Some consequences of generalized equipartition theorem! —

In the last lecture we have obtained the expression for generalized equipartition theorem as

$$\left\langle x_i \frac{\partial H}{\partial x_j} \right\rangle = \delta_{ij} k_B T \quad \text{——— (1)}$$

Now we take (1) $i=j$ and $x_i = p_i$, we obtain

$$\left\langle p_i \frac{\partial H}{\partial p_i} \right\rangle = k_B T \quad \text{——— (2)}$$

$(i=1, --, 3N)$

(2) $i=j$ and $x_i = r_i$, we have

$$\left\langle r_i \frac{\partial H}{\partial r_i} \right\rangle = k_B T \quad \text{——— (3)} \quad (i=1, ---3N)$$

From the canonical equations of motion

$$\frac{\partial H}{\partial r_i} = -\dot{p}_i$$

$$\boxed{\left\langle \sum_{i=1}^{3N} r_i \dot{p}_i \right\rangle = -3N k_B T} \quad \text{——— (4)}$$

Virial Theorem

In classical mechanics the sum of i-th coordinate times the ith component of the generalized force $(\sum r_i \dot{p}_i)$ is known as Virial theorem.

In many Physical system the Hamiltonians can be canonically transformed into the form

$$H = \sum_{i=1}^{3N} A_i P_i^2 + \sum_{i=1}^{3N} B_i Q_i^2$$

where P_i, Q_i are canonically conjugate variables and A_i, B_i are constants. For this kind of system we obtain

$$\sum_{i=1}^{3N} \left(P_i \frac{\partial H}{\partial P_i} + Q_i \frac{\partial H}{\partial Q_i} \right) = 2H \quad (5)$$

~~Let us take nonvanishing const A~~

If f is no. of A_i and B_i constants which are nonvanishing. Then from (2), (3) and (5)

$$2\langle H \rangle = f k_B T$$

$$\boxed{\langle H \rangle = \frac{1}{2} f k_B T}$$

$\Rightarrow$ Each harmonic term in the Hamiltonian contributes to $\frac{1}{2} k_B T$ to the average energy of the system.