

Problem 4:

a) The only two possible values are the energies $-\epsilon_0$ and ϵ_0 themselves. (2)

b) The probability for the two states in the canonical ensemble which is applicable to this situation are

$$p_1 = \frac{e^{-\frac{\epsilon_0}{k_B T}}}{e^{-\frac{\epsilon_0}{k_B T}} + e^{\frac{\epsilon_0}{k_B T}}} \quad p_2 = \frac{e^{\frac{\epsilon_0}{k_B T}}}{e^{-\frac{\epsilon_0}{k_B T}} + e^{\frac{\epsilon_0}{k_B T}}} \quad (2)$$

c)

$$U = p_1(-\epsilon_0) + p_2(+\epsilon_0) = -\epsilon_0 \frac{e^{-\frac{\epsilon_0}{k_B T}} - e^{\frac{\epsilon_0}{k_B T}}}{e^{-\frac{\epsilon_0}{k_B T}} + e^{\frac{\epsilon_0}{k_B T}}} \quad (1)$$
$$= -\epsilon_0 \tanh \frac{\epsilon_0}{k_B T} \quad (1)$$

d) $T \rightarrow 0 \Rightarrow \frac{\epsilon_0}{k_B T} \rightarrow +\infty \Rightarrow \tanh \frac{\epsilon_0}{k_B T} \rightarrow 1 \Rightarrow U \rightarrow -\epsilon_0$

$T \rightarrow \infty \Rightarrow \frac{\epsilon_0}{k_B T} \rightarrow 0 \Rightarrow U \rightarrow 0$ (1)

all values in between are possible, i.e., $[-\epsilon_0, 0]$ (1)

(if $T \rightarrow 0$ from below $U \rightarrow \epsilon_0$, i.e., if negative temperatures are possible (depends on the heat bath), the range is $[-\epsilon_0, \epsilon_0]$)

Problem 5:

$$a) Z(T) = \sum_{n_1 \in \{L, R, S\}} \dots \sum_{n_N \in \{L, R, S\}} e^{-\beta \sum_{i=1}^N \begin{cases} \epsilon & n_i \in \{L, R\} \\ 0 & n_i = S \end{cases}}$$

$$\stackrel{\textcircled{1}}{=} \left(\sum_{n \in \{L, R, S\}} e^{-\beta \begin{cases} \epsilon & n \in \{L, R\} \\ 0 & n = S \end{cases}} \right)^N$$

$$= (1 + 2e^{-\beta\epsilon})^N \textcircled{2}$$

$$b) U \stackrel{\textcircled{1}}{=} - \left(\frac{\partial \ln Z}{\partial \beta} \right)_N = -N \left(\frac{\partial \ln(1 + 2e^{-\beta\epsilon})}{\partial \beta} \right)_N = -N \frac{2e^{-\beta\epsilon}(-\epsilon)}{1 + 2e^{-\beta\epsilon}}$$
$$= \frac{2N\epsilon}{e^{\beta\epsilon} + 2} \textcircled{2}$$

c) They are identical. $\textcircled{2}$

If they are not identical because of some mistake in parts a) or b) accept only if it is acknowledged that something must be wrong.

Problem:

$$\begin{aligned}
 a) Z(T) &= \frac{1}{C_N} \int d\vec{x}^N e^{-\beta H(\vec{x}^N)} \\
 &= \frac{1}{h^{3N} N!} A^N \int_0^\infty dz_1 \dots \int_0^\infty dz_N \int d^3\vec{r}_1 \dots \int d^3\vec{r}_N e^{-\frac{\beta}{2m} \sum_{i=1}^N \vec{r}_i^2 - \beta mg \sum_{i=1}^N z_i} \quad (2) \\
 &= \frac{1}{h^{3N} N!} A^N \left(\int_0^\infty dz e^{-\beta mg z} \right)^N \left(\int d^3\vec{r} e^{-\frac{\beta}{2m} \vec{r}^2} \right)^N \\
 &= \frac{1}{N!} \left[\frac{A}{h^3} \frac{k_B T}{mg} (2\pi m k_B T)^{3/2} \right]^N \quad (2)
 \end{aligned}$$

$$\begin{aligned}
 b) \rho(\vec{r}) &= \int d\vec{x}^N \frac{e^{-\beta H(\vec{x}^N)}}{C_N Z(T)} \delta(\vec{r}_1 - \vec{r}) \quad (2) \\
 &= \left(\frac{mg}{A k_B T} \right)^N (2\pi m k_B T)^{-\frac{3N}{2}} \int d^3\vec{r}_1 \dots \int d^3\vec{r}_N \int d^3\vec{r}_N e^{-\frac{\beta}{2m} \sum_{i=1}^N \vec{r}_i^2 - \beta mg \sum_{i=1}^N z_i} \delta(\vec{r}_1 - \vec{r}) \\
 &= \left(\frac{mg}{A k_B T} \right)^N (2\pi m k_B T)^{-\frac{3N}{2}} \left(\int d^3\vec{r} e^{-\frac{\beta}{2m} \vec{r}^2} \right)^N A^{N-1} \left(\int_0^\infty dz e^{-\beta mg z} \right)^{N-1} \int d^3\vec{r}_1 e^{-\beta mg z_1} \delta(\vec{r}_1 - \vec{r}) \\
 &= \left(\frac{mg}{A k_B T} \right)^N (2\pi m k_B T)^{-\frac{3N}{2}} (2\pi m k_B T)^{\frac{3N}{2}} A^{N-1} \left(\frac{k_B T}{mg} \right)^{N-1} e^{-\beta mg z} \\
 &= \frac{mg}{A k_B T} e^{-\beta mg z} \quad (2)
 \end{aligned}$$

c) law of large numbers \rightarrow
 there are $N \rho(\vec{r}) A \Delta z$ particles within the volume $A \Delta z$ (1)

$$\begin{aligned}
 \Rightarrow P(z) \overbrace{A \Delta z}^V &= \overbrace{N \rho(\vec{r}) A \Delta z}^{N} k_B T \\
 \Rightarrow P(z) &= \rho(\vec{r}) N k_B T = \frac{N mg}{A} e^{-\frac{mgz}{k_B T}} = P(0) e^{-\frac{mgz}{k_B T}} \quad (1)
 \end{aligned}$$