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Problems in Advanced Statistical Physics

Problem 1: The Langmuir lattice gas

Consider a lattice of V sites, each of which is vacant with probability ρ or occupied by a single particle with probability $1-\rho$. Multiple occupancy is not allowed, i.e. the particles are subject to a *hard core interaction*.

a.) Calculate the variance of the particle number, and use the general relation given in the lectures to determine the isothermal compressibility of the lattice gas. Compare the result to the compressibility of the ideal classical gas computed from the ideal gas law.

b.) Write down an expression for the probability $P(N,V)$ to find exactly N particles in the system. Take the limit $V \to \infty$ keeping the mean particle number $\langle N \rangle = \rho V$ constant, and show that $P(N,V)$ then converges to a Poisson distribution.

c.) Now take $V \to \infty$ and $N \to \infty$ keeping the ratio $n = N/V$ fixed. Show that under this scaling

$$P(N,V) \sim \exp[-V s_\rho(n)] \tag{1}$$

and compute the *large deviation function* $s_\rho(n)$. Show that s_ρ is maximal at $n=\rho$. Expand to second order around this maximum to arrive at the Gaussian approximation to $P(N,V)$ predicted by the central limit theorem. Finally, compare the estimates for the probability $P(0,V)$ to find a completely empty lattice obtained from (i) the Gaussian approximation and (ii) the large deviation formula (1) with the exact result.

Problem 2: Shannon entropy

The Shannon entropy (or ignorance measure) of a probability distribution $P^{(s)}$ defined over a discrete set of states s is given by

$$S[P^{(s)}] = -k \sum_s P^{(s)} \ln P^{(s)}$$

where k is an arbitrary positive constant.

a.) Show that the canonical (grand-canonical) distribution maximizes the entropy under the constraint of fixed average energy (fixed average energy *and* particle number).

b.) Show that S satisfies the three properties (i) - (iii) listed in the lectures.

c.) Show, conversely, that these three properties uniquely define the ignorance measure. *Hint: Since S is required to be continuous, it is sufficient to consider rational probabilities.*[1]

Problem 3: Irreversibility of diffusion [2]

In the continuum limit the positional probability distribution $P(\vec{r}, t)$ of a random walker satisfies the diffusion equation

$$\frac{\partial P}{\partial t} = D\nabla^2 P.$$

The continuum analog of the Shannon entropy is

$$S[P] = -k \int d\vec{r}\; P(\vec{r}, t) \ln P(\vec{r}, t).$$

Show that $S[P]$ (provided it exists!) is a strictly increasing function of time.

Problem 4: Entropic elasticity [3]

As a simple model of a polymer, we consider a chain of N segments, each of length ℓ, which are aligned with the one-dimensional x-axis. With equal probability a link points parallel or antiparallel to the preceding one, i.e. the polymer is the trace of a one-dimensional random walk with step length ℓ. One end of the polymer is fixed at the origin $x = 0$.

a.) Compute the entropy of the polymer as a function of the position R of the free end. Expand the result to quadratic order in $R/\ell N$.

b.) The energy cost for stretching the polymer by an amount dR is equal to $f dR$, where f is the *tension*. Since the internal energy of the chain is always equal to zero, the first law of thermodynamics implies that

$$dE = TdS + fdR = 0$$

and hence the tension is given by $f = -T(\partial S/\partial R)$. Using the result of part a.), show that for small extensions the chain behaves like a harmonic spring. How does the spring constant depend on temperature? What does this imply for the temperature dependence of the length of a polymer under fixed tension? Compare to the behavior of a gas under constant pressure.

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[1] Exercise 5.17 in the book of Sethna.

[2] Exercise 5.10 in the book of Sethna.

[3] Exercise 5.12 in the book of Sethna.