Hand-in C

Consider a DNA-double helix. The helix consists of base pairs bound together: Adenine binds with Thymine with binding energy E_{A}, and Guanine binds with Cytosine with binding energy E_{C}. The bonds between AT and CG pairs can break and re-form in a process eventually leading to an equilibrium state, while the total energy E remains constant since the helix is isolated from the surroundings. The energy E is used to break n_{A} AT-pairs and n_{C} CG-pairs. Energy conservation gives

$$E = n_{\mathrm{A}} E_{\mathrm{A}} + n_{\mathrm{C}} E_{\mathrm{C}} \tag{1}$$

with $n_{\mathrm{A}} \leq N_{\mathrm{A}}$ and $n_{\mathrm{C}} \leq N_{\mathrm{C}}$ where N_{A} denotes the number of Adenine-Thymine (AT) pairs and N_{C} the number of Guanine-Cytosine (CG) pairs in the helix.

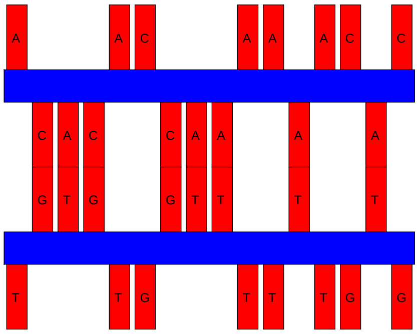

Figure 1: Simplified illustration of a piece of the considered DNA-double helix. The broken pairs stick out to the sides. Each broken AT pair contributes E_{A} to the total energy, and each broken CG pair contributes E_{C} to the total energy, when we measure energy relative to the case where all pairs are unbroken.

Question a:

Find the number of ways $\Omega(n_{\mathrm{A}}, n_{\mathrm{C}})$ one can break n_{A} AT-pairs and n_{C} CG-pairs. Show that for $n_i \gg 1$, $N_i \gg 1$, and $N_i - n_i \gg 1$ $(i = \mathrm{A}, \mathrm{C})$, the entropy S of the helix is

$$\begin{aligned} \frac{S}{k} = {} & N_{\mathrm{A}} \ln(N_{\mathrm{A}}) - n_{\mathrm{A}} \ln(n_{\mathrm{A}}) - (N_{\mathrm{A}} - n_{\mathrm{A}}) \ln(N_{\mathrm{A}} - n_{\mathrm{A}}) \\ & + N_{\mathrm{C}} \ln(N_{\mathrm{C}}) - n_{\mathrm{C}} \ln(n_{\mathrm{C}}) - (N_{\mathrm{C}} - n_{\mathrm{C}}) \ln(N_{\mathrm{C}} - n_{\mathrm{C}}) \end{aligned} \tag{2}$$

Question b:

Use Eq. (1) and Eq. (2) to show that in equilibrium

$$\frac{N_{\mathrm{A}} - n_{\mathrm{A}}^{\mathrm{eq}}}{n_{\mathrm{A}}^{\mathrm{eq}}} = \left(\frac{N_{\mathrm{C}} - n_{\mathrm{C}}^{\mathrm{eq}}}{n_{\mathrm{C}}^{\mathrm{eq}}} \right)^{\gamma}$$

and give a formula for γ. Here, n_i^{eq} are the equilibrium values of n_i.

Question c:

Consider now the special case $N_{\mathrm{A}} = N_{\mathrm{C}}$ and $E_{\mathrm{A}} = E_{\mathrm{C}}$. Calculate $S(E)$ and then the energy $E(T)$ as a function of temperature T. Interpret the limits $\lim_{T\to 0} E(T)$ and $\lim_{T\to\infty} E(T)$ physically.