

# More

## A Derivation of the Equipartition Theorem

The general derivation of the equipartition theorem involves statistical mechanics beyond the scope of our discussions, so we will do a special case using a familiar classical system, simple harmonic oscillators each consisting of a particle moving in one dimension under the action of an elastic restoring force such as a spring with force constant  $\kappa$ . The kinetic energy of the particle at any instant is  $\frac{1}{2}mv_x^2$  and its potential energy is  $\frac{1}{2}\kappa x^2$ , so the total energy is

$$E = \frac{1}{2}mv_x^2 + \frac{1}{2}\kappa x^2 \quad \mathbf{8-38}$$

From Equation 8-13 the Boltzmann distribution is

$$f_B(E) = Ae^{-E/kT} = Ae^{-(mv_x^2/2kT + \kappa x^2/2kT)} \quad \mathbf{8-39}$$

The probability that an oscillator will have energy  $E$  corresponding to  $v_x$  in  $dv_x$  and  $x$  in  $dx$  will be

$$f_B(E) dx dv_x = Ae^{-(mv_x^2/2kT + \kappa x^2/2kT)} dx dv_x \quad \mathbf{8-40}$$

where the constant  $A$  is determined from the normalization condition that the total probability is 1, i.e.,

$$\int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} Ae^{-(mv_x^2/2kT + \kappa x^2/2kT)} dx dv_x = 1 \quad \mathbf{8-41}$$

This rearranges to

$$A \int_{-\infty}^{+\infty} e^{-mv_x^2/2kT} dx_x \int_{-\infty}^{+\infty} e^{-\kappa x^2/2kT} dx = 1 \quad \mathbf{8-42}$$

The two integrals in Equation 8-42 are both of the same form. With the aid of Table B1-1, we have

$$A = \left( \frac{m}{2\pi kT} \right)^{1/2} \left( \frac{\kappa}{2\pi kT} \right)^{1/2} \quad \mathbf{8-43}$$

The average energy of an oscillator is then given by

$$\begin{aligned} \langle E \rangle &= \int \int E f_B(E) dx dv_x \\ &= A \int_{-\infty}^{+\infty} \left( \frac{1}{2} mv_x^2 + \frac{1}{2} \kappa x^2 \right) e^{-mv_x^2/2kT} e^{-\kappa x^2/2kT} dx dv_x \end{aligned} \quad \mathbf{8-44}$$

$$\langle E \rangle = A \int_{-\infty}^{+\infty} \frac{1}{2} m v_x^2 e^{-m v_x^2 / 2kT} dv_x \int_{-\infty}^{+\infty} e^{-\kappa x^2 / 2kT} dx + A \int_{-\infty}^{+\infty} e^{-m v_x^2 / 2kT} dv_x \int_{-\infty}^{+\infty} \frac{1}{2} \kappa x^2 e^{-\kappa x^2 / 2kT} dx \quad \mathbf{8-45}$$

Notice that the first term in Equation 8-45 is the integral of the kinetic energy times  $f_B(E)$ , i.e., it is the average kinetic energy of the oscillator. Similarly, the second term is the average potential energy. These integrals may also be evaluated with the aid of Table B1-1. The result, when multiplied by  $A$  as given by Equation 8-43, yields

$$\langle E \rangle = \left( \frac{1}{2} m v_x^2 \right)_{\text{av}} + \left( \frac{1}{2} \kappa x^2 \right)_{\text{av}} = \frac{1}{2} kT + \frac{1}{2} kT = kT \quad \mathbf{8-46}$$

The important features of this result are (1) that both the average kinetic energy and the average potential energy depend *only* on the absolute temperature and (2) that each average value is equal to  $\frac{1}{2} kT$ . This result for the harmonic oscillator is a special case of the general equipartition of energy theorem:

**In equilibrium, each degree of freedom contributes  $\frac{1}{2} kT$  to the average energy per molecule.**