Equipartition Theorem:—

Let p_i or q_i $(i = 1, 2, \ldots 3N)$ is denoted by x_i

Then we have to calculate $\left\langle x_i \frac{\partial H}{\partial x_j} \right\rangle$

where $H = H(\vec{r_i}, \vec{p_i})$ is the Hamiltonian

$$\left\langle x_i \frac{\partial H}{\partial x_j} \right\rangle = \frac{\int\limits_{E \le H \le E+\Delta} d\vec{r_i} \int d\vec{p_i}\; x_i \frac{\partial H}{\partial x_j} \times \cancel{\rho_0}}{\int\limits_{E \le H \le E+\Delta} d\vec{r_i} \int d\vec{p_i} \times \cancel{\rho_0}}$$

we have seen $\Gamma(E) = \int\limits_{E \le H \le E+\Delta} d\vec{r_i} \int d\vec{p_i}$

Thus $$\left\langle x_i \frac{\partial H}{\partial x_j} \right\rangle = \frac{1}{\Gamma(E)} \int\limits_{E \le H \le E+\Delta} d\vec{r_i} \int d\vec{p_i}\; x_i \frac{\partial H}{\partial x_j}$$

$$= \frac{1}{\Gamma(E)} \left[\int\limits_{H \le E+\Delta} d\vec{r_i} \int d\vec{p_i}\; x_i \frac{\partial H}{\partial x_j} - \int\limits_{H \le E} d\vec{r_i} \int d\vec{p_i}\, \frac{\partial H}{\partial x_j} \right]$$

Taylor's expansion $f(x+h) = f(x) + h f'(x) + \frac{h^2}{2!} f''(x) + \ldots$

$$\frac{1}{\Gamma(E)} \left[\int\limits_{H \le E} d\vec{r_i} \int d\vec{p_i}\, x_i \frac{\partial H}{\partial x_j} + \Delta \frac{\partial}{\partial E} \int\limits_{H \le E} d\vec{r_i} \int d\vec{p_i}\; x_i \frac{\partial H}{\partial x_j} + \ldots - \int\limits_{H \le E} d\vec{r_i} \int d\vec{p_i}\, \frac{\partial H}{\partial x_j} \right]$$

or $\left\langle x_i \frac{\partial H}{\partial x_j} \right\rangle = \frac{1}{\Gamma(E)} \Delta \frac{\partial}{\partial E} \int_{H \le E} d\vec{r}_\nu \int d\vec{p}_\nu \, x_\nu \frac{\partial H}{\partial x_j}$

Since $\frac{\partial E}{\partial x_j} = 0$, we can write the above expression as

$$\left\langle x_\nu \frac{\partial H}{\partial x_j} \right\rangle = \frac{\Delta}{\Gamma(E)} \frac{\partial}{\partial E} \left[\int_{H \le E} d\vec{r}_\nu \int d\vec{p}_\nu \, x_i \frac{\partial (H-E)}{\partial x_j} \right]$$

Next we have $\Gamma(E) = \Delta \omega(E)$ and doing some mathematical trick in the above expression

$$\left\langle x_\nu \frac{\partial H}{\partial x_j} \right\rangle = \frac{1}{\omega(E)} \frac{\partial}{\partial E} \left[\int_{H \le E} d\vec{r}_\nu \int d\vec{p}_\nu \left(\frac{\partial}{\partial x_j} \{ x_\nu (H-E) \} - (H-E) \frac{\partial x_\nu}{\partial x_j} \right) \right]$$

The first integral on the rhs is zero because it reduces to a surface integral on $H=E$ surface.

Thus we obtain

$$\left\langle x_i \frac{\partial H}{\partial x_j} \right\rangle = -\frac{1}{\omega(E)} \frac{\partial}{\partial E} \left[\int_{H \le E} d\vec{r}_\nu \int d\vec{p}_\nu (H-E) \delta_{ij} \right]$$

$$= \frac{-\delta_{ij}}{\omega(E)} \left[- \int_{H \le E} d\vec{r}_i \int d\vec{p}_i \right]$$

$$= \frac{\delta_{ij}}{\omega(E)} \Sigma(E) = \frac{\delta_{ij} \Sigma(E)}{\left(\frac{\partial \Sigma(E)}{\partial E} \right)}$$

$$= \delta_{ij} \left[\frac{\partial}{\partial E} \ln \Sigma(E) \right]^{-1} = \delta_{ij} \left[\frac{k_B}{\frac{\partial S}{\partial E}} \right]$$

or $$\boxed{\left\langle x_\nu \frac{\partial H}{\partial x_j} \right\rangle = \delta_{\nu j} k_B T}$$

Generalized equipartition theorem

H.W. Take $i = j$; $x_\nu = p_\nu$ and $\nu = j$; $x_\nu = \vec{r}_\nu$ and obtain the above result