VIVEKANANDA COLLEGE THAKURPUKUR KOLKATA-700063

NAAC ACCREDITED ‘A’ GRADE

Topic: Energy Fluctuation and Equipartition Theorem (https://www.youtube.com/watch?v=XVMacD60Xvw)

Course Title: Statistical Mechanics

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Name of the Department: Physics PG

Energy Fluctuation

$$U = \frac{\sum_r E_r e^{-\beta E_r}}{\sum_r e^{-\beta E_r}}$$

$$\Rightarrow \frac{\partial U}{\partial \beta} = \frac{\sum -E_r^2 e^{-\beta E_r}}{\sum e^{-\beta E_r}} - \frac{\sum E_r e^{-\beta E_r}}{(\sum e^{-\beta E_r})^2} \times \left(-\sum E_r e^{-\beta E_r}\right)$$

$$\frac{-\partial U}{\partial \beta} = \langle E^2 \rangle - \langle E \rangle^2$$

$$= \langle \Delta E^2 \rangle$$

$$\text{RMS} = \frac{\langle \Delta E^2 \rangle^{1/2}}{\langle E \rangle}$$

Rel. Root Mean Square Fluctuation in Energy

$$\langle \Delta E^2 \rangle = -\frac{\partial U}{\partial \beta} = KT^2 \frac{\partial U}{\partial T} = KT^2 C_V \propto N$$

as $C_V \propto N$

$E \propto N$

$$\frac{\langle \Delta E^2 \rangle^{1/2}}{E} = \frac{(O)N^{1/2}}{N} = \frac{1}{N^{1/2}}$$

Equipartition Theorem:

x_i, x_j coordinates in phase space

$$\left\langle x_i \frac{\partial H}{\partial x_j} \right\rangle = \frac{\int x_i \frac{\partial H}{\partial x_j} e^{-\beta H} d\omega}{\int e^{-\beta H} d\omega}$$

$\boxed{d\omega = d^{3N}q \, d^{3N}p}$

$$x_i \frac{\partial H}{\partial x_j} e^{-\beta H} = -\frac{x_i}{\beta} \frac{\partial}{\partial x_j} e^{-\beta H}$$

$$\int x_i \frac{\partial H}{\partial x_j} e^{-\beta H} d\omega = -\frac{1}{\beta} \int x_i \frac{\partial}{\partial x_j} e^{-\beta H} d\omega$$

Int. w.r.t dx_j (by parts)

$$-\frac{1}{\beta} \, x_i \, e^{-\beta H} \Big|_{x_j(1)}^{x_j(2)} d\omega_j + \frac{1}{\beta} \int \frac{\partial x_i}{\partial x_j} e^{-\beta H} dx_j \, d\omega_j$$

where $x_j(1)$ & $x_j(2)$ are extreme values of x_j

$d\omega_j \to d\omega$ devoid of dx_j

$$\left.\begin{array}{l} H(x_j(2)) \to \infty \\ H(x_j(1)) \to \infty \end{array}\right\} e^{-\beta H} \to 0 \;\; \& \;\; \frac{\partial x_i}{\partial x_j} = \delta_{ij}$$

$$= \frac{1}{\beta} \delta_{ij} \int e^{-\beta H} d\omega$$

$$\left\langle x_i \frac{\partial H}{\partial x_j} \right\rangle = \frac{\delta_{ij}}{\beta} = KT\delta_{ij}$$

For $x_i = p_i = x_j$ $\left\langle p_i \frac{\partial H}{\partial p_i} \right\rangle = \langle p_i \dot{q}_i \rangle = KT$

$x_i = q_i = x_j$ $\left\langle q_i \frac{\partial H}{\partial q_i} \right\rangle = -\langle q_i \dot{p}_i \rangle = KT$

$$\sum_{i=1}^{3N} \langle p_i \dot{q}_i \rangle = 3NKT$$

$$-\sum \langle q_i \dot{p}_i \rangle = 3NKT$$

Equipartition Theorem:

$$H = \sum_j A_j P_j^2 + \sum B_j Q_j^2$$

$$\sum\left(P_j \frac{\partial H}{\partial P_j} + Q_j \frac{\partial H}{\partial Q_j}\right) = 2H$$

Taking average.

$$\left\langle \sum\left(P_j \frac{\partial H}{\partial P_j} + Q_j \frac{\partial H}{\partial Q_j}\right)\right\rangle = 2\langle H\rangle$$

$$3NKT + 3NKT = 2\langle H\rangle$$

$$\langle H\rangle = \frac{6NKT}{2}$$

for $f \rightarrow$ degrees of freedom

$$\langle H\rangle = f\,\frac{KT}{2} \rightarrow$$