Canonical ensemble (NVT)

Maxwell-Boltzmann distribution: $P(p) = \left(\frac{\beta}{2\pi m}\right)^{3/2} e^{-(\beta p^2/2m)}$

Temperature $\longleftrightarrow$ kinetic energy: $k_B T = m\left\langle v_\alpha^2 \right\rangle$

$$\left\langle E_K \right\rangle = \tfrac{3}{2} N k_B T$$

- Berendsen thermostat: Velocity rescaling
- Anderson thermostat: Stochastic coupling
- Nosé-Hoover thermostat: Extended Lagrangian

Temperature fluctuation

$$\boxed{P(p) = \left(\frac{\beta}{2\pi m}\right)^{3/2} e^{-(\beta p^2/2m)}}$$

Relative variance of the kinetic energy:

$$\frac{\sigma_{p^2}^2}{\left\langle p^2 \right\rangle^2} \equiv \frac{\left\langle p^4 \right\rangle - \left\langle p^2 \right\rangle^2}{\left\langle p^2 \right\rangle^2} = \frac{2}{3}$$

Relative variance of temperature:

$$\frac{\sigma_T^2}{\left\langle T_K \right\rangle_{NVT}^2} \equiv \frac{\left\langle T_K^2 \right\rangle_{NVT} - \left\langle T_K \right\rangle_{NVT}^2}{\left\langle T_K \right\rangle_{NVT}^2}$$

$$= \frac{N\left\langle p^4 \right\rangle + N(N-1)\left\langle p^2 \right\rangle\left\langle p^2 \right\rangle - N^2\left\langle p^2 \right\rangle^2}{N^2\left\langle p^2 \right\rangle^2}$$

$$= \frac{1}{N}\frac{\left\langle p^4 \right\rangle - \left\langle p^2 \right\rangle^2}{\left\langle p^2 \right\rangle^2} = \frac{2}{3N}$$