Monte Carlo Simulation

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Microcanonical ensemble

first lets prove:

$$< E >= -\frac{d}{dZ}(\ln(Z))$$

We know:

$$< E >= \frac{\int Ee^{-\beta E}dv}{\int e^{-\beta E}dv}$$

also we can write:

$$\int Ee^{-\beta E}dv = -\frac{d}{d\beta}(\int e^{-\beta E}dv) \Rightarrow < E >= -1/Z\frac{d}{d\beta}(Z) \Rightarrow < E >= -\frac{d}{d\beta}(\ln(Z))$$

First part of this question solved, now let's continue to the next part. Now I have to prove:

$$\sigma_E^2 = \frac{d^2}{d\beta^2}(\ln(Z))$$

the process is similar as before:

$$\frac{d^2}{d\beta^2}(\ln(Z)) = -1/Z^2(\frac{dZ}{d\beta})^2 + 1/Z\frac{d^2Z}{d\beta^2} \qquad (*)$$

$$< E^2 >= 1/Z\int E^2e^{-\beta E}dv = 1/Z\frac{d^2Z}{d\beta^2}$$

From $(*)$ and the equation above, we will get:

$$< E^2 >=< E >^2 + \frac{d^2}{d\beta^2}(\ln(Z)) \Rightarrow \sigma_E^2 = \frac{d^2}{d\beta^2}(\ln(Z))$$

Now lets calculate Heat Capacity:

$$C_V = \frac{d < E >}{dT}$$

$$T = \frac{1}{k_B \beta} \Rightarrow dT = -\frac{1}{k_B \beta^2} d\beta$$

$$\Rightarrow C_V = -k_B \beta^2 \frac{d < E >}{d\beta} = -k_B \beta^2 \frac{d^2}{d\beta^2} (\ln(Z)) = -k_B \beta^2 \sigma_E^2$$