^5.4= (this is 3.2 to the power 5.4). The answer is 534.33

$$3.2^{5.4} = 534.3304$$

Next we study a special function that appears frequently in statistical physics problems: the gamma function. It is defined as an integral:

$$\text{gamma}(x) := \int_0^\infty e^{-t}\cdot t^{x-1}\,dt$$

The integral is performed from zero to infinity. To type infinity hit *<u>control shift z</u>*. We calculate a few values for gama function:

$\text{gamma}\left(\frac{1}{2}\right) = 1.77245$ **which is :** $\sqrt{\pi} = 1.77245$ $\quad\text{gamma}(1) = 1 \quad \text{gamma}(2) = 1$

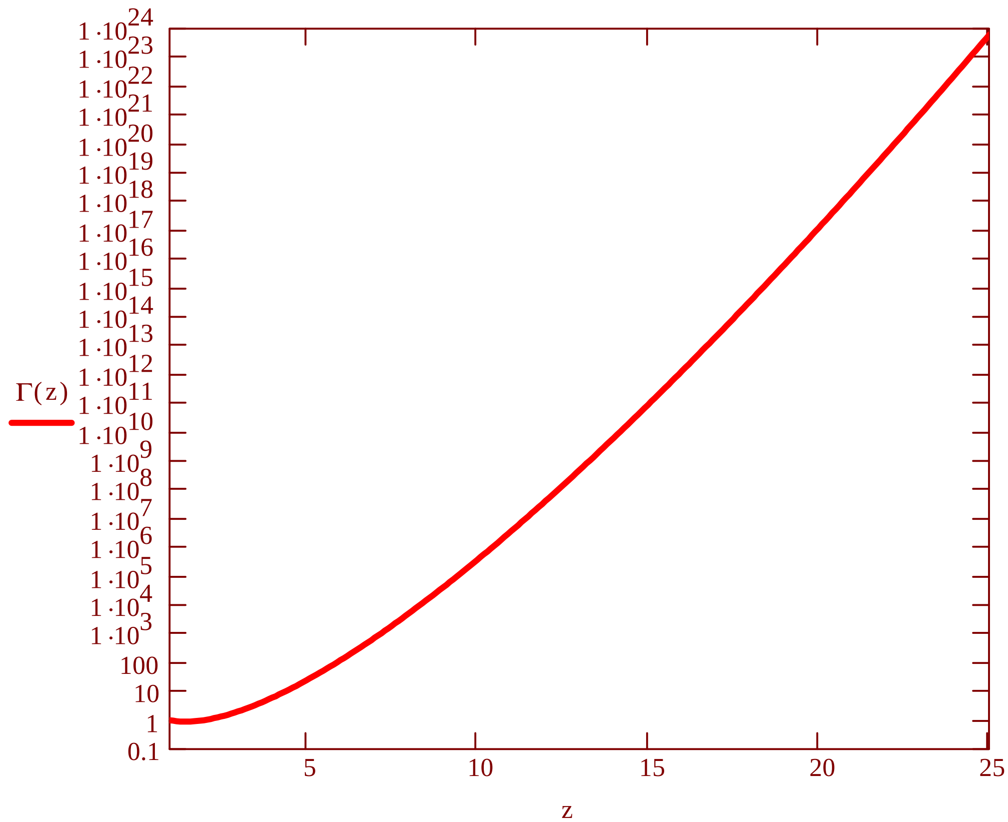
$\text{gamma}(3) = 2 \quad \text{gamma}(4) = 6 \quad \text{gamma}(5) = 24 \quad \text{gamma}(6) = 120$

One can show that for any natural number n: gamma(n) = (n-1)!.

Mathcad has the gamma function wired. To get it type the greek letter capital Γ.

We graph next the Gamma function Γ(z) versus z.

$z := 1., 1.1 .. 25.$



To get the Gamma function evaluated simbolically we write its integral definition and then hit the Evaluate Symbolically button from the Evalaution and Boolean toolbar.

