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## Harmonic oscillators

Our proof of the equipartition theorem depends crucially on the classical approximation. To see how quantum effects modify this result, let us examine a particularly simple system which we know how to analyze using both classical and quantum physics: *i.e.*, a simple harmonic oscillator. Consider a one-dimensional harmonic oscillator in equilibrium with a heat reservoir at temperature T. The energy of the oscillator is given by

$$E = \frac{p^2}{2m} + \frac{1}{2}\kappa x^2,\tag{467}$$

where the first term on the right-hand side is the kinetic energy, involving the momentum p and

mass m, and the second term is the potential energy, involving the displacement x and the force constant  $\kappa$ . Each of these terms is quadratic in the respective variable. So, in the classical approximation the equipartition theorem yields:

$$\frac{\overline{p^2}}{2m} = \frac{1}{2}kT, \tag{468}$$

$$\frac{1}{2}\kappa \overline{x^2} \qquad = \qquad \frac{1}{2}kT. \tag{469}$$

That is, the mean kinetic energy of the oscillator is equal to the mean potential energy which equals  $(1/2)\,k\,T$ . It follows that the mean total energy is

$$\overline{E} = \frac{1}{2} k T + \frac{1}{2} k T = k T. \tag{470}$$

According to quantum mechanics, the energy levels of a harmonic oscillator are equally spaced and satisfy

$$E_n = (n+1/2)\,\hbar\,\omega,\tag{471}$$

where  $\,n\,$  is a non-negative integer, and

$$\omega = \sqrt{\frac{\kappa}{m}}.\tag{472}$$

The partition function for such an oscillator is given by

$$Z = \sum_{n=0}^{\infty} \exp(-\beta E_n) = \exp[-(1/2)\beta \hbar \omega] \sum_{n=0}^{\infty} \exp(-n\beta \hbar \omega). \tag{473}$$

Now,

$$\sum_{n=0}^{\infty} \exp(-n\beta\hbar\omega) = 1 + \exp(-\beta\hbar\omega) + \exp(-2\beta\hbar\omega) + \cdots$$
 (474)

is simply the sum of an infinite geometric series, and can be evaluated immediately,

$$\sum_{n=0}^{\infty} \exp(-n\beta\hbar\omega) = \frac{1}{1 - \exp(-\beta\hbar\omega)}.$$
(475)

Thus, the partition function takes the form

$$Z = \frac{\exp[-(1/2)\beta\hbar\omega]}{1 - \exp(-\beta\hbar\omega)},\tag{476}$$

and

$$\ln Z = -\frac{1}{2} \beta \hbar \omega - \ln[1 - \exp(-\beta \hbar \omega)] \tag{477}$$

The mean energy of the oscillator is given by [see Eq. (399)]

$$\overline{E} = -\frac{\partial}{\partial \beta} \ln Z = -\left[ -\frac{1}{2} \hbar \omega - \frac{\exp(-\beta \hbar \omega) \hbar \omega}{1 - \exp(-\beta \hbar \omega)} \right], \tag{478}$$

οг

$$\overline{E} = \hbar \,\omega \left[ \frac{1}{2} + \frac{1}{\exp(\beta \,\hbar \,\omega) - 1} \right]. \tag{479}$$

Consider the limit

$$\beta \, \hbar \, \omega = \frac{\hbar \, \omega}{k \, T} \ll 1,\tag{480}$$

in which the thermal energy  $k\,T$  is large compared to the separation  $\hbar\,\omega$  between the energy levels. In this limit,

$$\exp(\beta \hbar \omega) \simeq 1 + \beta \hbar \omega, \tag{481}$$

$$\overline{E} \simeq \hbar \, \omega \left[ \frac{1}{2} + \frac{1}{\beta \, \hbar \, \omega} \right] \simeq \hbar \, \omega \left[ \frac{1}{\beta \, \hbar \, \omega} \right], \tag{482}$$

giving

$$\overline{E} \simeq \frac{1}{\beta} = kT. \tag{483}$$

Thus, the classical result (470) holds whenever the thermal energy greatly exceeds the typical spacing between quantum energy levels.

Consider the limit

$$\beta \, \hbar \, \omega = \frac{\hbar \, \omega}{k \, T} \gg 1,\tag{484}$$

in which the thermal energy is small compared to the separation between the energy levels. In this limit,

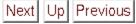
$$\exp(\beta \hbar \omega) \gg 1,$$
 (485)

and so

$$\overline{E} \simeq \hbar \,\omega \left[ 1/2 + \exp(-\beta \,\hbar \,\omega) \right] \simeq \frac{1}{2} \,\hbar \,\omega. \tag{486}$$

Thus, if the thermal energy is much less than the spacing between quantum states then the mean energy approaches that of the ground-state (the so-called zero point energy). Clearly, the equipartition theorem is only valid in the former limit, where  $k\,T\gg\hbar\,\omega$ , and the oscillator

possess sufficient thermal energy to explore many of its possible quantum states.



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