Equi-partition Theorem

In the classical limit, the average of \( z \frac{\partial H}{\partial z} \), where \( H \) is the Hamiltonian and \( z \) is a generalized coordinate or a conjugate momentum, can be expressed as a ratio of integrals over phase space:

\[
\langle z \frac{\partial H}{\partial z} \rangle = \int d\omega \left( z \frac{\partial H}{\partial z} \right) e^{-\beta H} \bigg/ \int d\omega e^{-\beta H}.
\]

The phase-space measure can be expressed as \( d\omega = d\omega' dz \). The integral over \( z \) in the numerator is

\[
\int_{z_{\text{min}}}^{z_{\text{max}}} dz \left( z \frac{\partial H}{\partial z} \right) e^{-\beta H}
\]

A. Express the integrand with a factor of \((\partial/\partial z)e^{-\beta H}\).

\[
z \frac{\partial H}{\partial z} e^{-\beta H} = -\frac{1}{\beta} z \frac{\partial}{\partial z} e^{-\beta H}
\]

B. Integrate by parts to get a term with integrand \( e^{-\beta H} \) and a boundary term.

\[
\int_{2_{\text{min}}}^{z_{\text{max}}} dz \left( -\frac{1}{\beta} z \frac{\partial}{\partial z} e^{-\beta H} \right) = -\frac{1}{\beta} z e^{-\beta H} \bigg|_{z_{\text{max}}}^{z_{\text{min}}} + \frac{1}{\beta} \int_{z_{\text{min}}}^{z_{\text{max}}} dz z e^{-\beta H}
\]

Show that if \( H \) approaches \(+\infty\) as \( z \) approaches its endpoints, the average reduces to

\[
\langle z \frac{\partial H}{\partial z} \rangle = \frac{0 + \frac{1}{\beta} \int d\omega e^{-\beta H}}{\int d\omega e^{-\beta H}} = \frac{1}{\beta} = T
\]

where \( T \) is the temperature.

C. Determine the average value of each of the following terms in \( H \):

- \( H \) depends on the momentum component \( p \) only through the term \( p^2/2m \)
  \[
P \left( \frac{\partial}{\partial p} \left( \frac{p^2}{2m} \right) \right) = 2 \left( \frac{p^2}{2m} \right) \implies 2 \langle \frac{p^2}{2m} \rangle = T \implies \langle \frac{p^2}{2m} \rangle = \frac{1}{2} T
  \]

- \( H \) depends on the coordinate \( x \) only through the term \( \frac{1}{4} \gamma x^4 \)
  \[
x \left( \frac{\partial}{\partial x} \left( \frac{1}{4} \gamma x^4 \right) \right) = 4 \left( \frac{1}{4} \gamma x^4 \right) \implies 4 \langle \frac{1}{4} \gamma x^4 \rangle = T \implies \langle \frac{1}{4} \gamma x^4 \rangle = \frac{1}{4} T
  \]

- \( H \) depends on the angular momentum component \( L \) only through the term \( L^2/2I \) (the moment of inertia \( I \) is positive)
  \[
  L \left( \frac{\partial}{\partial L} \left( \frac{L^2}{2I} \right) \right) = 2 \left( \frac{L^2}{2I} \right) \implies 2 \langle \frac{L^2}{2I} \rangle = T \implies \langle \frac{L^2}{2I} \rangle = \frac{1}{2} T
  \]

Compare your results with your neighbors.
Show your results to the instructor.
If \( z \) is a generalized coordinate or a conjugate momentum, then in the classical limit

\[
\left\langle z \frac{\partial H}{\partial z} \right\rangle = T,
\]

where \( T \) is the temperature.

D. Show that the operator \( z \partial / \partial z \) counts the powers of \( z \): \( (z \partial / \partial z) z^n = n z^n \).

\[
z \frac{\partial}{\partial z} z^n = z \cdot n z^{n-1} = n \cdot z^n
\]

Determine the average energy \( U \) in the classical limit for the following systems:

E. \( N \) atoms in a harmonic trapping potential with Hamiltonian

\[
H = \sum_{n=1}^{N} \left( \frac{1}{2m} \mathbf{p}_n^2 + \frac{1}{2} m \omega^2 r_n^2 \right).
\]

\[
U = \left\langle H \right\rangle = N \cdot \left( \frac{3}{2} T \right) + N \cdot \left( \frac{3}{3} T \right) = 3NT
\]

F. \( N \) quartic oscillators with Hamiltonian

\[
H = \sum_{n=1}^{N} \left( \frac{1}{2m} \mathbf{p}_n^2 + \frac{1}{4} \gamma x_n^4 \right).
\]

\[
U = \left\langle H \right\rangle = N \cdot \left( \frac{3}{4} \gamma \right) + N \cdot \left( \frac{1}{2} \gamma \right) = \frac{3}{4} \gamma NT
\]

G. an ideal gas of \( N \) diatomic molecules with atomic mass \( m \), vibrational frequency \( \omega \), and bond length \( R \). Its Hamiltonian can be approximated by

\[
H = \sum_{n=1}^{N} \left( \frac{1}{4m} \mathbf{p}_n^2 + \frac{1}{4} m \omega^2 z_n^2 + \frac{1}{mR^2} \left( L_{nx}^2 + L_{ny}^2 \right) \right),
\]

where \( R + z_n \) is the separation of the two atoms in the molecule and \( L_{nx} \) and \( L_{ny} \) are components of the internal angular momentum of the molecule.

\[
U = \left\langle H \right\rangle = N \left( \frac{3}{2} T \right) + N \cdot \left( \frac{1}{2} T \right) + N \cdot \left( \frac{5}{2} T \cdot 2 \right) = 3NT
\]

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