

(2.7) In one mole of gas at STP (standard temperature and pressure, i.e. 0 deg.C and 1 atm) a small fraction of the molecules have a kinetic energy  $\geq 15kT$ . (a) How many such molecules are there, and (b) what would their temperature be if they could be isolated?

As usual we begin by defining the values of the electron volt, eV, the Boltzmann constant,  $k$ , and the Avogadro number,  $N_A$  using data from Appendix III and IV:

$$eV := 1.6021773 \cdot 10^{-19} \cdot \text{joule} \quad k := 1.38066 \cdot 10^{-23} \cdot eV \cdot K^{-1} \quad N_A := 6.022137 \cdot 10^{23} \cdot \text{mole}^{-1}$$

Then we convert the temperature,  $T$ , from deg.C to deg.K as follows:

$$T := (0 + 273.15) \cdot K$$

(a) The number of  $kT$  units,  $x$ , is given and thus:

$$x := 15$$

In order to avoid numerical problems we only integrate eqn. (2.25) up to  $250kT$  as a substitute for infinity (otherwise the computer will experience an underflow exception):

$$f := \int_{x \cdot k \cdot T}^{250 \cdot k \cdot T} \frac{2 \cdot \sqrt{E}}{\sqrt{\pi} \cdot (k \cdot T)^{3/2}} \cdot \exp\left(-\frac{E}{k \cdot T}\right) dE \quad \text{eqn (2.25) without any rearrangements}$$

$$f = 3.002 \cdot 10^{-6} \quad f = 3.002 \cdot 10^{-4} \cdot \%$$

$$\text{Answer is : } f N_A = 1.808 \cdot 10^{18} \quad \text{molecules per mole}$$

(b) In order to calculate the corresponding temperature we begin by defining the integrand of eqn. (2.25) with the unknown energy (designated by  $z$ ) as a function of  $z$ :

$$g(z) := \frac{2 \cdot \sqrt{z}}{\sqrt{\pi} \cdot (k \cdot T)^{3/2}} \cdot \exp\left(-\frac{z}{k \cdot T}\right)$$

We then use eqn (2.21) to calculate the temperature from the average energy,  $E_{tr}$ :

$$E_{tr} := \frac{\int_{x \cdot k \cdot T}^{250 \cdot k \cdot T} E \cdot g(E) dE}{\int_{x \cdot k \cdot T}^{250 \cdot k \cdot T} g(E) dE} \quad \text{(This is the standard method to calculate the average of a function, in this case of } E, \text{ over an interval)}$$

$$T_{calc} := \frac{2}{3 \cdot k} \cdot E_{tr} \quad T_{calc} = 2737 \cdot K$$