Equipartition theorem

Let x_j be any component of $\mu = (\vec{q}, \vec{p})$. (That is, it can be any position or momentum component)

Expectation value

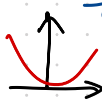
$$\left\langle x_j \frac{\partial H}{\partial x_k} \right\rangle = \frac{1}{Z} \int d\Gamma \, x_j \frac{\partial H}{\partial x_k} e^{-\beta H(\mu)}, \qquad d\Gamma = \prod_{j=1}^{N} d^3 q_j \, d^3 p_j$$

Notice that

$$\frac{\partial}{\partial x_k}\left[\frac{1}{\beta} e^{-\beta H(\mu)}\right] = -\frac{\partial H}{\partial x_k} e^{-\beta H(\mu)}$$

So I can perform the integration by parts on the numerator; if we define $d\Gamma_k$ to be the integration measure but without the coordinate dx_k, then

$$\int d\Gamma \, x_j \frac{\partial H}{\partial x_k} e^{-\beta H} = \left[-x_j \frac{\partial H}{\partial x_k} e^{-\beta H} \Big|_{-\infty}^{\infty} + \frac{1}{\beta} \int dx_k \cancelto{\delta_{jk}}{\frac{\partial x_j}{\partial x_k}} e^{-\beta H} \right]_{d\Gamma_k}$$

If the Hamiltonian is harmonic , then $H(\infty) = H(-\infty) = \infty$ and the first term vanishes. Consequently,

$$\left\langle x_j \frac{\partial H}{\partial x_k} \right\rangle = \frac{1}{\beta} \delta_{jk} \frac{\cancel{\int d\Gamma \, e^{-\beta H}}}{\cancel{Z}} = \boxed{\delta_{jk} k_B T}$$

What does this mean for a harmonic system? Suppose that

$$H = \sum_j a_j p_j^2 + \sum_j b_j q_j^2 .$$

Then $$\sum_j \left(p_j \underbrace{\frac{\partial H}{\partial p_j}}_{2a_j p_j} + q_j \underbrace{\frac{\partial H}{\partial q_j}}_{2b_j q_j} \right) = 2H$$

Thus,

$$\langle H \rangle = \frac{1}{2} \sum_{j=1}^{f/2} \left[\left\langle p_j \frac{\partial H}{\partial p_j} \right\rangle + \left\langle q_j \frac{\partial H}{\partial q_j} \right\rangle \right] = \boxed{\frac{1}{2} f k_B T}$$

where f is the total number of "harmonic" degrees of freedom that the system has. (Here p_j and q_j count as two different d.o.f.)