Thermodynamics Lecture Notes: Mathematical Notes

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1 Some Tricks for the calculation of Integrals – preparation for Chapter 5

How can we compute the following integral?

$$I_n(a) = \int_0^\infty x^n \exp\left(-ax^2\right) dx$$

Solution:
For $n = 0$, by introducing $x' = \sqrt{a}x$

$$I_0(a) = \int_0^\infty \exp\left(-ax^2\right) dx = \frac{1}{\sqrt{a}} \int_0^\infty \exp\left(-x'^2\right) dx'$$

We now consider the following integral:

$$\int_0^\infty \exp\left(-x^2\right) dx \int_0^\infty \exp\left(-y^2\right) dy = \int_0^\infty \int_0^\infty \exp\left(-x^2\right) \exp\left(-y^2\right) dxdy = \int_0^\infty \int_0^\infty \exp\left[-\left(x^2+y^2\right)\right] dxdy$$

By changing to the polar coordinate system, $x = r\cos\phi, y = r\sin\phi$, and $dxdy = rdrd\phi$, we have

$$\int_0^\infty \int_0^\infty \exp\left[-\left(x^2+y^2\right)\right] dxdy = \frac{1}{4}\int_0^\infty \int_0^{2\pi} r\exp\left(-r^2\right) drd\phi = \frac{\pi}{2}\int_0^\infty r\exp\left(-r^2\right) dr = -\frac{\pi}{4}\exp\left(-r^2\right)\Big]_{r=0}^{\infty} = \frac{\pi}{4}$$

leading to

$$\int_0^\infty \exp\left(-x^2\right) dx = \frac{\sqrt{\pi}}{2}$$

Finally, we obtain

$$I_0(a) = \int_0^\infty \exp\left(-ax^2\right) dx = \frac{1}{2}\sqrt{\frac{\pi}{a}}$$

For $n = 1$, it follows that

$$I_1(a) = \int_0^\infty x\exp\left(-ax^2\right) dx = -\frac{1}{2a}\exp\left(-ax^2\right)\Big]_0^\infty = \frac{1}{2a}$$

and for $n = 2$,

$$I_2(a) = \int_0^\infty x^2\exp\left(-ax^2\right) dx = -\frac{d}{da}I_0(a) = -\frac{\sqrt{\pi}}{2}\frac{d}{da}a^{-1/2} = \frac{\sqrt{\pi}}{4}a^{-3/2}$$

For n = 3 *and 4 , we have*

$$I_3(a) = \int_0^\infty x^3\exp\left(-ax^2\right) dx = -\frac{d}{da}I_1 = -\frac{1}{2}\frac{d}{da}a^{-1} = \frac{1}{2}a^{-2}$$

$$I_4(a) = \int_0^\infty x^4\exp\left(-ax^2\right) dx = -\frac{d}{da}I_2(a) = \frac{\sqrt{\pi}}{4}\frac{d}{da}a^{-3/2} = \frac{3\sqrt{\pi}}{8}a^{-5/2}$$

2 Recap on probabilities and probability distributions – preparation for Chapter 5

Let us consider a variable x, which can take a value between x_l to x_u. The variable x can be discrete, such as the number of population in the Swiss towns and villages, or continuous such as the absolute value of the speed of cars on the road. We then make n measurements of x, i.e. $x_1, x_2, \cdots$ to x_n.
Average and root mean squared are given by

$$\langle x \rangle = \frac{1}{n} \sum_{i=1}^{n} x_i$$

and

$$\sqrt{\langle (x - \langle x \rangle)^2 \rangle} = \sqrt{\langle x^2 \rangle - \langle x \rangle^2}$$

respectively, and a probability to have a value x_i by leading the average to be

$$P\left(x_i\right) = \frac{1}{n} x_i$$

$$\langle x \rangle = \sum_{i=1}^{n} P\left(x_i\right)$$

One can "bin" x with a finite interval, dx, and denote $n\left(x_i\right) dx$ to be the number of measurements where x is between x_i and $x_i + dx$. Then the average becomes

$$\langle x \rangle = \frac{1}{n} \sum_{i=1}^{n} x_i n\left(x_i\right) dx = \frac{1}{n} \sum_{x=x_l}^{x_u} x n(x) dx = \sum_{x=x_l}^{x_u} x P(x) dx$$

For continuous variables, in the limit of $n \to \infty$ and $dx \to 0, n(x)$ (so as $P(x)$) becomes a smooth function of x. Then the sum can be replaced by the integral, i.e.

$$\langle x \rangle = \frac{1}{N} \int_{x_l}^{x_u} x n(x) dx = \int_{x_l}^{x_u} x P(x) dx$$