Consider a system in which the energy E depends continuously on two variables: $E = E(x_i, x_j)$. Show that, given the canonical distribution, it follows that

$$\langle x_i \frac{\partial E}{\partial x_j} \rangle = k_B T \delta_{ij},$$

where δ_{ij} is the Kronecker delta.

Assume now that one has a harmonic oscillator with energy,

$$E(p, q) = \frac{p^2}{2m} + \frac{K}{2} q^2,$$

where m is the mass of the oscillator and K the spring constant. Use the results above to show that $\langle E \rangle = k_B T$ (equipartition of energy).

Consider a general system with the energy depending continuously on two variables:

$$E = E(x_i, x_j)$$

We calculate:

$$\langle x_i \frac{\partial E}{\partial x_j} \rangle = \frac{1}{Z} \int dx_i dx_j \; x_i \frac{\partial E}{\partial x_j} e^{-\beta E(x_i, x_j)} =$$

$$= \frac{1}{Z} \int dx_i dx_j \; x_i \left(-\frac{1}{\beta}\right) \frac{\partial}{\partial x_j} e^{-\beta E(x_i, x_j)}$$

$$= -\frac{k_B T}{Z} \int dx_i dx_j \; x_i \frac{\partial}{\partial x_j} e^{-\beta E(x_i, x_j)} =$$

integrate by parts

$$\stackrel{\downarrow}{=} \frac{k_B T}{Z} \int dx_i dx_j \left(\frac{\partial x_i}{\partial x_j}\right) e^{-\beta E(x_i, x_j)} = \boxed{k_B T \delta_{ij} = \langle x_i \frac{\partial E}{\partial x_j} \rangle}$$

Consider now a harmonic oscillator with energy

$$E(p, q) = \frac{p^2}{2m} + \frac{k}{2} q^2$$

where m is the mass and k the spring constant. Use the results above to show $\langle E \rangle = k_B T$

We have: $\langle E \rangle = \frac{1}{2m} \langle p^2 \rangle + \frac{k}{2} \langle q^2 \rangle$

But $\langle p \frac{\partial E}{\partial p} \rangle = \frac{1}{\cancel{2}m} \cancel{2} \langle p^2 \rangle = \frac{\langle p^2 \rangle}{m} = k_B T$ as given above,

$$\langle q \frac{\partial E}{\partial q} \rangle = \frac{k}{2} 2 \langle q^2 \rangle = k \langle q^2 \rangle = k_B T$$

$$\Rightarrow \langle E \rangle = \frac{1}{2\cancel{m}} (k_B T \cancel{m}) + \frac{\cancel{k}}{2} \frac{k_B T}{\cancel{k}} = \frac{1}{2} k_B T + \frac{1}{2} k_B T = k_B T$$