Task I : analytical derivation

MB: $P(p) = \sqrt{\frac{2\beta}{\pi m}} \exp\left(-\frac{\beta p^2}{2m}\right)$, $\beta = \frac{1}{k_B T}$

Show: $\frac{\sigma_{p^2}^2}{\langle \sigma^2 \rangle^2} = 1$ and $\frac{\sigma_T^2}{\langle T \rangle_{NVT}^2} = \frac{1}{N}$

1) calculate $\langle p^2 \rangle$, $\langle p^4 \rangle$

2) $\sigma_{p^2}^2 = \langle p^4 \rangle - \langle p^2 \rangle^2$

$$\langle p^2 \rangle = \int_0^\infty p^2 P(p)\, dp$$

$$= \int_0^\infty p^2 \sqrt{\frac{2\beta}{\pi m}} \exp\left(-\frac{\beta p^2}{2m}\right) dp$$

Let $u = \frac{\beta p^2}{2m} \Leftrightarrow p^2 = \frac{u\, 2m}{\beta}$ with $u \propto p^2$ $\Rightarrow u \to 0,\ p \to 0$; $u \to \infty,\ p \to \infty$

$$\frac{du}{dp} = \frac{\beta}{\cancel{2}m}\cancel{2}p \Leftrightarrow dp = du\,\frac{m}{\beta p} = du\,\frac{m}{\beta}\sqrt{\frac{\beta}{u 2m}}$$

$$= \int_0^\infty \frac{u\, 2m}{\beta} \sqrt{\frac{2\beta}{\pi m}} \exp(-u)\, du\, \frac{m}{\beta}\sqrt{\frac{\beta}{u 2m}}$$

$$= \frac{\cancel{2}m}{\cancel{\beta}} \sqrt{\frac{\cancel{2\beta}}{\cancel{\pi m}}}\, \frac{\cancel{m}}{\beta} \sqrt{\frac{\cancel{\beta}}{\cancel{2m}}}\ \underbrace{\int_0^\infty \sqrt{u}\, \exp(-u)\, du}_{\frac{\sqrt{\cancel{\pi}}}{\cancel{2}}}$$

$$= \frac{m}{\beta}$$

$$\langle p^4 \rangle = \int_0^\infty p^4 \cdot P(p)\, dp$$

$$= \int_0^\infty p^4 \sqrt{\frac{2\beta}{\pi m}} \exp\left(-\frac{\beta p^2}{2m}\right) dp$$

Let $u = \frac{\beta p^2}{2m} \iff p^2 = \frac{u 2m}{\beta}$, $p^4 = \left(\frac{u 2m}{\beta}\right)^2$

$$\frac{du}{dp} = \frac{\beta}{\cancel{2}m} \cancel{2}p \iff dp = du \frac{m}{\beta p} = du \frac{m}{\beta} \sqrt{\frac{\beta}{u 2m}}$$

$$= \left(\frac{2m}{\beta}\right)^2 \sqrt{\frac{2\beta}{\pi m}} \int_0^\infty u^2 \exp(-u)\, du \frac{m}{\beta} \sqrt{\frac{\beta}{u 2m}}$$

$$= \frac{2^2 m^2}{\beta^2} \sqrt{\frac{2\beta}{\pi m}} \frac{m}{\beta} \sqrt{\frac{\beta}{2m}} \underbrace{\int_0^\infty \frac{1}{\sqrt{u}} u^2 \exp(-u)\, du}_{\frac{3}{4}\sqrt{\pi}}$$

$$= \frac{\cancel{4} m^2}{\beta^2} \frac{\cancel{\sqrt{2}}\, \cancel{\beta}}{\cancel{\sqrt{\pi}}\, \cancel{m} \cancel{\sqrt{2}}} \frac{\cancel{m}}{\cancel{\beta}} \frac{3}{\cancel{4}} \cancel{\sqrt{\pi}}$$

$$= 3 \frac{m^2}{\beta^2}$$

$$\sigma_{p^2}^2 = \langle p^4 \rangle - \langle p^2 \rangle^2$$

$$= \frac{3m^2}{\beta^2} - \left(\frac{m}{\beta}\right)^2 = 2\frac{m^2}{\beta^2}$$

$$\frac{\sigma_{p^2}^2}{\langle p^2 \rangle^2} = \frac{2\,\frac{m^2}{\beta^2}}{\frac{m^2}{\beta^2}} = 2$$

$\lightning$

in 2D, due to the degrees of freedom a factor $\times \frac{1}{2}$ has to be applied.

$$2 \times \frac{1}{2} = \underline{\underline{1}}$$

Show

$$\frac{\sigma_T^2}{\langle T \rangle^2_{NVT}} = \frac{1}{N}$$

Without going into too much thermodynamical Details:

For small temperature fluctuations σ_T^2 may be expressed as follows:

$$\sigma_T^2 \approx \frac{\sigma_E^2}{(N k_B)^2}$$

some correction factors (like 1,25 are ignored)

with the energy fluctuation σ_E^2

The variance in Energy $\sigma_E^2 = \langle E^2 \rangle - \langle E \rangle^2$ is given from thermal physics as

(1) $\sigma_E^2 = k_B T^2 C_V$ with the heat capacity C_V.

With $C_V := \left.\frac{\partial E}{\partial T}\right|_V$ and the $KE = \frac{1}{2} k_B T N$

$\Rightarrow$ $C_V = N k_B$ (2)

for N particles with 2 degrees of Freedom in 2D

$\Rightarrow$ (2) in (1)

$$\sigma_E^2 = k_B T^2 N k_B = k_B^2 T^2 N^2$$

$$\Rightarrow \sigma_T^2 \approx \frac{\cancel{k_B^2} T^2 \cancel{N}}{N^2 \cancel{k_B^2}} = \frac{T^2}{N}$$

and with $\langle T \rangle^2 = T^2$

$$\Rightarrow \frac{\sigma_T^2}{\langle T \rangle^2} = \frac{T^2}{N T^2} = \frac{1}{N}$$

$\square$

Consequences

$\frac{\sigma_T^2}{\langle T \rangle^2} = \frac{1}{N}$ $\Rightarrow$ for large N the temperature fluctuates very littl.

$\Rightarrow$ for large systems (N big) the temperature is stable, for smaller systems it can vary more

Since $T \propto \langle E \rangle \propto p$: for large systems individual momenta of the particles fluctuate less