

We first derive the equipartition theorem for a system with a quadratic energy given by

Source: Schroeder,
Intro to Thermal Physics

$$E(q) = cq^2,$$

where q could be the position, momentum, etc. We suppose $q \in (-\infty, \infty)$ is continuous, and that our system is in equilibrium with a thermal bath at temperature T . We compute $\langle E \rangle$.

$$\begin{aligned} Z &= \frac{1}{2\pi\hbar} \int_{-\infty}^{\infty} e^{-\beta cq^2} dq = \frac{1}{2\pi\hbar} \cdot \frac{1}{\sqrt{\beta c}} \int_{-\infty}^{\infty} e^{-\beta cq^2} d\sqrt{\beta c} q \\ &= \frac{1}{2\pi\hbar} \cdot \frac{1}{\sqrt{\beta c}} \int_{-\infty}^{\infty} e^{-x^2} dx = \frac{1}{2\hbar} \frac{1}{\sqrt{\beta c\pi}}. \end{aligned}$$

$$\langle E \rangle = -\frac{\partial}{\partial \beta} \ln Z = -\frac{1}{Z} \frac{\partial Z}{\partial \beta} =$$

$$-2\hbar \sqrt{\beta c\pi} \cdot \frac{1}{2\hbar \sqrt{\beta c}} \cdot -\frac{1}{2} \beta^{-3/2} = \frac{1}{2\beta} = \frac{1}{2} k_B T.$$

This is the equipartition theorem for a system with a single quadratic degree of freedom: the average energy associated with that degree of freedom is $\frac{1}{2} k_B T$.

We next derive the equipartition theorem for system with a single linear degree of freedom.

Source: Schroeder, Intro Thermal Physics, Problem 6.7

Consider a system in equilibrium with a thermal bath at temperature T , with energy given by $E(q) = c|q|$, $q \in (-\infty, \infty)$. We compute its average energy:

$$Z = \frac{1}{2\pi\hbar} \int_{-\infty}^{\infty} e^{-\beta E(q)} dq = \frac{1}{\pi\hbar} \int_0^{\infty} e^{-\beta c q} dq =$$

$$\frac{1}{\pi\hbar\beta c} \int_0^{\infty} e^{-x} dx = \frac{1}{\pi\hbar\beta c}. \quad \text{We can now compute the average}$$

energy

$$\langle E \rangle = -\frac{\partial}{\partial \beta} \ln Z = -\frac{1}{Z} \frac{\partial Z}{\partial \beta} = -\pi\hbar\beta c \cdot -\frac{1}{\pi\hbar c \beta^2}$$

$$= \frac{1}{\beta} = \boxed{k_B T}$$

Thus, the equipartition theorem for a system with a single linear degree of freedom is simply the statement that the average energy for that DOF is $k_B T$.

Next, consider a system where the energy is given by

$$E(q) = c|q|^n \quad (\text{we include the absolute value to ensure decay for large } q \text{ and odd } n.)$$

Its partition function is given by

$$Z = \frac{1}{2\pi\hbar} \int_{-\infty}^{\infty} e^{-\beta c|z|^n} dz = \frac{1}{2\pi\hbar (\beta c)^{1/n}} \int_{-\infty}^{\infty} e^{-|x|^n} dx$$

$$= \frac{2}{\pi\hbar (\beta c)^{1/n}} \frac{1}{n} \Gamma\left(\frac{1}{n}\right).$$

It follows that the average energy for this system is given by

$$\langle E \rangle = -\frac{\partial}{\partial \beta} \ln Z = -\frac{1}{Z} \frac{\partial Z}{\partial \beta} = -\frac{\pi\hbar (\beta c)^{1/n} n}{2\Gamma(1/n)} \cdot \frac{2\Gamma(1/n)}{\pi\hbar c^{1/n} n} \left(-\frac{1}{n}\right) \beta^{-1/n-1}$$

$$\frac{1}{\beta n} = \boxed{\frac{k_B T}{n}}$$

So more generally, the equipartition theorem for a single degree-of-freedom DOF states that the average energy for that DOF is $k_B T/n$.

Finally, consider a system with many degree-of-freedom (DOF) whose energy is given by

$$E(q_1, \dots, q_m) = c_1 |q_1|^n + \dots + c_m |q_m|^n$$

In this case, the partition function is given by

$$\begin{aligned} Z &= \frac{1}{(2\pi\hbar)^m} \int_{-\infty}^{\infty} \dots \int_{-\infty}^{\infty} dq_1 \dots dq_m e^{-\beta(c_1 |q_1|^n + \dots + c_m |q_m|^n)} \\ &= \frac{1}{(2\pi\hbar)^m} \left(\int_{-\infty}^{\infty} e^{-\beta c_1 |q_1|^n} dq_1 \right) \dots \left(\int_{-\infty}^{\infty} e^{-\beta c_m |q_m|^n} dq_m \right) \\ &= \frac{1}{(2\pi\hbar)^m} \cdot \frac{1}{\beta^{m/n}} \cdot \frac{2^m}{(c_1 \dots c_m)^{1/n}} \frac{1}{n^m} \Gamma\left(\frac{1}{n}\right)^m, \text{ which implies} \end{aligned}$$

that

$$\begin{aligned} \langle E \rangle &= -\frac{\partial}{\partial \beta} \ln Z = -\frac{1}{Z} \frac{\partial Z}{\partial \beta} = \\ &= (c_1 \dots c_m)^{1/n} \left(\frac{2\pi\hbar \beta^{1/n} n}{2\Gamma(1/n)} \right)^m \left(\frac{2\Gamma(1/n)}{2\pi\hbar n} \right)^m \frac{1}{(c_1 \dots c_m)^{1/n}} (-m/n) \beta^{-m/n-1} \\ &= \frac{m}{n} = \boxed{\frac{m \cdot k_B T}{n}} \end{aligned}$$

Thus, we arrive at a more general version of the equipartition theorem:
For a system with m degree-of-freedom DOFs,

$$\frac{\langle E \rangle}{m} = \frac{k_B T}{2}$$

That is, the average energy per DOF is $k_B T/2$, and equivalently,
the average total energy is $m \cdot k_B T/2$.