This is Γ(1/2): $\int_0^\infty e^{-x} \cdot x^{-.5}\,dx \rightarrow \pi^{\left(\frac{1}{2}\right)}$

This is Γ(3/2): $\int_0^\infty e^{-x} \cdot x^{.5}\,dx \rightarrow \frac{1}{2} \cdot \pi^{\left(\frac{1}{2}\right)}$

This is Γ(5/2): $\int_0^{\infty} e^{-x} \cdot x^{1.5}\,dx \rightarrow \frac{3}{4} \cdot \pi^{\left(\frac{1}{2}\right)}$

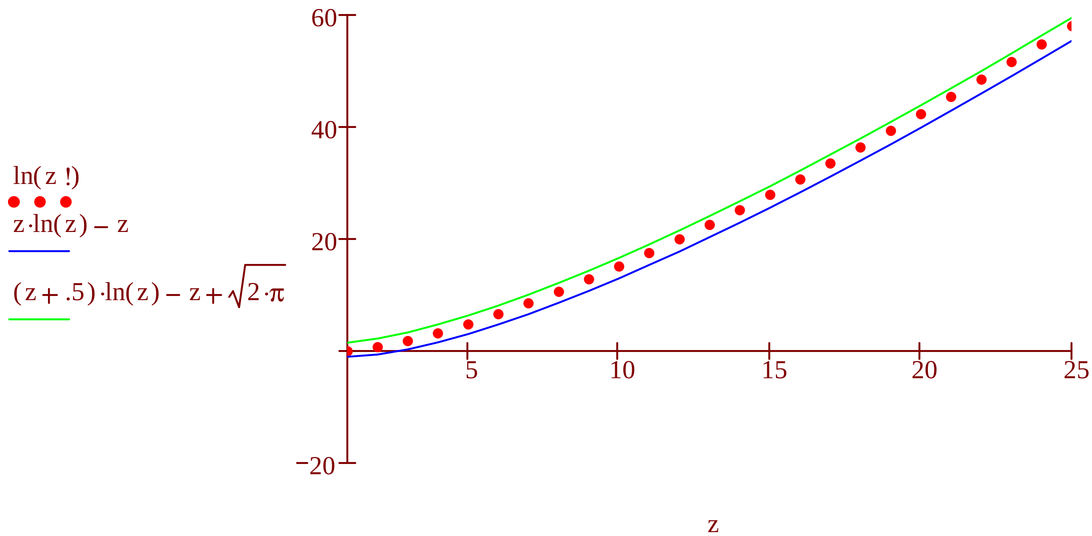
This is Γ(7/2): $\int_0^{\infty} e^{-x} \cdot x^{2.5}\,dx \rightarrow \frac{15}{8} \cdot \pi^{\left(\frac{1}{2}\right)}$

This is Γ(9/2): $\int_0^{\infty} e^{-x} \cdot x^{3.5}\,dx \rightarrow \frac{105}{16} \cdot \pi^{\left(\frac{1}{2}\right)}$

This is Γ(11/2): $\int_0^{\infty} e^{-x} \cdot x^{4.5}\,dx \rightarrow \frac{945}{32} \cdot \pi^{\left(\frac{1}{2}\right)}$

In the following graph we compare ln(Γ(z+1)) = ln(z!) to the Stirling approximation ln(z!) ~ zln(z)- z and to the improved Stirling approximation:
ln(z!) ~ (z + 0.5)ln(z) - z + 0.5ln(2π). The Stirling approximation is valid for large values of z.

$z := 0 .. 25$



We now compute the fractional errors made by approximating ln(z!) with the Stirling approximation and the improved Stirling approximation and graph them versus z. You will note that for z > 20 the error made by using the Stirling approximation is less than 6%

$z := 1 .. 150$

$$\frac{\left| z \cdot \ln(z) - z - \ln(z!) \right|}{\ln(z!)}$$

$$\frac{\left| \left[(z + .5) \cdot \ln(z) - z + \sqrt{2 \cdot \pi} \right] - \ln(z!) \right|}{\ln(z!)}$$