DNA, the genetic molecule deoxyribonucleic acid, exists as a pair of long molecules. The two molecules can be linked by up to N base pairs. It requires energy ϵ (> 0) to unlink each base pair, and the only configurations accessible to the system are those of the form shown in the figure, in which the first n base pairs are unlinked and the remaining $N - n$ base pairs are linked. The base pair at one end of the molecule (i.e., the N^{th} base pair) is prevented from unlinking. When n base pairs are unlinked then the degeneracy of the configuration is g^n (where $g > 1$), owing to the variety of orientational states available to the unlinked base pairs. The molecule is in equilibrium at temperature T, and Boltzmann's constant is denoted by κ.

(a) Show that the canonical partition function Z, when expressed as a function of N and the variable x [$\equiv g\exp(-\epsilon/\kappa T)$], has the form

$$Z = A\,\frac{x^N - 1}{x - 1},$$

and determine the number A.

(b) Determine, in closed form, the mean fraction of unlinked base pairs $\langle n\rangle/N$, expressing your answer in terms of N and x.

(c) For N large but finite, sketch the mean fraction of unlinked pairs as a function of x. Give the limiting values of this mean fraction at low and high temperatures.

(d) By considering the two quantities

$$\lim_{x\to 1-}\ \lim_{N\to\infty} \langle n\rangle/N \qquad \text{and} \qquad \lim_{x\to 1+}\ \lim_{N\to\infty} \langle n\rangle/N,$$

and taking care with the limits, show that when $N \to \infty$ the system exhibits a phase transition (viz. a discontinuity in the mean fraction of unlinked base pairs), as a function of x, at the value $x = 1$. Note that $\lim_{x\to 1-}$ and $\lim_{x\to 1+}$ respectively denote limits taken through values of x *less* than and *greater* than 1.

(e) Discuss briefly the origin of the transition, in terms of a competition between energy and entropy.

(f) State, giving brief reasons, whether or not you expect the system to exhibit a phase transition in each of the following two situations:
(i) $T > 0$ and N finite? (ii) $g = 1$?

You may use without derivation the following results:

$$\sum_{n=0}^{N-1} t^n = \frac{t^N - 1}{t - 1} \quad \text{and} \quad \sum_{n=0}^{N-1} n\,t^n = t\frac{d}{dt}\sum_{n=0}^{N-1} t^n .$$