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Übung zur Vorlesung
Mathematische Statistische Physik
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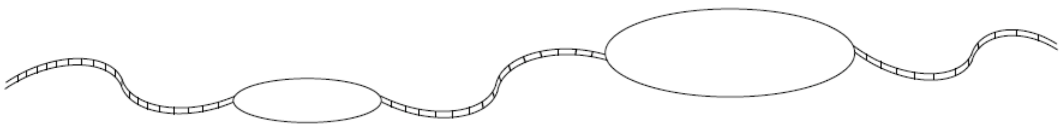
Problem 20

The **Poland-Scheraga model** is a simplified model for thermal denaturation of DNA. It describes the microscopic configurations of DNA as an alternating sequence of bound segments and denaturated loops. The configuration starts and ends with bound segments. For simplicity, the configurational entropy of a bound segment associated with its embedding in ambient space is neglected. The statistical weight of a bound sequence of length l is given by $w^l = \exp(-\beta\epsilon l)$, where ϵ is a binding energy per unit length. A denaturated loop does not carry an energy and its statistical weight is derived from its degeneracy. Assume that its configurations are random walks such that for large l the statistical weight has the form $\Omega(l) = s^l/l^c$, where $s > 1$ is a non-universal constant and the exponent c is determined by the properties of the loop configurations; for an unconstrained random walk in d spatial dimensions $c = d/2$.



(a) Calculate the grand canonical partition sum $Z_G(z) = \sum_{L=0}^{\infty} z^L Z(L)$ with z the fugacity and the canonical partition sum for a DNA of total length L given by

$$Z(L) = \sum_{l_1, l_2, \cdots} e^{-\beta\epsilon l_1}\Omega(l_2)e^{-\beta\epsilon l_3}\Omega(l_4)\cdots\delta_{l_1+l_2+\ldots,L}$$

The result reads:

$$Z_G(z) = \frac{V(z)}{1 - U(z)V(z)}$$

with $U(z) = \sum_{l=1}^{\infty} \frac{(zs)^l}{l^c}$ and $V(z) = \sum_{l=1}^{\infty}(zw)^l = zw/(1-zw)$.

(b) To set the average chain length $\langle L\rangle$ one has to choose a fugacity z such that $\langle L\rangle = \partial \ln Z_G(z)/\partial \ln z$. This implies that the thermodynamic limit, $\langle L\rangle \to \infty$, is obtained by letting z approach the lowest fugacity z^* for which the grand canonical partition sum diverges, i.e. $U(z^*)V(z^*) = 1$. Show that this gives the condition

$$U(z^*) = \frac{1}{wz^*} - 1$$

whose solution gives the fugacity $z^*(w)$ as a function of the temperature.

(c) The fraction of bound monomer pairs $\Theta := N_b/\langle L\rangle$, with $N_b := \partial \ln Z_G(z)/\partial \ln w$ the number of bound pairs, is the experimentally measured quantity and the order parameter of the model. Show that

$$\Theta = \frac{\partial z^*}{\partial w}$$

(d) Show that for $c \leq 1$ the function $U(z)$ is finite for $z < 1/s$ and monotonically increases to infinity as z approaches $1/s$. Study the solution of $U(z^*)V(z^*) = 1$ and show that there is no phase transition.

(e) Show that for $1 < c \leq 2$, $U(z)$ monotonically increases towards a finite value with an infinite slope as $z \to 1/s$. Show that now there is a phase transition and determine the behavior of the order parameter close to the critical temperature.

Problem 21

Consider a one-dimensional **spin–$\frac{1}{2}$ quantum xy-model** with the Hamiltonian

$$\mathcal{H} = -J \sum_{\langle ij\rangle} \left(\tau_i^x \tau_j^x + \tau_i^y \tau_j^y\right)$$

where $i = 1, 2, \cdots, N$ and the τ's obey the anti-commutation relations $\{\tau_i^x, \tau_i^y\} = 0$, $\{\tau_i^x, \tau_i^x\} = \{\tau_i^y, \tau_i^y\} = 2$ and commutation relations $[\tau_i^x, \tau_j^x] = 0$ etc. for $i \neq j$.

(a) Define the operators $\tau_j^{\pm} = \frac{1}{2}(\tau_j^x \pm i\tau_j^y)$ and show that $\mathcal{H} = -2J \sum_{\langle ij\rangle} \left(\tau_i^+ \tau_j^- + \tau_i^- \tau_j^+\right)$ with $\{\tau_i^{\pm}, \tau_i^{\pm}\} = 0$, $\{\tau_i^+, \tau_i^-\} = 1$, and $[\tau_i^{\pm}, \tau_j^{\pm}] = 0$ for $i \neq j$.

(b) Use the Jordan-Wigner transformation $c_j = (-1)^{N_j} \tau_j^-$ with $N_j = \sum_{l<j} \tau_l^+ \tau_l^-$. Show that the operators c_i and $c_i^\dagger$ obey the usual Fermion anti-commutation relations, and the Hamiltonian becomes $\mathcal{H} = -2J \sum_{i=1}^{N-1} \left(c_{i+1}^\dagger c_i - c_{i+1} c_i^\dagger\right)$

(c) Show that the boundary terms $c_1^\dagger c_N + c_N^\dagger c_1$ will not affect the free energy

$$-\beta f(\beta) = \lim_{N\to\infty} \frac{1}{N} \log \mathrm{Tr}(e^{-\beta\mathcal{H}})$$

such that the Hamiltonian can be taken as $\mathcal{H} = \sum_{i,j} M_{ij} c_i^\dagger c_j$ with $M_{ij} = -2J$ for $i = j \pm 1(\mathrm{mod} N)$.

(d) Upon diagonalizing the Hamiltonian show that the free energy in the thermodynamic limit is given by

$$-\beta f(\beta) = \int_0^1 \log\left[\frac{1}{2}\left(1 + e^{4\beta J \cos(2\pi x)}\right)\right] dx$$

For a further discussion of the one-dimensional xy-model see the discussion in the review article: Thompson, C.J., "One-dimensional models – short range forces" in Phase Transitions and Critical Phenomena, ed. by C. Domb and M.S. Green, vol. 1, pp 177-226 (London, Academic Press, 1972).