SISSA ISAS

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Physics and Chemistry of Biological Systems
Entrance Exam- Spring Session 2007

Solve **one** of the following problems (no extra credit is given for attempts to solve more than one problem). Write out solutions clearly and concisely. State each approximation used. Diagrams welcome. Number page, problem, and question clearly. Do not write your name on the problem sheet, but use extra envelope.

PROBLEM 1

Consider a one dimensional chain of N Ising spins, regularly spaced at unit distances. Each spin takes on the values $\sigma_i = \{+1, -1\}$ and interacts with its nearest neighbours with a ferromagnetic exchange interaction of unit strength.

$$\mathcal{H} = -\sum_{i=1}^{N-1} \sigma_i \sigma_{i+1} \quad . \tag{1}$$

1. Calculate the free energy of the system at a temperature T.
2. Compare the previous result with the free energy calculated in the case where the last spin is constrained to be up: $\sigma_N = +1$. Comment on the effect of boundary conditions on the system properties. Discuss qualitatively how would the thermodynamics be affected by closed boundary conditions, $\sigma_1 = \sigma_N$.
3. Repeat the calculation of point [1] when the spins are subject to an external field h and the chain length N is very large:

$$\mathcal{H} = -\sum_{i=1}^{N-1} \sigma_i \sigma_{i+1} - \sum_{i=1}^{N} h\sigma_i \quad . \tag{2}$$

4. Consider an infinitely-long chain, in the absence of the external field. Consider the correlation function, $g(l)$, of two spins at a distance l along the chain

$$g(l) = \langle \sigma_i \sigma_{i+l} \rangle - \langle \sigma_i \rangle \langle \sigma_{i+l} \rangle \tag{3}$$

(i is arbitrary given the infinite length of the chain and the brackets denote the canonical average). Discuss how $g(l)$ decays as a function of l

PROBLEM 2

Two dipoles in thermal equilibrium

Consider two particles of dipole moments $\mathbf{d}$ and $\mathbf{d}'$. The first particle is in the origin, the second is at position $\mathbf{r}$. Their interaction potential is given by

$$V(\mathbf{r}) = -\frac{1}{r^5}\left[3(\mathbf{d}\cdot\mathbf{r})(\mathbf{d}'\cdot\mathbf{r}) - r^2(\mathbf{d}\cdot\mathbf{d}')\right]$$

These particles are assumed to be in thermal equilibrium at a temperature T and their dipoles are free to rotate.

- Determine the canonical partition function of the system for $r = |\mathbf{r}|$ fixed, assuming that both d and d' are much smaller than $\sqrt{k_B T r^3}$(Hint: use spherical coordinates, with z axis in the direction of $\mathbf{r}$).
- Using this approximation for Z, derive an expression for the mean force between the dipoles. With which law does this force decay to zero?
- How would the last result change if the system would live in two dimensions (instead of three)?
- Compute the free energy of the system as a function of r, always assuming that r is large.
- Describe a possible physical situation for which this model could be appropriate.

PROBLEM 3

The candidate should address one and only one of the following points (that is, address either A) or B), or C) or D))

A) Describe a biological system of pharmacological relevance and discuss at least one computational technique that can be used to study it.

B) Summarize a paper in computational pharmacology which has been of great interest to you.

C) Describe shortly a project you would like to pursue in drug design in the next future.

D) Address at least two of the following issues

(i) Use and limitation of molecular docking techniques

(ii) Principles of structure-based drug design

(iii) Relevance of NMR spectroscopy for drug discovery

(iv) New synthetic approaches for use in the contemporary drug discovery research

PROBLEM 4

Problem for candidates who are applying for the Experimental Curriculum of the SMB PhD Program.

Pretend that you are writing a research proposal in the field of Biophysics, Biotechnology or Nanotechnology and write a few pages about what you would study experimentally if you had at your disposal a set of instruments that you can specify regardless of practical considerations such as cost and space requirements. In each of approximately three and 1/2 pages please explain:
1) The overall problem that you want to address.
2) What instrument(s) you would like to use and why.
3) The reasons why YOU find the problem interesting i.e. how thw problem relates to your culture.
In the last 1/2 page the candidate will write a summary of the whole proposal as self-consistently as possible. A paper that will contain also numbers with units (for instance about sensitivity levels) will be rated higher than a paper that contains only vague statements. Of course the proposal does not need to be original but, please, pay attention to the paper's organization and logic that will need to be present especially in absence of original ideas and specific numbers.